PREDICTION OF THERMODYNAMIC PROPERTIES BY STUCTURE-BASED GROUP CONTRIBUTION APPROACHES

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Thesis

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ABSTRACT

This research suggests two new group contribution methods to facilitate phase behavior calculation when reliable experimental data are lacking. The first method pertains to the implementation of an updated version of the Elliott and Natarajan method to the Statistical Associating Fluid Theory (SAFT) and Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) equations of state. Shape factor parameters have been correlated for 878 compounds including different variety of families and the parameters from Elliott and Natarajan have been updated to improve accuracy for alcohols. Thereafter, thermodynamic properties such as boiling temperatures and vapor pressures have been predicted. We obtain 36%, 65%, and 32% AAD% in pressures for the ESD, SAFT, and PC-SAFT equations of state. Additionally, we have compared our GC-PC-SAFT to the one by Tihic et al., applying their suggested First-Order and Second-Order groups for 650 non-associating compounds. We observed higher accuracy for our method relative to the Tihic et al. The resulting P AAD% were 53% for Tihic FOG and 42% for Tihic SOG.

The second method suggests a new group contribution model for Tb at 760mmHg and Tb at 10 mmHg. These correlations recognize a finite limit in boiling temperature as infinite molecular weight is approached. The availability of two vapor pressures enables

straightforward application of the Clausius-Clapeyron equation to estimate boiling temperatures at other points. In the presented approach, there are 3 parameters and 72 functional groups for each temperature which are regressed through a database consisting of 336 hydrocarbons and 642 non-hydrocarbons. The average absolute percent deviations (AAD%) between the correlated and experimental temperatures are calculated in comparison with Joback-Reid and Gani approaches. We obtain 3.5, 4.7, and 4.1 AAD% in temperature for the present work, Joback, and Gani methods, respectively. Additionally, the accuracy of the present work is evaluated by calculating the vapor pressures from the DIPPR correlation at the predicted temperatures of each model. We obtained 33.2, 104.3 and 48.1 AAD% in pressure for the present work, Joback, and Gani methods. Finally, the accuracy of the presented correlations are tested against Asher and Pankow model, UNIFAC-$P_L°$, for 66 volatile compounds in the temperature range of 290 – 320 K. For the vapor pressure at the 10mmHg boiling temperature, we obtain 36.9 AAD% for the present work and 94.5 AAD% for the Asher method.

Overall, these group contribution methods establish a standard for comparison of more fundamental methods like molecular simulations with transferable potentials. Transferable potentials generally provide accuracy of 10-30AAD% in pressure, but have only been developed for relatively small databases over narrow temperature ranges.

DEDICATION

To

My Dear Mother and Father

In Recognition of Their Worth, Love, and Respect

ACKNOWLEDGEMENTS

I would like to warmly acknowledge the help and support I received from my best friend ever, my companion every time, and my love, Amir. Also, I would like to respectfully thank my Professor Dr. Richard Elliott for advising me throughout my research.

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CHAPTER I

INTRODUCTION

The prediction of thermodynamic properties of fluids is crucial in the chemical, biochemical, petroleum, and related industries. Thermodynamic properties of a large variety of chemical species in a vast range of temperatures and pressures are of industrial importance. For instance, phase behavior determination of mixtures is the basis for distillation processes. Lack of reliable experimental data compels developing predictive approaches especially for complex chemicals. Polymers are an example of ever-increasing segments in chemical industry[1]. Predicting the thermodynamic behavior of polymeric solutions is demanding [2-6], but necessary. New pharmaceutical compounds are being invented every day which are needed to be thermodynamically characterized and it is not always practical but expensive to run experiments whenever the need arises. In these cases, the components must be characterized entirely in terms of their chemical structure. Group contribution methods have the advantage of being simple and quick. With this background this research is trying to develop reliable group contribution methods to estimate the physical and thermodynamic properties of compounds and extend it to polymers. The first method pertains to the group contribution estimation by fundamentally sound equations of state[7-10]. In the second method we follow a

correlative group contribution method, which can successfully predict the asymptotic trend of the boiling temperature when the infinite chain length is approached.

1.1 Research Objectives

In this research we propose completely structure-based methods to predict the phase behavior of pure fluids. The study is divided to two main sections as following:

1. Develop group contribution methods to predict vapor pressures of pure species using the Elliott-Suresh-Donohue (ESD), Statistical associating fluid theory (SAFT), and Perturbed-Chain Statistical associating fluid theory (PC-SAFT) models. The analysis consists of two steps. First, calculating the species parameters of each equation of state using an experimental database. Second, proposing a group contribution formula and the regressing the parameters of interest for the functional groups.
2. Propose correlative group contribution formulas for Tb at 760 mmHg and Tb at 10 mmHg which have finite limits when the infinite molecular weight is approached.

These methods should also be evaluated for their ability to predict vapor pressures At the end of each chapter, we compare the proposed approaches by already existed models.

CHAPTER II

METHODOLOGY

2.1 Implementing the Elliott and Natarajan method for SAFT and PC-SAFT models

Statistical mechanic analysis provides different semi-empirical equations of state (EOS) based on strong theoretical foundation. Among these equations of state, the ones based on Wertheim's Perturbation Theory[11] show good agreement with experimental data. Wertheim's theory is based on a rigorous analysis of cluster diagram expansions[12-15]. As such, it includes both the entropic and enthalpic contributions to hydrogen bonding subject to the assumptions of the potential model. The potential model is composed of square-well attractive sites strategically located to model steric hindrance and short range, linear bonding. Chapman et al. compared the results obtained from Wertheim's theory against the Monte Carlo simulation[16]. From these statistical models SAFT[17] and ESD[7] are of interest because of their accuracy to predict the thermodynamic properties of species. Thereafter, several modifications have been developed to increase the accuracy of SAFT EOS. Simplified SAFT[18], LJ-SAF[19, 20], SAFT-VR[21], PC-SAFT[9], and Simplified-PC-SAFT[22] are some versions

developed from SAFT EOS. The last two versions of SAFT have shown the best results in predicting the phase behavior of various compounds. This is noticeable that the simplified-PC-SAFT would reduce to the original PC-SAFT when pure species are involved. In the present work, we have adapted the SAFT[8, 23] and PC-SAFT[9] equations of state to an updated Elliott and Natarajan group contribution approach. This method enables us to encompass the polymeric compounds analysis in a consistent way as small molecules. Furthermore, we have calculated vapor pressures for a large numbers of compounds as criteria to evaluate the accuracy of the model. Previous works have addressed the prediction of the vapor pressure by group contribution methods to varying extent. Jensen et al. [24] and later Yair[25] have developed UNIFAC-based group contribution methods to calculate the vapor pressures. Along with their approach Asher et al. [26, 27] updated the groups and reported the accuracy of the vapor pressure within a factor of 1.8. They used the temperature range of 290-320 K to regress the model coefficients for 148 compounds. Some narrowly developed group contribution methods for SAFT,VR-SAFT, and PC-SAFT EOS has been reported by Thi[28] and Tamouza[29, 30] applicable to limited families like alkanes, ethers, and esters. They have reported the vapor pressure with high accuracy; however, the application of their approaches is very limited. The most recent work on GC-PC-SAFT is published by Tihic et al[31]. Their study includes both first-order and second-order groups and consists of a variety of different families but no associating compounds. A comparison between the present work and Tihic approach has been performed and the results are reported in Chapter 3. In this research we have developed a group contribution method for SAFT and PC-SAFT equations of state based on an updated version of Elliott and Natarajan method. Through

a detailed analysis of the vapor pressures estimated by the group contribution approach we observed peculiar behavior of the alcohols with two or more hydroxyl groups. The reason could be intramolecular hydrogen bonding. Therefore, they are omitted from the database. In this way, we could reduce the vapor pressure error from ~80% AAD to ~40% for GC-ESD.

As mentioned before, this analysis consists of two steps. The first step is to calculate the parameter corresponding of states using the experimental data. Therefore, a reliable database was needed which includes the boiling temperatures at 760 and 10 mmHg, and structural functional groups for each compound. We have used the database provided by ChemStations, Inc. in their process simulation software package ChemCAD. Their data are taken primarily from the DIPPR compilation. Although, UNIFAC groups have already been assigned to all compounds in the ChemCAD database, we observed several mistakes in the assigned functional groups or in the boiling temperatures. Therefore, we updated the database including near 950 compounds.

Thereafter, derivations were required for each equation of state to characterize the internal energy departure function, second virial coefficient and so on, After obtaining the needed relationships a code was written for each EOS to set up all the equations and calculate the parameters corresponding state using the experimental data. The shape parameter was of particular interest since group contribution correlations previously existed for density and solubility parameter. This code was written in FORTRAN and incorporated the HYBRD algorithm of Argonne labs to solve the non-linear system of equations. The next step was to regress the group contributions for all the functional groups. The procedure was to set up a table including all the compounds and their

constructive groups. A formula was suggested for the shape factor, then its value for all of the compounds was calculated using the functional groups. Then the group contribution values were regressed minimizing the root mean square, rms, deviation between the parameter obtaining from the group contribution formula and those calculated from experimental data. The next step was to write another program for each equation of state which picks the group contribution shape factors and calculates the other two remaining parameters to be consistent with the density and solubility parameter. Then the accuracy of the proposed method was tested. Vapor pressures and boiling temperatures were calculated at three different points, 760, 100, and 10 mmHg for each EOS. Another code was written to perform these calculations.

At the next step, a detailed analysis based on the obtained results and their deviations and bias was performed for each family in the database. Through this observation we recognized the peculiar behavior of the alcohols which have more than one hydroxyl groups. This may be attributable to the intramolecular hydrogen bonds in these kind of molecules. The same behavior is existed for acids for the same reason. Therefore these compounds were deleted from the database. Thereafter, all the procedures were started over by the new set of compounds.

The next step was comparing the accuracy of the proposed GC-PC-SAFT method with a most recently reported approach by Tihic et al[31]. They have suggested a group contribution method for the simplified PC-SAFT providing a set of first order groups, FOG, with an optional set of second order groups, SOG. Comparing these methods required another attempt in the database to assign the SOG to compounds if

possible. Then a code was written to calculate the properties using Tihic method. Finally, the results was tabulated and reported.

2.2 Proposing a correlation for Tb at 760 and 10 mmHg and T_c

In the fourth chapter we focus on the asymptotic trend of the critical and boiling temperatures when the infinite molecular weight is approached. To date, several methods have been developed to estimate the critical properties and boiling temperatures as key quantities in chemical industries. Levelt et al.[32] characterized the critical properties by using the scaling function and the universal critical exponent. Albright et al.[33] suggested a crossover formalism in the critical region using van der Waals equation of state to predict the classical behavior of the fluid. Later Kiselev[34] proposed a crossover form of the SAFT equation of state and as another follow-up study, a crossover EOS for square-well fluids[35]. Some other types of approach use the molecular descriptors to calculate the physio-chemical properties of the molecules. These methods use the logical and mathematical procedure to encode the chemical information into some meaningful numbers. Then physical properties of the molecules could be correlated using statistical knowledge and QSAR/QSPR step-wise regression methods. These methods are only based on the chemical structure and have been used to correlate the boiling points by Egolf et al.[36] , Hall and Story[37], Breindl et al.[38], and Beck et al.[39] Critical properties are also correlated by similar approaches by Egolf et al.[36]and Hall and

Story[37]. In 1987, Joback and Reid[40] developed a group contribution correlation based on 41 simple first-order groups which provides the possibility of building a lot of functional groups. The Constantinou and Gani[41] is another well-known method which facilitates the calculations based on 78 UNIFAC groups with optional set of second-order groups. The availability of the heats of vaporization at 298 for these methods provides the possibility of calculating the boiling temperatures at any other point using Clausius-Clapeyron equation. This means that we have assumed the heat of vaporization is constant in our temperature range. However, Kolska et al.[42] have reported an updated set of heat of vaporization at boiling temperature which will result in more accurate results for calculations. However, many of these approaches are questionable because of their accuracy. In this regard, Lue et al.[43] have shown that all EOS models with linear dependence on molecular weight must conform to $Zc \rightarrow ⅓$. This [44]observation suggests a possible limitation to the EOS approach since experimental observations do not appear to be consistent with $Zc \rightarrow ⅓$. From the other hand, according to some studies published by Nikitin et.al[45], Tsonopoulos and Tan[46], and Elliott and Gray[47], a finite limit is expected for the boiling temperatures as the infinite molecular weight is approached.

By this background, the purpose of this chapter is to present new correlations for the normal boiling temperature (760 mmHg) and a similar correlation for the boiling temperature at 10 mmHg. Availability of an additional boiling temperature, e.g. 10mmHg, enables the interpolation through the Clausius-Clapeyron equation. Thus estimation of the boiling temperature is made possible at any pressure below roughly 0.2 MPa. Finally, we evaluate the relative accuracy of these correlations by comparing to the Joback[40], Gani[41, 42], and Asher-Pankow[27] methods.

For this part we started with our updated database. After suggesting the group contribution formulas for each boiling temperature along with the critical temperature based on theoretical facts, the properties were calculated. As before, the rms error was minimized to regress the group contribution values. Also, we calculated the quantities of interest by Joback-Reid and Gani group contribution methods to compare the accuracy of the models. Another spreadsheet or code was needed to calculate the vapor pressures for Asher and Pankow model. Another performed analysis pertained to the behavior and trends of the SPEAD EOS[48] near the critical region and at infinite molecular weight. After all, the results were tabulated and reported.

CHAPTER III

GROUP CONTRIBUTION PREDICTION OF VAPOR PRESSURE WITH SAFT, PC-SAFT AND ESD EQUATIONS OF STATE

3.1 Introduction

Prospective applications and new compounds often require knowledge of properties and phase behavior that have not been measured. For example, polymeric materials are an ever-increasing segment of the chemical industry, both as end products and intermediates. Representation of polymer mixtures by equations of state for this task is a fairly mature area.[3] The phase equilibria of mixtures of polymers in organic liquid solvents and in supercritical fluids has been a subject of some research.[5, 6, 49] Nevertheless, existing methods do not generally include explicit treatment of hydrogen-bonding contributions and there is a need for predictive rather than correlative models. As another example, alternative energy and pharmaceutical applications often encounter compounds that have not been extensively characterized. Experimental values for the melting temperature and the density may be all that is available. In these cases, the components must be characterized entirely in terms of their chemical structure. With this

background, the present research describes a group contribution method for solvents from several families that extends naturally to polymer species and their solution phase behavior.

Our method is based on EOS models that adapt Wertheim's theory to characterize hydrogen bonding as an explicit contribution to the free energy. We consider two variants of statistical associating fluid theory (SAFT)[8, 9] and we update the ESD treatment considered by Elliott and Natarajan.[7, 10] Wertheim's theory is based on a rigorous analysis of cluster diagram expansions.[12] As such, it includes both the entropic and enthalpic contributions to hydrogen bonding subject to the assumptions of the potential model. The potential model is composed of square-well attractive sites strategically located to model steric hindrance and short range, linear bonding.

In optimizing the group contributions, vapor pressure was selected as a sensitive and valuable property for characterizing the shape factor. Consequently, the results provide a basis for vapor pressure prediction that is evaluated crudely by computing the vapor pressures in the database that result from applying the group contribution correlation developed here.

Previous work has addressed group contribution predictions of polymer properties and solvent vapor pressures to varying extents. Benzaghou et al.[50] correlated EOS parameters in terms of various functional groups and extrapolated them to the polymer limit, but did not report on vapor pressure accuracy. Jansen et al.[24] and later Yair and coworkers[25] developed a UNIFAC group contribution method for predicting vapor pressures of pure compounds. They claimed a percent average absolute deviation (%AAD) of roughly 4% for vapor pressure. On the other hand, Asher et al[26] recently

updated the UNIFAC method for 76 typical aerosol compounds, but they reported accuracy within a factor of two (ie. -50-100 %AAD). They also reported deviations for the Lee-Kesler method and several others to be roughly within a factor of three (-70-200%AAD). A follow-up study by Asher and Pankow[26, 27] showed similar accuracy for an additional 208 hydrocarbons. Similarly, Bureau et al.[51] reported deviations of 16-285%AAD for seven esters using the UNIFAC method.

In work closely related to the present effort, Elliott and Natarajan[10] developed a correlation for polymer parameters and evaluated accuracy for vapor-liquid equilibrium in polymer solutions. They presented a group-contribution approach for the ESD equation,[27] an equation similar to SAFT and PC-SAFT, to estimate the shape parameter. They did not evaluate the accuracy of vapor pressures computed from the correlated group contributions, however. Group contribution correlations for boiling temperature and heat of vaporization like those of Constantinou et al.[41] and Kolska et al.[42] can also be used for vapor pressure prediction. The accuracy of this approach generally yields 50-100%AAD. This approach does not provide a consistent basis for extension to solution properties, however, placing it outside the scope of the current study. We plan to evaluate this approach in greater detail separately.

Recently, Tamouza et al.[29, 30], Nguyen Thi[28] and Huynh et al.[52] have developed group contributions for the SAFT approach applied to pure compounds and binary mixtures of esters and aromatic compounds. Although they have reported vapor pressure accuracy of 10-50%AAD for 35 esters, 25 hydrocarbons, and 9 alcohols, their analysis focuses on limited variability in molecular structure (e.g. only linear alkyl

formates) and applies a very different approach from the one developed in the present work.

The most recent work on GC-SAFT families has been done by Tihic et al.[31] with application to polymer solution phase equilibria using first order and second order groups with 400 hydrocarbons of low molecular weight. Unfortunately, they have not reported the details of the chemical families in their database. Furthermore, their training compounds do not include associating compounds. Finally, they have not reported the vapor pressure accuracy for their method.

In this paper, the method developed by Elliott and Natarajan[10] is adapted to the statistical associating fluid theory (SAFT) model[8] and perturbed-chain statistical associating fluid theory (PC-SAFT)[9] model. The present group contribution (GC) method is developed in two stages. Initially, pure component parameters of each EOS were obtained by matching their boiling temperatures at 10 or 760 mmHg and available GC estimates of solubility parameter and liquid density, while applying standard hydrogen-bonding parameters. Then, group contributions were regressed for the shape factor parameters of each EOS. Group contributions are presented for 84 first-order functional groups (FOG). Given the GC shape factors, the same GC estimates of solubility parameter and liquid density can be applied to estimate all EOS parameters on a GC basis. The resulting correlation enables three-parameter corresponding states predictions without any experimental data. The difference between the present work and one for Elliott and Natarajan[10] is that alcohols with multiple hydroxyl segments have been omitted. We observed that properties varied too strongly when second or third hydroxyl segments were located at different positions in the molecule, possibly related to

intramolecular hydrogen bonding. Therefore, considering alcohols with multiple hydroxyls must be the subject of a future study. Excluding these alcohols has reduced the %AADP obtaining by GC-ESD from ~81% to ~40%. Thermodynamic properties were correlated and predicted for a database of 878 compounds, including associating compounds. Association contributions were treated with Wertheim's theory. Our database includes 181 associating compounds. The database covers nineteen chemical families including: hydrocarbons, cyclic hydrocarbons, aromatic hydrocarbons, alcohols, amines, nitriles, thiols, sulfides, aldehydes, ketones, esters, ethers, halocarbons, and silicones. The updated group contribution shape factors are reported for the ESD[10] model along with new SAFT[8] and PC-SAFT[9] groups in Table3. 1 In addition, we evaluate the resulting method for vapor pressure prediction as well as boiling temperature of a database of 871 organic compounds. Based on the present work, vapor pressure average absolute percent deviations (P AAD%) were 36% for ESD, 65% for SAFT, 32% PC-SAFT. For comparison, the reported FOG and SOG by Tihic et al. have been used for prediction of vapor pressure of ~650 non-associating compounds. The resulting P AAD% were 53% for Tihic FOG and 42% for Tihic SOG.

An alternative characterization of accuracy is the average absolute deviation ($|\Delta T|$) between experimental and calculated saturated temperature. These were 8 K, 12 K, 8 K , 10 K and 9 K for ESD, SAFT, PC-SAFT, Tihic FOG and Tihic SOG equations, respectively.

3.2 Group Contribution form of SAFT and PC-SAFT Equations

Generally, the SAFT and PC-SAFT models characterize each pure component in terms of three parameters. The parameters for the SAFT EOS are: the temperature-independent segment volume, v^{∞}, the shape parameter, m, and the temperature-independent dispersion energy of interaction between segments, u°/k. For PC-SAFT the parameters are: the temperature-independent segment diameter, σ, the depth of the potential which is related to Barker-Henderson[53] approach, ε/k, and the number of segments per chain, m. ESD also has three parameters, a molecular volume, b, a shape parameter, c, and a van der Waals attractive energy, ε/κ. To establish a correspondence between the three EOSs we have focused on b, molecular volume. For SAFT models, $b = \pi m\sigma^3/6$.

Meanwhile, all three models apply three additional parameters for hydrogen-bonding species: the number of hydrogen-bonding segments per molecule, N_d; the bonding volume, K^{AD}; and the hydrogen-bonding energy, ε^{HB}. Following Elliott and Natarajan, the present work computes ε^{HB}/k from the hydrogen-bonding group contribution method effectively as an average over bonding sites: 4kcal/mol for hydroxyl groups and 1.25kcal/mol for amine, amide, nitrile, and aldehydes groups. These values were derived from previous studies of hydrogen-bonding energies for a wide range of components.[54] The number of adjustable parameters can be further reduced by noting other trends pertinent to hydrogen bonding. N_d is obvious from the molecular structure, and we can correlate the bonding volume, K^{AD}, in terms of b and m.

$$K^{AD} = 0.035b/m \quad (1)$$

Elliott and Natarajan[10] used K^{AD} =0.025 *b/c* as a similar equality for the ESD model. We have assigned two association sites to all associating components (often referred to as the 2B model[55]). Consequently, we only need three parameters, $v^{\circ\circ}$, *m*, and u°/k for the SAFT EOS and σ, *m*, and ε for the PC-SAFT EOS, and *b, c* and ε for ESD EOS to be characterized for each component.

At this point, the task is to calculate three parameters of any EOS by satisfying three criteria. Firstly, the estimated compressibility factors must be consistent, using molar volumes presented by Hoy[56] et al. as extended by Elliott and Natarajan. This effectively fixes the molecular volume, *b*.

$$Z_L^{298} = \frac{0.1V_L^{298}}{298R} \quad (2)$$

where, V_L^{298} is the liquid molar volume at 298 K, and *R* is the universal gas constant. Note that this constraint is slightly different from $Z_L^{298} = 0$, as applied by Elliott and Natarajan.

The extended Hoy[56] correlation has the form

$$V_L^{298} = 12.1 + \sum \nu_i \Delta V_i \quad (3)$$

where ΔV_i is the UNIFAC group contribution for liquid molar volumes as cited in Table3. 1.

Secondly, the internal energy departure functions should be consistent with the internal energy estimated from liquid molar volume and heat of vaporization provided by the Constantinou and Gani[41] GC method. We use the relationship of the solubility

parameter, $\delta = [(H_{vap}^{298} - 298R)/V_L^{298}]^{1/2}$, in terms the internal energy departure function for each EOS, neglecting the departure function of the vapor.

$$\frac{\delta^2 V_L^{298}}{298R} = -\frac{U}{298R} \tag{4}$$

We can readily derive the internal energy departure function from the Helmholtz energy. Detailed expressions for the internal energy and the solubility parameter in terms of the SAFT and PC-SAFT models are given in Appendix A.

Thirdly, the shape factor is determined in one of two ways, depending on whether an optimal value is being determined for inclusion in the database, or whether one seeks the result of the group contribution correlation. For an optimal value, the last constraint to be satisfied is the equality of fugacity of vapor and liquid phases at the temperature of interest (boiling temperature at 760 or 10mmHg, whichever is nearer to 400K).

$$\ln \varphi^L = \ln \varphi^V \tag{5}$$

$$\ln \varphi = \beta \mu^{res}(T,K) - \ln Z \tag{6}$$

$$\frac{\mu^{res}(T,K)}{kT} = \tilde{A}^{res} + (Z-1) \tag{7}$$

$$\tilde{A}^{res} = \frac{A^{res}}{NkT} \tag{8}$$

where, $\tilde{A}^{res}$ is the reduced Helmholtz free energy which their relations are presented in the Appendix A for SAFT and PC-SAFT EOSs.

In the calculation of vapor phase fugacity, a truncated virial expansion after its second coefficient is used as follows

$$Z_V^{sat} = P^{sat} b/\eta^V RT = 1 + B_2 \eta^v \tag{9}$$

The relations for the second viral coefficient are given in Appendix A. The saturated liquid and vapor densities at this condition are computed based on the experimental vapor pressure.

When the group contribution result is sought, shape factors are computed from

$$m = 1 + (\sum \upsilon_i \Delta m_i) \tag{10}$$

where, Δm_i is the group contribution and 1 is the number assigned to a spherical molecule.

The optimal shape parameters for all compounds were tabulated with the ones in terms of the group contribution correlations. This table was formulated as an Excel worksheet using the "sumproduct" operator to compute the GC values and the Excel solver was applied to minimize %*RMSm* between m^{opt} and m^{GC} by changing the functional group factors. The RMS error plays the role of an objective function and has the form of below:

$$\%RMSm = 100\sqrt{\frac{\sum\left(\frac{m^{opt} - m^{GC}}{m^{opt}}\right)^2}{NDP}} \tag{11}$$

where, *NDP* is the number of data points.

Table3. 1 Group Contribution for Estimating the Shape Parameter, the Liquid Molar Volume, and the Heat of Vaporization[a]

	PC-SAFT	SAFT	ESD		
Group	Δm	Δm	Δc	ΔV_{298}^{L}	ΔH_{298}^{vap}
CH3-	0.483	0.995	0.228	21.6	4.116
CH2<	0.390	0.462	0.207	15.6	4.650
>CH-	-0.187	-0.331	0.019	9.6	2.771
>C<	-0.515	-0.994	-0.090	3.6	1.284
CH2=CH	0.180	0.457	0.135	32.4	6.714
CH=CH	-0.118	-0.091	0.040	26.4	7.370
CH2=C	0.054	-0.122	0.112	26.4	6.797
CH=C	0.134	0.470	0.162	20.4	8.178
C=C	0.117	-0.386	-0.022	14.4	9.342
ACH	0.150	0.363	0.109	13.4	4.098
AC-	1.824	2.287	0.917	7.4	12.552
ACCH3	0.681	1.115	0.416	29.0	9.776
ACCH2	0.640	-0.133	0.358	23.0	10.185
ACCH	0.496	0.345	0.345	17.0	8.834
OH	0.636	1.853	0.378	12.5	24.529
ACOH	3.613	6.028	1.765	19.9	40.246
CH3CO	0.965	2.244	0.664	38.9	18.999
CH2CO	1.169	2.289	0.787	32.9	20.041
CHO	-0.042	0.922	0.243	23.3	12.909
CH3COO	2.502	4.290	1.241	43.0	22.709
CH2COO	0.847	0.891	0.639	37.0	17.759
HCOO	0.785	1.047	0.556	***43.3***	14.500
CH3O	1.383	2.650	0.688	28.0	10.919
CH2O	-0.230	0.471	0.129	22.0	7.478
CH-O	-0.083	-0.322	0.057	16.0	5.708
FCH2O	-0.018	1.452	0.188	33.2	11.227
CH2NH2	0.133	1.190	0.296	32.6	14.599
CHNH2	0.031	-0.199	0.144	26.6	11.876
CH3NH	0.776	1.734	0.444	32.6	14.452
CH2NH	0.329	1.419	0.510	26.6	14.481
CHNH	2.430	3.885	1.092	20.6	14.000
CH3-RN	0.222	0.478	0.104	28.2	6.947
CH2-RN	0.222	0.478	0.104	28.2	6.918
ACNH2	2.322	3.690	1.310	24.4	28.453
C5H4N	1.277	2.037	0.885	***75.7***	31.523
C5H3N	1.639	2.367	2.367	***69.7***	31.005
CH2CN	0.032	0.663	0.233	38.7	23.340
CH2CL	0.604	1.004	0.376	35.1	13.780

[a] Bold-italic values are Elliott and Natarajan additions to Hoy's volumetric parameters.

Table3.1 Group Contribution for Estimating the Shape Parameter, the Liquid Molar Volume, and the Heat of Vaporization (Continued)

CHCL	0.533	1.008	0.392	29.1	11.985
CCL	0.342	0.619	0.295	23.1	9.818
CHCL2	1.036	2.249	0.655	48.6	19.208
CCL2	1.841	3.061	0.923	42.6	17.574
CCL3	5.475	8.850	2.269	62.1	33.400
ACCL	0.523	0.448	0.345	26.9	11.883
CH2NO2	1.935	3.312	1.151	***50.2***	30.644
CHNO2	1.225	1.749	0.805	***46.3***	26.277
ACNO2	0.044	-0.213	0.194	***31.4***	19.700
CH2SH	0.293	0.474	0.292	***46.7***	14.931
I	-0.048	-0.105	0.105	***42.6***	14.364
Br	0.353	0.975	0.324	***25.3***	11.423
CH<->C	0.167	0.723	0.168	***40.2***	7.751
C<->C	0.696	2.778	0.755	***28.8***	11.549
CL(C=C)	0.631	1.389	0.376	19.5	7.000
ACF	0.467	0.815	0.246	18.6	4.877
CF3	4.878	6.629	1.546	37.2	8.901
CF2	2.426	4.316	0.759	26.0	1.860
CF	2.487	-4.458	0.805	14.8	8.901
COO	0.401	1.008	0.498	25.7	13.4
SiH3	0.408	0.329	0.215	***21.6***	3.4
SiH2	0.408	0.329	0.215	***58.4***	3.4
SiH	0.408	0.329	0.215	***53.7***	3.4
Si	0.408	0.329	0.215	***50.3***	3.4
SiH2O	1.819	2.537	2.537	***33.8***	6.8
SiHO	1.819	2.537	2.537	***33.8***	6.8
SiO	1.676	2.672	0.796	***33.8***	6.8
TERT-N	-1.129	0.467	-0.337	12.6	4.190
CCL2F	0.647	0.976	0.413	53.8	13.322
CCLF2	0.993	2.213	0.382	45.5	8.301
CONH2	0.707	2.875	0.695	34.3	41.9
CONHCH3	8.837	14.293	14.293	49.9	38.5
CONHCH2	8.722	13.854	13.854	43.9	51.787
CON(CH3)2	9.340	15.368	15.368	***78.9***	38.9
CONCH3CH2	9.225	14.929	14.929	***72.9***	39.1
CON(CH2)2	9.110	14.490	14.490	***66.9***	39.3
C2H5O2	0.791	5.054	5.054	50.0	36.657
C2H4O2	0.210	0.273	0.273	44.0	14.956
CH3S	0.884	1.464	0.498	39.6	16.921

Table3.1 Group Contribution for Estimating the Shape Parameter, the Liquid Molar Volume, and the Heat of Vaporization (Continued)

CH2S	1.167	1.763	0.654	33.6	17.117
CHS	0.038	-0.027	-0.027	27.6	13.265
C4H3S	0.127	-0.063	-0.063	65.7	27.966
C4H2S	0.068	-0.124	-0.124	59.7	28
RCH2<	0.294	0.467	0.180	15.6	4.650
>RCH-	-0.060	-0.148	-0.013	9.6	2.771
>RC<	-0.275	-1.031	-0.124	3.6	1.284

Table3.2 Coverage of Compounds in the database and Percent Error in the Correlation for the Shape Parameters of Different Equations of States and liquid molar volume

	no. in database	rms% error in Δm PC-SAFT	rms% error in Δm SAFT	rms% error in Δc ESD	rms% error in v
Alcohols	77	14.85	30.76	10.03	7.14
Amines	55	19.89	34.16	11.64	8.93
Nitriles	10	20.68	39.81	14.75	6.95
Silanes	10	16.84	17.62	13.86	21.02
Imines	7	9.80	14.01	7.45	9.81
tert-Ns	6	26.71	16.23	17.95	7.60
Nitrates	19	19.33	35.62	11.04	9.11
Thiols	27	14.16	17.87	8.44	8.39
Aldehydes	23	22.81	24.53	13.39	6.23
Epoxides	13	24.23	12.14	18.89	8.69
Ethers	38	17.77	40.71	8.01	8.43
Formates	16	13.04	25.22	7.52	10.33
Esters	92	12.84	19.00	7.18	5.44
Ketones	28	13.68	18.66	7.31	3.96
Alcohol-Ethers	18	26.54	55.97	17.35	5.27
Aliphatic hydrocarbons	157	12.47	19.56	9.40	9.58
Cyclic Hydrocarbons	41	12.74	15.92	7.29	5.88
Aromatic Hydrocarbons	137	10.82	26.55	6.55	6.61
Halocarbons	103	24.04	54.82	11.52	10.12
Overall	**878**	**16.34**	**30.97**	**9.80**	**8.27**

3.3 Results and discussions

Optimized group contribution values are listed in Table3. 1 for all three EOS models, along with the contributions for the V^{L}_{298} and H^{va}. Note that Table3. 1 does not report any value for carboxylic acid groups owing to the peculiar hydrogen bonding behavior in these complexes. A revised association model for carboxylic acids is the subject of an upcoming study. The coverage of families of compounds is given in Table 3.2, where the deviations correspond to the deviations of the correlated shape parameters from the optimized values. The correlation errors are generally around 17% for PC-SAFT, 31% for SAFT and 10% for ESD. The fairly large deviations are due to the sensitivity of the shape parameters to the accuracy of the solubility parameter estimation. As before, we recommend that the group contribution estimation of the shape parameter correlation should only be applied when reliable vapor pressures or critical constants are not available. Note that most of the engineering methods for predicting vapor pressure based on molecular structure are somewhat limited and based on predicting the boiling temperature.[57] Hence, we consider the boiling temperature deviations first in assessing the quality of vapor pressure predictions resulting from the shape factor correlation. Table3. 3 summarizes the boiling point temperature deviations for all organic families considered here. The deviations in Table3. 3 correspond to the boiling point temperatures of pure compounds for several different families at pressures of 760 mmHg, 100 mmHg and 10 mmHg. Keep in mind that our objective function minimized %RMS*m,* not %AAD *P* or %AAD *T*. As demonstrated in Table3. 3, the average value of ΔT is around 10 K

for all EOS models, demonstrating the feasibility of this approach when no experimental data are available.

Table3. 3 Average Boiling Temperature Errors at 760, 100 and 10 mmHg for GC-PC-SAFT, GC-SAFT and GC-ESD and also Tihic el at[31]. Approach

	no. of Occ.	T AAD%	T Bias%	$100\ln(T^{calc}/T^{exp})$	ΔT	$\lvert\Delta T\rvert$
SAFT	878	3.45	-1.76	-1.87	-5.41	12.48
PCSAFT	878	2.20	0.52	0.46	1.43	8.12
ESD	878	2.21	-0.05	-0.11	-1.00	8.13
Tihic FOG	643	2.79	-0.43	-0.53	-0.16	9.91
Tihic SOG	666	2.67	-0.48	-0.57	-0.40	9.52

Table3. 4 shows a detailed analysis of vapor pressure deviations for various families of organic compounds as an average at the three boiling temperatures: 760 mmHg, 100 mmHg and 10 mmHg. A detailed table of vapor pressure deviations is available in the supplemental information. Note that the best results obtain at the normal boiling temperature. Also, PC-SAFT and ESD generally have close prediction of *P* AAD% and close to 35%. This is because the ESD model is effectively a simplified form of SAFT equation of state with an alternative approximation for the radial distribution function. PC-SAFT and ESD may have better results because their disperse attraction contributions were characterized with direct consideration of non-spherical molecules whereas the SAFT model is based on adaptation of a disperse attraction term that has been optimized for spherical molecules.[53, 58-60]. Among these organic compounds, a few families have distinctly large deviations: epoxides (176 *P*AAD% for SAFT, 57 *P*AAD% for PC-SAFT and 83 *P*AAD% for ESD), alcohol-ether (110 *P P* AAD% for

SAFT, 54 *P* AAD% for PC-SAFT and 63 *P* AAD% for ESD). These large deviations are attributed to the peculiar chemical structures of the epoxides (ie. 1,2-epoxy-2-methylpropane) and the dual functionality of alcohol-ether compounds (e.g. carbitol, acetovanillone, ethyl lactate). The behavior of alcohol-ether compounds may reflect interaction between the functional groups that undermines the group additivity. On the other hand, hydrocarbons have the best results with vapor pressure deviations of 51 AAD%*P* for SAFT, 19 AAD%*P* for PC-SAFT and 22 AAD%*P* for ESD. These small deviations reflect effective group additivity.

Table3. 5 and Table3. 6 provide a comparison between our current approach with the FOG and SOG used in the simplified PC-SAFT EOS by Tihic and coworkers[31]. Note that the simplified PC-SAFT EOS is the same as PC-SAFT EOS for pure compounds. According to Table3. 5 and Table3. 6, the FOG and SOG of Tihic et al.[31] have larger vapor pressure deviations, 53 *P* AAD% for Tihic FOG and 42 *P* AAD % for Tihic SOG at 10, 100 and 760 mmHg boiling point temperatures compared to ~28 % with the present work for the same compounds. Readers are referred to the supplemental materials for detailed vapor pressure deviations for each EOS. The perfluoro groups (i.e. CF3 and CF2) represent a particular case of interest. For example, a deviation of 3000% was obtained for 111trifluoroethane with the Tihic correlation, compared to 70% by the present work. Generally, the high vapor pressure deviations for perfluoro compounds relate to low heat of vaporization and high vapor pressure relative to compounds with similar molecular volume. Sans and Elliott[61] explained this peculiar behavior using a soft shoulder in their transferable potential. They reported 8% *P*AAD and 3% in liquid density for these compounds. Finally, Tihic et al. reported that the density deviations

improve when using SOG. A similar observation applies to the vapor pressure deviations, and it is more obvious at lower pressures. Maximum deviations obtained for vapor pressures and boiling temperature are summarized in Table 3.7 and Table 3.8.

It is notable that a few compounds have been excluded from our database because they are very small molecules or have peculiar molecular structures. For instance, compounds like 1,1 difluoroethane, propyleneimine, 1,3propyleneoxide, and 1,2propyleneoxide are too small to exhibit group additivity. Also, if the structure of a molecule be too complicated then some other interactions between the structural groups would come into effect. Trioxane and dimethylmaleate are examples. Moreover, as mentioned before, some fluorinated species are problematic such as dichlorofluoromethane, 1,2dibromotetrafluoroethane, and octafluorocyclobutane. Some other compounds like ethyl fluoride and furan would have smaller shape factor than one when we want to calculate their parameters by this method, which is disallowed. Shape factor is representative for the sphericity of the molecule and the most spherical compound is methane which its assigned shape factor is one; therefore, all other compounds should have greater shape factors than one. Another issue to be considered is the acceptance of the experimental data. The Othmer-Yu and Riedel references in the DIPPR database are not based on experimental data, although they often form the basis of DIPPR's "accepted" values. 1,2 Epoxy butane was excluded for this reason. Overall, these 12 compounds out of 890 have been deleted from our database in addition to the alcohols with multiple hydrodroxyl groups.

Table3. 4 Average vapor pressure deviations at 760, 100 and 10 mmHg for different families of organic compounds

Family	EOS	no. of Occ.	*P* AAD%	*P* Bias%	$\ln(P^{calc}/P^{exp})$
Alcohols	SAFT	77	73.57	63.07	35.48
C3-C24	PC-SAFT		32.62	8.22	-0.78
	ESD		39.44	23.10	11.79
Amines	SAFT	55	99.61	86.09	35.33
C2-C14	PC-SAFT		48.55	7.02	-13.42
	ESD		59.21	25.78	-0.06
Nitriles	SAFT	10	150.58	149.91	70.25
C3-C8	PC-SAFT		43.23	9.68	-3.93
	ESD		39.93	-6.56	-18.84
Silanes	SAFT	10	63.29	63.29	46.84
C-C12	PC-SAFT		29.40	0.80	-5.85
	ESD		33.86	14.20	6.72
Imines	SAFT	7	191.90	191.59	81.91
C5-C13	PC-SAFT		34.57	24.57	16.99
(e.g. Acridine)	ESD		55.60	46.92	28.72
tert-Ns	SAFT	6	139.69	53.34	62.76
C3-C15	PC-SAFT		37.76	-11.14	-15.06
(e.g. Trimethylamine)	ESD		37.50	-10.69	-14.88
Nitrates	SAFT	19	78.12	51.10	13.92
C2-C18	PC-SAFT		47.52	-0.37	-23.85
	ESD		47.25	-8.57	-34.12
Alcohol-Ethers	SAFT	18	110.75	95.17	44.64
C3-C10	PC-SAFT		53.71	-19.33	-47.64
(e.g. carbitol)	ESD		62.96	17.39	-10.03

Table3.4 Average vapor pressure deviations at 760, 100 and 10 mmHg for different families of organic compounds (Continued)

Cyclic - Hydrocarbons C3-C16	SAFT	41	41.28	39.01	30.15
	PC-SAFT		14.28	1.59	-0.73
	ESD		12.67	-4.31	-6.08
Aromatic - Hydrocarbons C4[b]-C24	SAFT	138	54.00	35.46	17.54
	PC-SAFT		35.33	19.84	7.02
	ESD		53.33	39.69	16.19
Thiols C2-C12	SAFT	27	53.25	41.51	24.80
	PC-SAFT		25.14	2.18	-4.03
	ESD		24.67	7.50	0.86
Aldehydes C2-C13	SAFT	23	95.68	89.09	45.61
	PC-SAFT		34.56	29.86	18.02
	ESD		34.96	21.33	10.59
Epoxides C3-C7	SAFT	13	176.53	176.49	73.25
	PC-SAFT		56.89	26.59	7.88
	ESD		82.95	60.13	22.87
Ethers C2-C16	SAFT	38	77.23	71.40	42.34
	PC-SAFT		31.30	-14.19	-24.24
	ESD		27.67	6.78	-0.14
Formates C2-C11	SAFT	16	103.80	93.43	41.04
	PC-SAFT		18.77	-0.94	-4.32
	ESD		19.46	8.17	4.04
Esters C3-C28	SAFT	92	45.66	18.99	2.66
	PC-SAFT		26.56	-11.41	-18.67
	ESD		27.53	8.46	1.98

[b] Conjugated double bonds (e.g. 1,3-Butadiene) behave like aromatic hydrocarbons.

Table3.4 Average vapor pressure deviations at 760, 100 and 10 mmHg for different families of organic compounds (Continued)

Ketones	SAFT	28	80.42	76.05	38.70
C3-C12	PC-SAFT		52.41	11.77	-13.30
	ESD		59.77	28.65	-3.74
Hydrocarbons	SAFT	157	51.09	38.15	22.97
C3-C36	PC-SAFT		18.83	6.02	1.84
	ESD		22.31	8.88	3.61
Halocarbons	SAFT	103	77.19	51.60	4.01
C3-C10	PC-SAFT		48.50	5.87	-36.68
	ESD		37.76	-5.40	-37.98
Total	**SAFT**	**878**	69.30	54.07	24.18
	PC-SAFT		32.21	4.63	-8.74
	ESD		38.26	15.81	-0.42

Table3. 5 A comparison between the current study and FOG of Tihic et al.[31] in terms of vapor pressure errors

Group		no. of Occ.	P AAD%	P Bias%	$\ln(P^{calc}/P^{exp})$
Nitriles	Tihic FOG	18	35.58	-23.81	-41.05
	This Work		46.98	2.79	-20.44
Thiols	Tihic FOG	27	122.34	111.04	53.28
	This Work		25.14	2.18	-4.03
Epoxides	Tihic FOG	13	124.15	107.23	39.62
	This Work		56.89	26.59	7.88
Ethers	Tihic FOG	38	33.08	-12.55	-24.90
	This Work		31.30	-14.19	-24.24
Formates	Tihic FOG	16	47.88	31.59	14.96
	This Work		18.77	-0.94	-4.32
Esters	Tihic FOG	92	33.16	17.09	1.35
	This Work		26.56	-11.41	-18.67
Ketones	Tihic FOG	28	108.27	72.48	2.11
	This Work		52.56	11.77	-13.30
Hydrocarbons	Tihic FOG	157	22.87	5.58	0.35
	This Work		18.83	6.02	1.84
Cyclic Hydrocarbons	Tihic FOG	41	96.06	95.56	55.44
	This Work		14.28	1.59	-0.73
Aromatics	Tihic FOG	138	24.54	-6.38	-14.05
	This Work		35.33	19.84	7.02
Halocarbons	Tihic FOG	71	123.01	94.72	13.97
	This Work		48.25	13.94	-29.49
Total	**Tihic FOG**	**643**	**53.71**	**28.53**	**3.24**
	This Work		**28.50**	**4.02**	**-7.43**

Table3. 6 A Comparison Between the Current Study and SOG of Tihic et al.[31] in Terms of Vapor Pressure Errors

Group		no. of Occ.	*P* AAD%	*P* Bias%	$\ln(P^{calc}/P^{exp})$
Nitriles	Tihic SOG	18	35.58	-23.81	-41.05
	This Work		46.98	2.79	-20.44
Thiols	Tihic SOG	27	109.14	100.64	52.45
	This Work		25.14	2.18	-4.03
Aldehydes	Tihic SOG	23	35.04	15.07	4.87
	This Work		34.56	29.86	18.02
Epoxides	Tihic SOG	13	121.54	109.83	43.11
	This Work		56.89	26.59	7.88
Ethers	Tihic SOG	38	31.15	-10.62	-21.51
	This Work		31.30	-14.19	-24.24
Formates	Tihic SOG	16	47.07	32.39	16.06
	This Work		18.77	-0.94	-4.32
Esters	Tihic SOG	92	54.36	35.27	14.44
	This Work		26.56	-11.41	-18.67
Ketones	Tihic SOG	27	37.02	3.35	-9.09
	This Work		28.72	-13.42	-21.05
Hydrocarbons	Tihic SOG	157	24.97	13.71	7.82
	This Work		18.83	6.02	1.84
Cyclic Hydrocarbons	Tihic SOG	41	50.48	17.27	0.37
	This Work		14.28	1.59	-0.73
Aromatics	Tihic SOG	137	24.32	-4.81	-12.68
	This Work		35.33	19.84	7.02
Halocarbons	Tihic SOG	71	123.06	96.39	15.79
	This Work		34.71	0.40	-31.54
Total	**Tihic SOG**	**666**	**42.35**	**32.29**	**16.21**
	This Work		**27.70**	**4.15**	**-6.68**

Table3. 7 Maximum deviations in vapor pressures by PC-SAFT, SAFT, and ESD equations of state

	no. in database	Max PAAD% by PC-SAFT	Max PAAD% by SAFT	Max PAAD% by ESD
Alcohols	77	277.0	479.0	251.5
Amines	55	758.7	1579.0	1056.8
Nitriles	10	232.5	1029.7	206.4
Silanes	10	90.5	125.6	131.0
Imines	7	137.9	1335.0	267.2
tert-Ns	6	350.9	2448.5	479.7
Nitrates	19	366.7	458.7	296.8
Thiols	27	147.6	378.0	190.5
Aldehydes	23	446.0	944.9	386.0
Epoxides	13	322.7	912.7	513.3
Ethers	38	147.9	746.3	291.3
Formates	16	144.9	302.9	178.6
Esters	92	126.9	347.0	177.4
Ketones	28	1184.1	1519.5	1581.2
Alcohol-Ethers	18	263.3	830.4	484.1
Aliphatic hydrocarbons	157	129.2	392.7	181.0
Cyclic Hydrocarbons	41	72.1	159.7	65.7
Aromatic Hydrocarbons	137	881.5	441.4	1368.2
Halocarbons	103	242.3	1001.6	195.8
Overall	**878**	**1184.1**	**2448.5**	**1581.2**

Table3. 8 Maximum boiling temperature deviations in vapor pressures by PC-SAFT, SAFT, and ESD equations of state

	no. in database	Max TAAD% by PC-SAFT	Max TAAD% by SAFT	Max TAAD% by ESD
Alcohols	77	7.6	10.7	8.1
Amines	55	15.6	17.2	14.8
Nitriles	10	12.3	15.2	10.3
Silanes	10	3.9	6.1	5.7
Imines	7	6.3	16.9	9.1
tert-Ns	6	9.7	19.6	11.1
Nitrates	19	15.3	20.0	16.1
Thiols	27	7.8	10.4	7.8
Aldehydes	23	10.6	14.8	10.1
Epoxides	13	9.8	14.9	11.9
Ethers	38	18.5	13.4	8.7
Formates	16	5.5	8.8	6.3
Esters	92	8.8	13.4	6.7
Ketones	28	16.3	18.5	17.7
Alcohol-Ethers	18	12.9	11.9	9.0
Aliphatic hydrocarbons	157	18.4	11.8	15.8
Cyclic Hydrocarbons	41	7.8	5.9	6.7
Aromatic Hydrocarbons	137	14.3	10.9	14.9
Halocarbons	103	46.5	45.8	44.2
Overall	**878**	**46.5**	**45.8**	**44.2**

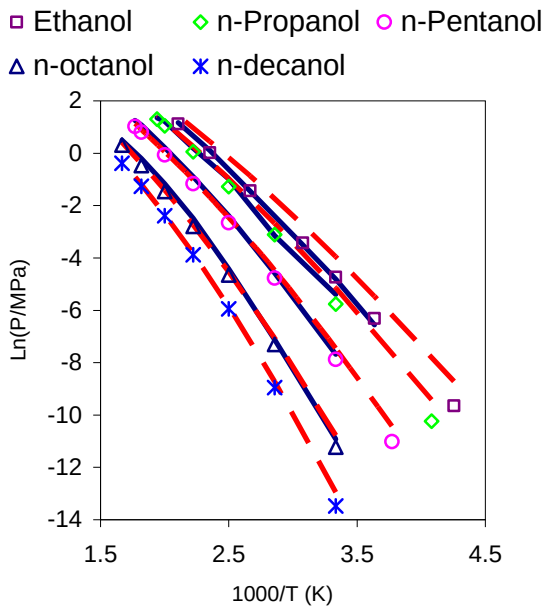


Figure 3. 1 The plot of the saturated vapor pressure versus the inverse of the temperature for alcohols. Experimental data[62] are shown with points. The solid lines and the dashed lines represent the TraPPE[63] and GC-PC-SAFT, respectively.

The pressure-temperature diagram is presented in Figure 3. 1 for several alcohols. The predicted pressure by the presented method is plotted using GC-PC-SAFT (red dashed lines). As shown in the plot, the GC-PC-SAFT overestimates the vapor pressure of small alcohols (e.g. ethanol); also molecules like methanol can not be treated by this method at all, which is not plotted because its curves overlaps with ethanol and decreases the clarity of the plot. However, the fact is that the group contribution method is not intended for small molecules, since the experimental data are available. On the other hand, accurate agreement is observed between the experimental and estimated vapor pressures for larger alcohols (e.g. n-pentanol and n-octanol). Furthermore, our method can be applied simply and rapidly. For example, TraPPE predictions for n-decanol are not available while the present method has been applied simply, with very small

deviations from the experimental data. Also it is noticeable that this method has been used at low temperatures (e.g. less than 0.45 reduced temperatures) while the TraPPE method has not generally been applied below reduced temperatures of 0.6. According to Table3. 4 the lowest vapor pressure deviations for alcohols can be achieved by using PC-SAFT as the basis, and slightly larger deviations are achieved with ESD and SAFT.

Figure 3. 2 shows the predictions for olefins by GC-ESD and GC-SAFT compared with experimental and TraPPE data. As before, small molecules like ethylene can not be treated with this approach. Also for small compounds the deviation between the GC-ESD and experimental data are large. Again, our model can successfully predict the vapor pressure at low temperatures where TraPPE has not been applied. PC-SAFT results in slightly lower deviations than SAFT or ESD. Figure 3. 3 provides a similar illustration for n-alkanes with GC-SAFT alone.

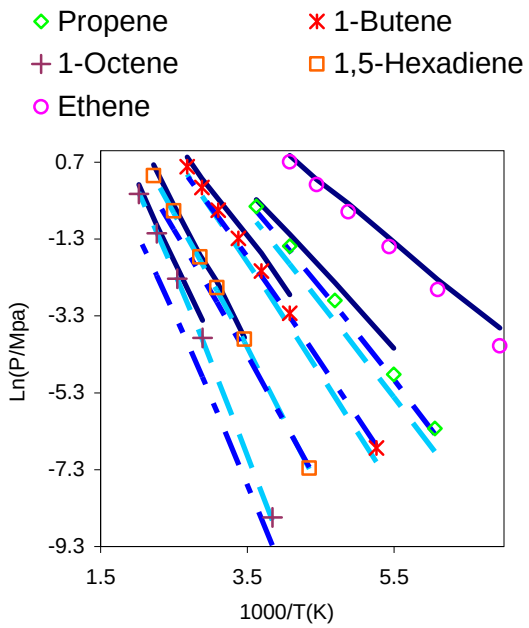


Figure 3. 2 The plot of the saturated vapor pressure versus the inverse of the temperature for olefins. Experimental data[62] are shown with points. The solid lines represent the TraPPE[64] model, the dashed lines represent GC-ESD, and the dashed-dot lines represent the GC-SAFT results.

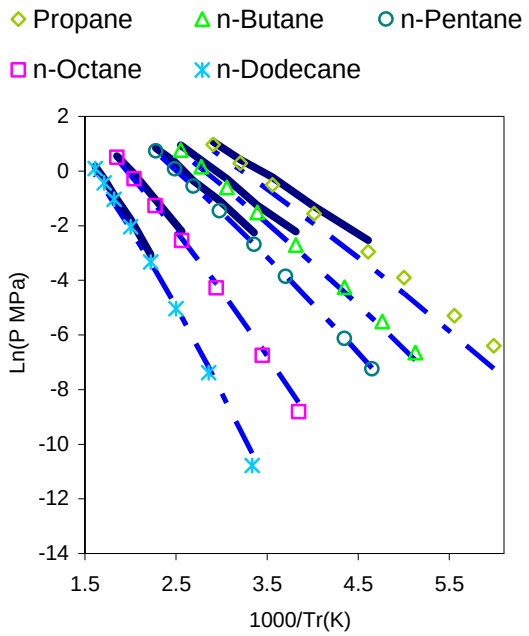


Figure 3. 3 plot of the saturated vapor pressure versus the inverse of the temperature for n-alkanes. Experimental data[62] are shown with points, solid lines show the TraPPE[65] results and blue dashed lines represent the GC-SAFT.

3.4 Conclusions

We have proposed a generalized group contribution approach based on the principle of three-parameter corresponding states for 16 different families of compounds. In this method, SAFT and PC-SAFT models were used to demonstrate the group contribution approach, along with an updated version of the Elliott and Natarajan correlation for the ESD model. The results are more accurate than many previous group contribution methods for predicting thermodynamic properties such as vapor pressure and boiling temperature. A distinctive part of this work is proposing groups for varied associating compounds with the SAFT methodology. The PC-SAFT and ESD models provided accuracy of roughly 40% *P* AAD. This is comparable to the accuracy achieved by the TraPPE[65] method involving molecular simulation, but less accurate than the AUA[65, 66] or SPEADMD[57] molecular simulation methods (10-20% *P*AAD). Going forward, we expect this group contribution method to set an upper bound on % *P*AAD to be accepted from vapor pressure predictions of more detailed molecular models. In future research, this method could be readily extended to mixtures including polymer solutions as demonstrated by Elliott and Natarajan. Associating blends and their compatibilization would be of particular interest. Also, proposing a method for treating carboxylic acids and hydrogen fluoride is challenging. We hope to address the carboxylic acids in the very near future. Furthermore, predicting other thermodynamic properties such as entropy, speed of sound, and heat capacity can be the subject of future studies. Basically, once we obtain the EOS parameters by the present approach we can calculate many other quantities through the equation of state.

3.5 Sample Calculations

Here, we show the detailed calculation of three compounds to elaborate the method more clearly. The first example is 1-Hexadecanol whose step by step calculations are shown by GC-SAFT method. The second example illustrates application to polymers with polymethyl-methacrylate, calculated by the ESD EOS. The third example illustrates application to a cyclic ether, tetrahydrofuran, using the PC-SAFT EOS.

3.5.1 Example1. (1-Hexadecanol, GC-SAFT)

1-Hexadecanol is composed of : 1 CH3, 15CH2 & 1 OH; and has a molecular weight of 242.446 kg/mol. Using Hoy values for liquid molar Volume, we obtain:

$$V_{298}^{L} = 12.1 + (21.6 + 15 \times 15.6 + 12.5) = 279.35\ cc/mol \tag{12}$$

By governing Gani's approach for heat of vaporization, we get:

$$H_{298}^{vap} = 6.829 + (4.116 + 15 \times 4.65 + 24.529) = 105.224\ kJ/mol \tag{13}$$

Therefore, solubility parameter can be readily calculated as:

$$\delta[(J/cc)^{0.5}] = [\frac{H_{vap}^{298}[J/mol] - 298[K]R[J/mol.K]}{V_L^{298}[cc/mol]}]^{1/2} = \left[\frac{105.224 \times 1000 - 298 \times 8.314}{279.35}\right]$$

(14)

The group contribution shape factor for SAFT EOS is equal to:

$$m^{GC-SAFT} = 1 + (0.995 + 15 \times 0.462 + 1.853) = 10.772 \quad (15)$$

At this point, we have one parameter (shape factor) of SAFT EOS, and we have to calculate the other two ones (the temperature-independent segment volume, v^{∞} temperature-independent dispersion energy of interaction between segments, u°/k). For this reason we can use the following equations:

$$Z_{L,298}^{calc} = \frac{0.1\,[MPa] \times V_L^{298}[cc/mol]}{298\,[K] \times R\,[J/mol.K]} \quad (16)$$

Using Hoy values for liquid molar volume at 298K and 1 bar we obtain:

$$\frac{0.1V_L^{298}}{298R} = \frac{0.1 \times 279.35}{298 \times 8.314} = 0.011275$$

This value should be equal to the calculated compressibility factor calculated by SAFT EOS. This is our first constraint.

$$-\frac{U^{calc}}{298R}=\frac{\delta^2[J/cc]\ V_L^{298}\ [cc/mol]}{298[K]\ R[J/mol.K]} \qquad (17)$$

$\frac{\delta^2 V_L^{298}}{298R}=\frac{19.17825^2\times 279.35}{298\times 8.314}=41.4706$ This equation is our second constraint.

By satisfying these two equations we can readily calculate remained parameters.

$v^{\circ\circ}=14.00\left[mlit/mol\right]$ & $\frac{u^{\circ}}{k}=240.02\left[K\right]$

Using this approach to estimate the vapor pressures at 760, 100 and 10 mmHg one will get ~29.3% error as an average.

3.5.2 Example2.(poly methyl methacrylate, Mw=20024, GC-ESD)

The repeat unit of this polymer is methyl methacrylate which consists of 2 CH3, 1CH2, 1 >C< and 1 COO. The molecular weight of the repeat cell is equal to 100.12, therefore to get the Mw of the polymer we almost need 200 of the repeat cell which means we now have 400 CH3, 200CH2, 200 >C< and 200 COO. At this time we can calculate the parameters as the same way explained in the previous example:

$V_{298}^{L}=12.1+(400\times 21.55+200\times 15.55+200\times 3.56+200\times 25.7)=17594.1 cc/mol$

$H_{298}^{vap}=5520.03\ kJ/mol\ ,\ \delta[(J/cc)^{0.5}]=8.66\left(cal/cc\right)^{0.5}$

$$c^{GC-ESD} = 1 + (400 \times 0.228 + 200 \times 0.207 + 200 \times (-0.090) + 200 \times 0.498) = 215.21$$

Then by satisfying Equation (16) and (17) we can calculate the size parameter, b, and the dept of potential, ε. The results are as following:

$$b = 6851.65 \ cc/mol, \ \frac{\varepsilon}{k} = 340.36 K$$

3.5.3 Example 3. (Tetrahydrofuran, GC-PC-SAFT)

Tetrahydrofuran consists of 3 RCH2 and 1 CH2O; and its molecular weight is 72.1057 kg/mol. By the same way as explained in the previous example we can calculate the liquid molar volume , heat of vaporization and solubility parameter as below:

$$V_L^{298} = 80.75 \ [cc/mol], \quad H_{vap}^{298} = 28.257 \ [KJ/mol] \ \ \& \ \ \delta = 17.87 \ [(J/cc)^{0.5}]$$

The group contribution shape factor would be obtained as:

$$m^{GC-PCSAFT} = 1 + 3 \times 0.294 + 1 \times (-0.229) = 1.653$$

After Solving two constraints stated in Example B.1 we get :

$$\sigma = 4.07[A^{\circ}] \quad \& \quad \frac{\varepsilon}{k} = 340.36\,[K]$$

which would result in ~85% error in vapor pressure as an average. Again, we have to stress that this method is suggested only when the experimental data are unavailable.

Readers are referred to the available spreadsheets at the link given below to facilitate their calculations:

http://gozips.uakron.edu/~elliot1/

CHAPTER IV

FINITELY LIMITED GROUP CONTRIBUTION CORRELATIONS FOR BOILING TEMPERATURES

4.1 Introduction

Estimates of boiling temperatures can be extremely valuable in modeling many chemical processes. Boiling temperatures are direct measures of the vapor-liquid equilibria (VLE) of pure fluids, and accurate VLE for pure fluids is essential for accurate VLE of mixtures. Mixture VLE plays a crucial role in distillation processes and a related role in other separation processes like supercritical fluid extraction. Generally, one would like to know as much as possible about the boiling properties of a substance, including the vapor pressure from the triple point to the critical point. On the other hand, knowledge of the boiling temperatures at key pressures like 760 and 10 mmHg can go a long way toward providing the necessary information when coupled with the Clausius-Clapeyron equation. While such data exist for many compounds, it is often the case that a new compound is being considered for which data are few or non-existent. Examples might include compressor lubricants for ozone-friendly refrigerants, components in

distillation of biofuels, or oxidation products of volatile organic compounds. In cases like these, the boiling temperatures are key indicators of volatility and solubility. Clearly, it would be desirable to have a reasonable prediction of the vapor pressure, even if the estimated error in the prediction were significant.

When considering boiling property predictions, the compounds of interest usually contain multiple functional groups and boil at high temperatures. High boiling temperatures generally preclude measurement of the entire vapor pressure curve because compounds tend to thermally decompose above 400°C,[67] In these cases, the critical properties must be estimated and properties defined in terms of the critical properties, like the acentric factor, must be treated with care. Then, the boiling properties play an even more important role. Functional group multiplicity also decreases the likelihood of reliable experimental measurements. Experimental studies tend to focus on homologous series. Hence, it is easy to understand how boiling point correlation methods based on nothing but molecular structure may often be necessary.

Reinhard and Drefahl [68] provide a review of many boiling point estimation methods. These methods can be classified as group contribution methods or more generically "structure based" relationships. Generically structure based methods include correlations in terms of connectivity[69],graph theory[70] or any number of descriptors that can be applied to a molecular structure. With this approach, the possibility exists to correlate the properties in terms of many subtle details of the molecular structure, improving precision. On the other hand, the user interface for specifying these details becomes more complex. While graphical methods of specifying molecular structure are becoming more common, present "structure based" correlations are limited to

homologous series and databases containing the properties of interest and all the possible structure based descriptors are relatively uncommon. Group contribution methods, on the other hand, offer advantages of simple user input and wide applicability to a broad range of compounds and properties. Two group contribution methods provide particularly good examples of these advantages: the Joback-Reid[40] and the Constantinou and Gani[41] approaches. The Joback-Reid method is based on 41 simple first-order groups. Stein and Brown[71] extended the Joback-Reid method by increasing the number of groups to 85 and analyzing a database of 11,010 compounds. They retained the Joback-Reid model equation, however. The method of Constantinou and Gani[41] is based primarily on 78 UNIFAC groups[72], with the optional inclusion of second order groups when available. Also, Asher and Pankow[27] have suggested a new UNIFAC-based group contribution method to predict the behavior of organic aerosols in the temperature range of 290-320 K. Their correlation follows the methodology of Jensen et al.[24] and Yair and Fredenslund[25], which correlate the vapor pressure directly, instead of interpolating between boiling temperatures.

The purpose of the present article is to present new correlations for the normal boiling temperature (760 mmHg) and a similar correlation for the additional boiling temperature at 10 mmHg along with the critical temperatue. The group contributions are based on UNIFAC groups to facilitate simultaneous group identification for estimation of activity coefficients. These correlations recognize a finite limit in boiling temperature as well as critical temperature as infinite molecular weight is approached. The rationale for this assumption is explained in the background section. In the present correlations, there are 3 parameters for the boiling temperature correlations and 1 parameter for the critical

temperature plus 72 functional groups for each which are regressed through a database consisting of 336 hydrocarbons and 642 non-hydrocarbons. The database consists of various chemical families including aliphatics, olefinics, naphthenics, aromatics, alcohols, amines, nitriles, thiols, sulfides, aldehydes, ketones, esters, ethers, halocarbons, silicones and acids. Heats of vaporization at 298 K are available for the Joback model which make calculations possible at 10 mmHg by assuming that ΔH is almost constant in this range. Also, Kolska and Gani have reported a correlation for heat of vaporization at the normal boiling point which is used in this study. The utility of having an additional boiling temperature available at, say, 10 mmHg is that, it enables interpolation through the Clausius-Clapeyron equation. Thus estimation of the boiling temperature is made possible at any pressure below roughly 0.2 MPa.. We evaluate the relative accuracy of these correlations by comparing to the Joback, Gani. We obtain 3.5, 4.7, and 4.1 AAD% in temperature for the present work, Joback-Reid, and Gani methods, respectively. Additionally, the accuracy of the present work is evaluated by calculating the vapor pressures from the DIPPR correlation at the predicted temperatures of each model. We obtained 33, 104 and 48 AAD% in pressure for the present work, Joback-Reid, and Gani methods. Also the critical temperature correlation results in 2.6 AAD% in critical temperature. Asher and Pankow have reported UNIFAC-$P_L°$ method to predict the vapor pressure of oxygen-containing compounds to model the behavior of organic aerosols. Their correlation has been regressed in the temperature range of 290 – 320 K. The Asher et al. model is compared to this approach for 66 volatile species. For the vapor pressure at the 10mmHg boiling temperature, we obtain 37 AAD% for the present work and 95 AAD% for the Asher-Pankow method.

4.2 Background

The assumption of a finite limit in the boiling temperature is suggested by: (1) experimental data for pure n-alkanes[45, 73], (2) experimental data for polymer solutions[74] (3) equation of state analysis, [7, 46, 75], and (4) molecular simulation results, [76, 77]. All of these data and analyses suggest that the reciprocal critical temperature should vary as $MW^{-½}$, where MW is the molecular weight, and that the intercept at infinite molecular weight should be non-zero. The critical temperature represents the terminus of the boiling temperature at the molecular weight where the critical pressure approaches 760 or 10 mmHg. Therefore, a finite limit for the critical temperature implies a finite intercept for the boiling temperature curve. In the 10mmHg case, we can estimate the difference between its intercept and that of the critical temperature correlation to be negligible. Therefore, we have based our critical temperature correlation upon boiling temperature at 10mmHg and designed our correlations such that the critical temperature and Tb at 10mmHg curves converge at very high molecular weight. Following Nikitin study[45], the critical pressure approaches 760 mmHg near a carbon number of C_{116} and it approaches 10 mmHg when the carbon number approaches $C_{2200.}$ These trends are illustrated in Figure 4.1 and Figure4.2. These estimates are crude in the sense that they are far from the experimental data, but they serve to establish a rough estimate of the termini of the boiling curves. The termination of the 760 mmHg curve obscures the fact that we assume a common intercept with the 10

mmHg curve. Regression analysis on the two experimental data sets independently showed that the intercepts were within one estimated standard deviation of each other, making any distinction statistically insignificant.

Support for a finite limit in critical temperature can also be found in several related analyses. The data for critical temperatures of polymer solutions like polystyrene in cyclohexane[74], approach very high molecular weights, and these indicate a clearly finite limit. On the other hand, these are not exactly the same things as critical temperatures of pure compounds. It is possible to study the pure compound critical temperature within the context of an assumed equation of state, as shown by Tsonopoulos and Tan [46] for the Flory EOS and Elliott and Lira[75] for the Elliott-Suresh-Donohue (ESD) model. The analysis for the ESD model is relatively simple but helps to illustrate several key points and limitations. The ESD model is:

$$Z \equiv \frac{P}{\rho RT} = 1 + \frac{4cb\rho}{1-1.9b\rho} - \frac{9.5qYb\rho}{1-1.7745Yb\rho} - \frac{Nd(1-X^A)}{1-1.9b\rho} \qquad (18)$$

Where c is a shape factor and proportional to the molecular weight and $q = 1 + 1.90476(c-1)$. The term involving (1-X^A) accounts for hydrogen bonding and is neglected in the present analysis

An advantage of the simple form for the ESD model is that an analytical solution for critical properties is available for non-associating components:

$$Z_c = (1 + 0.115/c^{1/2} - 0.186/c + 0.217/c^{3/2} - 0.173/c^2)/3 \qquad (19)$$

$$B_c = \frac{bP_c}{RT_c} = \frac{Z_c^2[-(1.9k_1Z_c + 3a) + \sqrt{(1.9k_1Z_c + 3a)^2 + 4a(4c-1.9)(9.5q - k_1)/Z_c}}{2a(4c-1.9)}$$

(20)

$$Y_c = \frac{Z_c^3}{a}\left(\frac{RT}{bP_c}\right)^2 \tag{21}$$

$$\varepsilon / k = T_c \ln(Y_c + 1.0617) \tag{22}$$

where, $a = 1.9(9.5q - k_1) + 4ck_1 \quad and \quad k_1 = 1.7745$

Taking the limit as $c \to \infty$, we obtain $Z_c \to 1/3$.

Also, at $c \to \infty$, $a \to \infty$ and $q \to \infty$. Therefore, the dimensionless critical pressure becomes:

$$B_c \sim \frac{-3a + \sqrt{(3a)^2 + 16ac(9.5q)\times 3}}{8ac} \sim \frac{c^{3/2}}{c^2} \sim c^{-1/2}$$

$$B_c \sim \frac{-3a + \sqrt{(3a)^2 + 16ac(9.5q)\times 3}}{8ac} \sim \frac{c^{3/2}}{c^2} \sim c^{-1/2} \tag{23}$$

And subsequently Y_c becomes proportional to a constant:

$$Y_c \sim \frac{(c^{-1/2})^2}{c} \sim 1 \tag{24}$$

Solubility parameter represents a standardized scale of the attractive energy (ε) density and is known to be independent of molecular weight for polymers. Therefore, it is inferable from Eq(22) that a finite limit is indicated for the critical temperature. This result is common to many EOS models, including those involving Statistical Associating Fluid Theory (SAFT). In fact, [43] have shown that all EOS models with linear dependence on molecular weight must conform to $Z_c \to ⅓$. This observation suggests a possible limitation to the EOS approach since experimental observations do not appear to

be consistent with $Z_c \rightarrow ⅓$, [43]. Nevertheless, the finite limit in T_c is supported by both the EOS analysis and the available experimental data.

Molecular simulations can artificially overcome the thermal decomposition problem. Smit et al.[78] obtained the critical properties up to C48 by a configurational-bias Monte Carlo simulation. Later, Escobedo and de Pablo[76] simulated SW-chains up to 100 segments and fitted the simulation results to the rectilinear diameter rule to calculate the critical points. They obtained 2.6 for $T_\infty^{c*}(k_{\mathbf{B}}T_\infty^c/\varepsilon)$ of infinite SW-chains. Recent work by Elliott and Gray[77] permits an extrapolation to the long chain limit by SPEAD equation of state[48]. The asymptotic trends observed by Elliott and Gray[77] also indicate that a finite critical temperature is approached, although it is lower than the experimental trend. Furthermore, the trend for Z_c is decreasing until a value of roughly 0.25 at N_c=100 and η_c=0.057, but then Z_c increases to 1/3, consistent with the assessment of Lue et al. The trend in this case is obscured by the presence of two inflections in the critical region for $N_c>15$, indicating a need for greater care in the regression of A_2 in the critical region at high molecular weight. Further work would be required to resolve this problem completely, but the indication of a finite limit in T_c even while N_c goes to infinity is our primary interest in the present work. Readers are referred to Gerek and Elliott[48] and also Elliott and Gray[77] for further details about the SPEAD EOS.

Altogether, these data and analyses could be ignored individually as merely indirect inferences because of the problem with thermal decomposition and the inability to directly measure the boiling properties at infinite molecular weight. Taken together, however, the observation that all these inferences point consistently to the same model equation, suggests adopting that equation for further analyses.

4.3 Database and Methods

Two sources comprise the database applied in the present study. The first is the database used by ChemStations, Inc. in their process simulation software package ChemCAD. These data are taken primarily from the DIPPR compilation. UNIFAC groups have already been assigned to all compounds in the ChemCAD database, along with coefficients of the vapor pressure equation and limits on the range of applicability when available. In all cases, 10 mmHg and 760 mmHg were within the range of the available vapor pressure correlations. A number of compounds were individual groups, either recognized within the UNIFAC framework (e.g. water) or not (e.g. CO2), were deleted from the database.

For several compounds, UNIFAC groups were not exactly applicable. Notably, these include anhydrides, organometallics, lactones, secondary thiols and cyanides, peroxides, phenyl –thiols and -cyanides, and isocyanates. In this context, it must be pointed out that the UNIFAC groups have a disadvantage in that many common molecular structures have been omitted in the current formulation. Nevertheless, the UNIFAC method has received broad acceptance in the estimation of activity coefficients. Since activity coefficients and boiling points are of similar importance in separation processes, it is advantageous to have a universal group specification method, especially since the identification of the most representative UNIFAC group sometimes requires judgment on the user's part. Furthermore, applications to activity coefficients have

necessitated construction of fairly large databases in which corresponding groups and properties are readily available. As with any group contribution method, it is always possible to imagine adding more groups. At present, we opt for the UNIFAC group definitions as a compromise between general coverage and general utility.

For non-volatile hydrocarbons, additional data were available in the form of the API 42 project [79]. These data are focused on vapor pressures between 1 and 10 mmHg. The 10 mmHg data were selected for compilation and correlation. UNIFAC groups were assigned and the ChemStations and API 42 databases were combined for the hydrocarbons.

With these adjustments the database was reduced to 336 hydrocarbons and 642 non-hydrocarbons. The distribution of compound functionalities is summarized within Table 4.2. The procedure for developing the correlations was to regress the hydrocarbons first, then, leave the hydrocarbon groups unchanged while optimizing the non-hydrocarbon group characterizations. Minimization of the average absolute error in temperature was the objective function. The solver utility in Microsoft Excel® was used to perform the non-linear regressions. The proposed model equation for the normal boiling point is given by:

$$T_b / K = \frac{1000}{C_1 + \frac{C_2}{\sqrt{\sum \nu_k \left(\Delta T_b\right)_k}} + \frac{1000}{C_3 + \sum \nu_k \left(\Delta T_b\right)_k}} \tag{25}$$

At a pressure of 760 mmHg, C_1=0.5, C_2=38.36, and C_3=256.6. For a pressure of 10 mmHg, the constants are C_1=0.5, C_2=59.15, C_3=274.22.

In the same way as described above, we have regressed a correlation for critical temperature based on boiling temperature at 10 mmHg. The proposed correlation is as follows:

$$T_c / K = T_b^{10\,mmHg}\left(1+\frac{1}{0.596+\sum \nu_k (\Delta T_c)_k}\right) \tag{26}$$

The group characterizations for critical temperature and boiling temperatures are given at Table4.3.

The accuracy of the proposed boiling temperature correlations has been compared with Joback-Reid [40] and Constantinou-Gani[41] group contribution methods.

The Joback model equation for calculating the normal boiling temperature is given by:

$$T_b / K = 198.2 + \sum \nu_k \left(\Delta T_b\right)_k \tag{27}$$

The Constantinou and Gani formula for normal boiling temperature is:

$$T_b / K = 204.359 \times \ln\left[\sum \nu_k (\Delta T_b)_k\right] \tag{28}$$

Calculating the temperature at other pressures is possible using the Clausius-Clapyron equation and having the heat of vaporization. Heats of vaporization at 298 K for Joback model [40] are given by:

$$\Delta H^{\circ}_{v,298} = 15.3 + \sum \nu_k \, \Delta H_k \;\; kJ / mol \tag{29}$$

By considering that the heat of vaporization is almost constant within this temperature range, we can calculate the boiling temperature at 10 mmHg. On the other hand, Kolska and Gani[42] have reported heats of vaporization at the normal boiling

point for Constantinou-Gani groups. These give lower deviations and are used in this study . The suggested model equation is:

$$\Delta H^{\circ}_{v,298} = 14.876 + \sum \nu_k \, \Delta H_k \;\; kJ / mol \tag{30}$$

Average absolute deviations for temperatures at 760 and 10 are summarized at Table 4.4.

As criteria for the accuracy of this model, vapor pressures at 760 and 10 mmHg are calculated with the DIPPR correlation presented by Daubert and Danner[73]. The correlation is as below:

$$P = \exp\left[A + \frac{B}{T} + C \ln T + DT^E \right]; \;\; P[Pa], T[K] \tag{31}$$

DIPPR coefficients are available at DIPPR (2004)[62].

A comparison between the correlated vapor pressures by this approach, Joback and Gani is performed and is shown in

4.5.

Asher and Pankow[27] have proposed a UNIFAC-based method, UNIFAC-$P_L°$, to predict the vapor pressure of volatile oxygen-containing compounds in order to model the partitioning of the atmospheric particulate materials in organic aerosol systems. They have suggested the following equation in order to calculate the liquid vapor pressure of pure compounds as a function of temperature, $P^{\circ}_{L,i}(T)$.

$$RT \ln P^{\circ}_{L,i}(T) = \sum_{k=1}^{N} \nu_{k,i} \Delta g_k + \sum_{k=1}^{N} \nu_{k,i} \Delta \Gamma_{k,i} \tag{32}$$

where, R is the gas constant, T is the system temperature, $\nu_{k,i}$ is the number of groups of type k in compound i, Δg_k is the difference between the free energy of the

compound at temperature T in the pure liquid and in the ideal gas at 1 *atm*, and $\Delta\Gamma_{k,i}$ is the UNIFAC residual term. According to the Asher[26] approach, Δg_k can be defined as:

$$\Delta g_k = \frac{A_{k,1}}{T} + A_{k,2} + A_{k,3}T + A_{k,4}\ln T \qquad (33)$$

Vapor pressures are calculated for 66 compounds at 10 mmHg by the present model and compared with Asher et al. approach and are summarized at Table 4.8

4.4 Results and Discussion

The resulting group characterizations for boiling temperatures at 760 and 10mmHg are given in Table 4.3, which are optimized for a database including 978 compounds. The coverage of different families in the database is provided in Table 4.2. The % average absolute deviations for temperature, *T*AAD%, and the absolute temperature differences, $|\Delta T|$, between correlated temperatures and experimental ones are tabulated at Table 4.4. Note that the number of compounds has been reduced from 978 to 942 because some group such as Si, have not been reported by Joback[40] and Constantinou [41] Also, there are some other groups like CCl2, ACNO2, >N- which are not reported by Kolska[42] to calculate the heat of vaporization at normal boiling points for the Gani model. Therefore, to make the comparison consistent we have reduced the database in a way that every compound can be treated by all three models. A complete list of excluded compounds is provided in the Appendix F. For comparison, the deviations of correlated temperatures by the Joback and the Gani methods are also

summarized in Table 4.4. It is evident from Table4.4 and Figure 4.1 that the Joback-Reid method exhibits higher deviations than either of the other two methods. The Gani method appears to approach a finite value for the intercept in Figure 4.1, but consideration of their model equation indicates that the intercept must actually approach zero and this is evident in near infinite molecular weight. This discrepancy has a larger impact at 10 mmHg than at 760 mmHg, as shown in Table 4.1. Whereas the %AAD at 760mmHg is 3.1 for Gani's method compared to 2.9% for the present work, this increases to 5.2% vs. 4.1% at 10mmHg. A partial explanation for this behavior is that the 10 mmHg curve approaches the T_c curve more closely than the 760 mmHg curve at high molecular weights. Table 4.5 shows the results of vapor pressure calculations and their deviations. The maximum deviations obtained for the temperatures are given in Table 4.6. As mentioned before the utility of having two boiling temperatures available is that, it enables interpolation through the Clausius-Clapeyron equation. As an example we predicted boiling temperature at 100mmHg and compared them with Joback and Gani methods. The results are summarized in Table 4.7. Additionally, Figure 4.3, Figure 4.4 , and depict a comparison for all three models for some olefins, ethers and halocarbons. Halocarbons having 3 carbons or less shows high deviations for all three models. Table 4.5, Figure 4.3, Figure 4.4, and Figure 4.5 show that the present method can predict the vapor pressures more accurately than the other two approaches. Detailed analysis of the regression results shows that the improved accuracy of the proposed correlations is most significant for the compounds with highest molecular weights. This observation is consistent with our hypothesis that the model equation should follow the general trend illustrated in Figure 4.1 and Figure 4.2. Additionally, the predicted vapor pressures for 66

compounds are compared with the ones using Asher and Pankow[27] method at 10 mmHg. Note that the saturation temperatures for all of these compounds are in the same range that Asher et al. has used to regress their coefficients which makes the comparison fair. The results are shown in Table 4.8. It is observed that the Asher et al. method can predict the vapor pressures of alcohols more accurately, while the present method is more accurate for other compound families. A detailed table of compounds and their estimated vapor pressures by Asher et al. approach has been provided in the Appendix G.

Table 4.1. AAD% in boiling temperature at 760 and 10 mmHg for 942 compounds

P(mmHg)	Present work	Joback-Reid	Gani
760	2.9	4.1	3.1
10	4.1	5.2	5.2
Combined Avg	3.5	4.7	4.1

The primary limitations of the proposed correlations have to do with accuracy for the various functional groups and the lack of general coverage of molecular structures of the current UNIFAC formulation. In both cases, a simple solution is to add more functional groups. To improve accuracy, secondary groups could be added. To improve general coverage, additional primary groups could be included. In both cases, one must be concerned about the availability of sufficient data to reliably characterize the groups and the utility of the user interface. Advances in graphical interfaces may improve the flexibility in designing the user interface, but we note that computer methods are improving in general. In particular, we note that molecular simulation techniques are advancing to the point that viable predictions of properties like boiling and critical

temperatures may be available in the foreseeable future. Molecular simulations using united atom models can be likened to first order and higher order group contribution methods simultaneously. The group identifications in united atom models are similar to first order groups like CH_2 or CH. But the molecular geometry is also implied by the molecular model, accounting for the physical basis that gives rise to higher order effects. In our estimation, future generations of group contribution methods should derive from steadily closer relations to molecular simulation methodology.

Table 4.2 Distribution of various families in the data base to characterize the functional group boiling points.

Families	No. of Occ.	Example
Alcohols	108	Inositol
Amines	56	Benzylamine
Nitriles	10	Propionitrile
Silanes	10	Dimethyl Silane
Imines	7	Acridine
Tert-Ns	6	Trimethylamine
Nitrates	19	O-Nitrotoluene
Thiols	27	Cyclohexyl mercaptan
Aldehydes	23	Methacrolein
Epoxides	18	1,2 Epoxybutane
Ethers	38	Acetal
Formates	16	Methyl formate
Esters	93	Isobutyl acetate
Ketones	28	Cyclohexanone
Alcohol-Ethers	18	Carbitol
Hydrocarbons	157	Propyne
Cyclic hydrocarbons	41	Cis-decalin , Cyclooctane
Aromatic hydrocarbons	138	Styrene , 1,4 Pentadiene
Halocarbons	108	Allyl chloride , Freon 13B1
Acids	57	Cinnamic Acid
Total	**978**	

Table 4.3 Group characterizations for critical temperature and boiling temperatures at 760 and 10 mmHg

Groups	No. of Occ.	Tb at 760 mmHg	Tb at 10 mmHg	T_c
CH3	665	116.284	76.569	0.086
CH2	517	123.631	111.400	0.041
RCH2	82	133.831	110.859	0.036
CH	164	95.944	111.000	-0.009
RCH	42	111.630	101.100	0.015
C	65	58.450	90.711	-0.086
RC	12	36.300	72.857	0.038
CH2=CH	72	229.791	178.000	0.112
CH=CH	57	258.038	225.819	0.079
CH2=C	32	240.287	208.545	0.050
CH=C	17	266.852	264.290	0.025
C=C	3	188.120	180.000	-0.176
ACH	240	132.609	108.000	0.037
AC	101	204.558	192.740	0.004
ACCH3	63	282.512	243.180	0.099
ACCH2	51	273.625	267.900	0.054
ACCH	10	226.530	248.000	-0.005
OH	99	412.000	397.860	0.225
ACOH	26	525.221	571.449	0.163
CH3CO	22	518.749	447.547	0.193
CH2CO	14	493.090	468.100	0.167
CHO	25	384.480	332.500	0.180
CH3COO	23	520.791	462.720	0.222
CH2COO	33	497.163	472.520	0.204
HCOO	16	409.000	360.579	0.188
CH3O	23	250.000	207.642	0.145
CH2O	56	245.957	234.651	0.108
CH-O	6	213.800	188.000	0.046
FCH2O	1	337.000	256.000	0.112
CH2NH2	19	409.408	367.300	0.189
CHNH2	4	351.959	323.100	0.105
CH3NH	3	325.300	308.000	0.148
CH2NH	9	325.300	308.000	0.105
CHNH	2	325.300	308.000	0.137
CH3N	1	142.000	217.681	0.144
CH2N	5	142.000	217.681	0.008

Table 4.3 Group characterizations for critical temperature and boiling temperatures at 760 and 10 mmHg (Continued)

ACNH2	13	611.200	546.553	0.112
C5H4N	3	925.245	828.662	0.196
CH2CN	10	734.001	628.005	0.179
COOH	58	800.052	797.129	0.317
CH2CL	23	399.999	346.591	0.129
CHCL	12	312.000	265.517	0.074
CCL	4	275.600	236.610	0.066
CHCL2	7	568.324	474.200	0.161
CCL2	3	469.500	375.331	0.087
CCL3	7	647.410	519.421	0.148
ACCL	13	366.305	310.470	0.080
CH2NO2	2	797.000	696.000	0.220
CHNO2	1	744.000	672.000	0.174
ACNO2	16	733.000	671.000	0.164
CH2SH	20	501.000	418.277	0.129
I	5	509.000	424.420	0.072
Br	25	201.724	125.556	-0.023
CH===C	12	263.387	210.342	0.106
C===C	7	309.648	97.538	-0.185
CL<C=C>	7	183.171	140.000	0.092
ACF	2	131.000	112.323	0.071
CF3	12	0.001	0.001	-0.122
CF2	11	90.000	10.000	-0.088
CF	4	110.000	92.000	0.107
COO	43	385.893	361.331	0.150
SiH3	1	167.864	137.000	0.071
SiH2	1	160.000	153.000	0.029
SiH	1	133.000	144.000	-0.026
Si	3	94.000	135.000	-0.051
SiO	5	108.481	138.000	0.026
TERT-N	5	94.000	140.000	-0.041
CCL2F	2	408.557	344.181	0.161
CCLF2	5	14.500	37.700	-0.145
CONH2	3	1371.950	1066.585	0.125
CH3S	2	464.600	411.035	0.119
CH2S	5	464.600	411.035	0.091

Table4.4Temperature average absolute deviations for various models at 760 and 10mmHg

		T AAD%			| ΔT |		
Families	No. of Occ.	This	Joback	Gani	This	Joback	Gani
Alcohols	106	3.3	4.5	2.9	14.1	20.9	13.0
C3-C24 amines	56	3.2	4.9	4.0	12.3	18.7	14.9
C2-C14 Nitriles	10	4.4	3.9	5.9	20.6	16.9	26.6
C3-C8 Imines	5	3.0	3.8	3.6	11.2	13.4	13.0
C5-C10 Tert-N	4	2.5	4.0	2.6	10.1	15.5	9.9
C6-C15 Nitrates	3	0.8	3.2	1.0	2.6	11.5	3.5
C2-C3 thiols	27	1.9	5.0	3.4	7.4	18.3	12.5
C2-C12 aldehydes	23	1.9	3.8	2.6	6.3	13.1	8.7
C2-C13 Epoxides	18	3.8	6.5	9.5	11.9	19.4	27.9
C3-C7 Ethers	38	1.6	3.5	3.5	5.4	12.4	11.6
C2-C18 Formates	16	1.1	2.3	2.0	3.4	8.2	6.9
C2-C11 Esters	93	1.6	4.7	2.3	6.9	23.7	9.6
C3-C28 Ketones	28	2.0	3.6	3.8	7.2	12.4	13.3
C3-C12 Alcohol-Ethers	18	3.6	5.1	3.9	14.2	20.1	15.6
C3-C10 Hydrocarbons	156	1.8	4.1	3.2	6.0	15.0	11.0
C3-C32 Cyclic Hydrocarbons	41	1.6	2.7	3.9	5.4	20.4	12.6
C3-C16 Aromatic Hydrocarbons	138	1.8	4.1	3.9	8.2	18.6	16.7
C4-C24 Halocarbons	105	10.0	6.0	5.8	25.8	18.0	15.7
C3-C10 Acids	57	9.6	9.9	12.5	51.6	53.1	66.3
C3-C18 Total	942	3.5	4.7	4.1	12.2	20.2	16.7

4.5 Pressure average absolute deviations for different models at 760 and 10 mmHg

Families	No. of Compounds	This	Joback	Gani
Alcohols C3-C24	106	45.5	123.4	47.0
amines C2-C14	56	39.0	71.0	47.7
Nitriles C3-C8	10	40.0	40.6	49.5
Imines C5-C10	5	33.9	65.9	38.8
Tert-N C6-C15	4	57.9	82.7	53.8
Nitrates C2-C3	3	11.3	49.1	15.4
thiols C2-C12	27	27.0	49.7	39.1
aldehydes C2-C13	23	28.3	41.9	40.6
Epoxides C3-C7	18	37.0	56.3	63.4
Ethers C2-C18	38	23.1	44.0	42.4
Formates C2-C11	16	22.2	40.6	34.5
Esters C3-C28	93	29.0	238.0	31.5
Ketones C3-C12	28	28.1	41.2	44.5
Alcohol-Ethers	18	65.4	118.5	87.6

Table 4.5 Pressure average absolute deviations for different models at 760 and 10 mmHg (Continued)

C3-C10				
Hydrocarbons C3-C32	156	25.3	93.6	40.8
Cyclic Hydrocarbons C3-C16	41	23.7	40.8	40.0
Aromatic Hydrocarbons C4*-C24	138	26.6	62.4	43.5
Halocarbons C3-C10	105	45.0	79.1	116.7
Acids C3-C18	57	51.2	248.9	65.5
Total	**942**	**33.2**	**104.3**	**48.1**

* Conjugated double bonds (e.g. 1,3-Butadiene) act like aromatic hydrocarbons.

Table 4. 6 Maximum deviations in boiling temperatures and vapor pressures using the present approach

Families	No. of Occ.	Max T AAD %	Max | ΔT |	Max P AAD %
Alcohols C3-C24	106	18.5	75.9	209.3
amines C2-C14	56	17.6	57.9	204.5
Nitriles C3-C8	10	13.5	59.9	95.1
Imines C5-C10	5	6.8	25.0	60.9
Tert-N C6-C15	4	5.2	19.4	166.0
Nitrates	3	2.3	6.7	37.4

Table 4.6 Maximum deviations in boiling temperatures and vapor pressures using the present approach (Continued)

C2-C3 thiols	27	5.9	24.8	141.0
C2-C12 aldehydes	23	8.7	27.9	177.0
C2-C13 Epoxides	18	12.5	44.8	81.2
C3-C7 Ethers	38	5.1	17.9	155.8
C2-C18 Formates	16	6.0	15.3	93.5
C2-C11 Esters	93	8.9	58.4	233.5
C3-C28 Ketones	28	14.2	56.7	249.3
C3-C12 Alcohol-Ethers	18	8.8	42.0	278.8
C3-C10 Hydrocarbons	156	25.5	55.7	219.5
C3-C32 Cyclic Hydrocarbons	41	8.1	16.7	221.4
C3-C16 Aromatic Hydrocarbons	138	20.3	68.5	204.4
C4-C24 Halocarbons	105	13.9	28.7	100.0
C3-C10 Acids	57	34.8	257.5	118.94
C3-C18 Total	942	34.8	257.5	278.8

Table 4. 7 Boiling temperature deviations at 100 mmHg predicted by the present approach, Joback, and Gani models.

Families	No. of Comp.	T AAD% at 100 mmHg			| ΔT | at 100 mmHg		
		This	Joback	Gani	This	Joback	Gani
Alcohols	106	3.1	4.5	2.6	13.3	20.4	11.6
C3-C24 amines	56	2.9	4.7	3.4	11.3	17.9	12.7
C2-C14 Nitriles	10	4.3	3.5	5.3	20.1	15.8	24.8
C3-C8 Imines	5	2.4	3.7	2.9	8.8	13.1	11.1
C5-C10 Tert-N	4	2.3	3.8	1.6	8.8	15.0	6.4
C6-C15 Nitrates	3	0.8	3.5	0.9	2.9	11.9	3.0
C2-C3 thiols	27	1.8	4.5	3.1	6.6	16.9	11.4
C2-C12 aldehydes	23	1.5	3.4	2.0	4.7	12.0	6.3
C2-C13 Epoxides	18	3.6	6.1	9.0	10.7	18.6	25.9
C3-C7 Ethers	38	1.4	2.9	2.7	4.9	10.5	9.1
C2-C18 Formates	16	0.9	1.5	1.6	2.6	4.9	5.1
C2-C11 Esters	93	1.5	4.4	1.9	6.5	22.0	7.9
C3-C28 Ketones	28	1.8	3.3	3.0	6.6	11.8	10.7
C3-C12 Alcohol-Ethers	18	3.6	5.1	4.1	14.2	19.8	16.1
C3-C10 Hydrocarbons	156	1.5	3.7	2.2	5.1	13.8	8.0
C3-C32 Cyclic Hydrocarbons	41	1.5	2.1	3.5	4.7	6.6	11.8
C3-C16 Aromatic Hydrocarbons	138	1.7	3.6	3.3	7.3	16.4	14.8
C4-C24 Halocarbons	105	10.2	5.7	5.4	26.0	16.9	14.4

Table 4.7 Boiling temperature deviations at 100 mmHg predicted by the present approach, Joback, and Gani models.(Continued)

C3-C10 Acids	57	4.2	6.0	7.1	23.7	33.0	37.9
C3-C18 Total	942	3.0	4.2	3.4	10.7	17.1	13.2

Table 4. 8 A comparison between the estimated vapor pressures at 10 mmHg by this method and Asher approach [27] for 68 compounds. (all temperatures are in the scope of Asher et al. regression, i.e. between 290 and 320).

		This	**Asher et.at 2006**
Families	**No. of Comp.**	**%AAD**	**%AAD**
alcohos	12	48.6	27.0
aldehyde	4	16.4	27.1
ketone	9	52.4	261.5
Hydrocarbones	21	36.3	62.6
Cyclic Hydrocarbons	8	25.4	175.6
Aromatics Hydrocarbons	12	24.3	61.7
Total	**66**	**36.9**	**94.5**

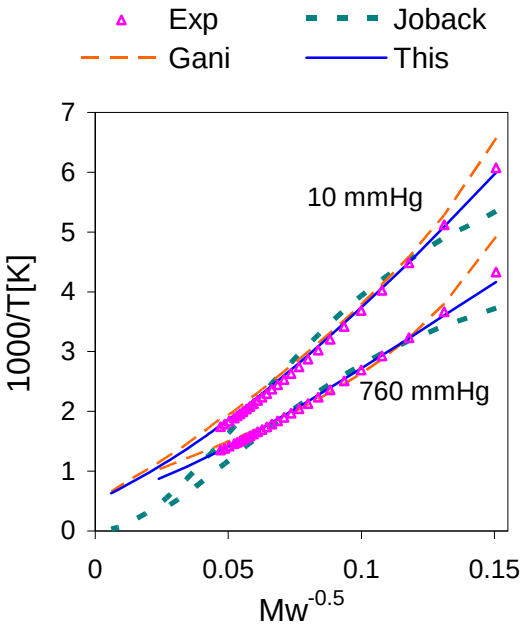


Figure 4.1 Boiling temperatures of n-alkanes versus molecular weight.

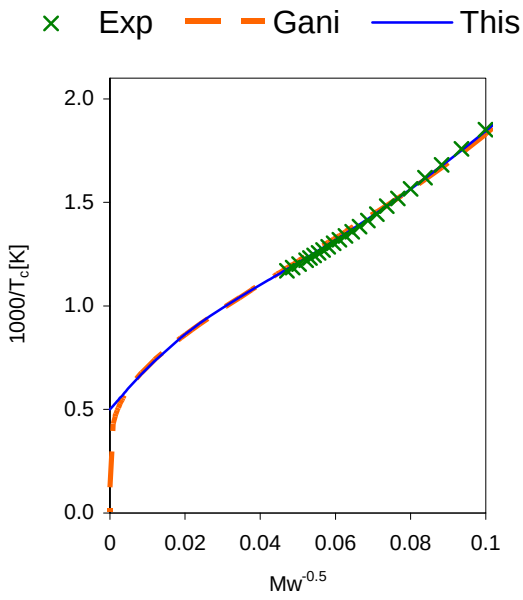


Figure 4. 2 Critical Temperature of n-alkanes versus molecular weight.

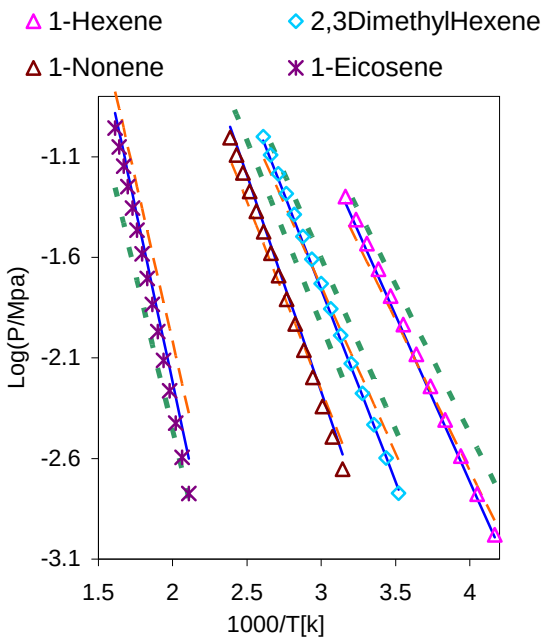


Figure 4. 3 Vapor pressure versus temperature for some olefins. Experimental data are shown by points. The solid line, doted line and dashed lines represent for This, Joback and Gani approaches, respectively.

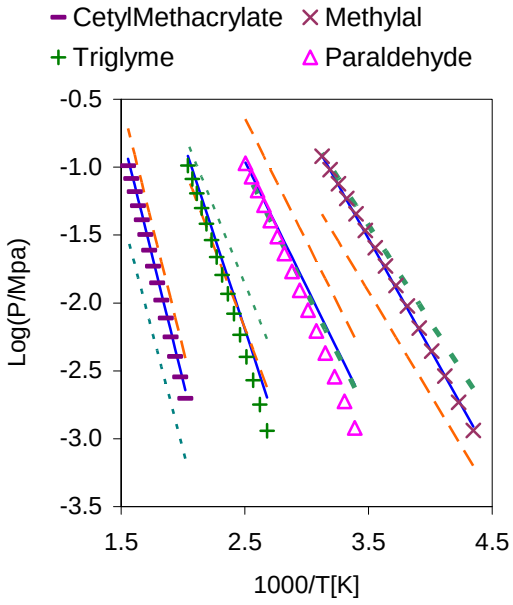


Figure 4. 4 Vapor pressure versus temperature for some Ether and Esters. Experimental data are shown by points. The solid line, doted line and dashed lines represent for This, Joback and Gani approaches, respectively.

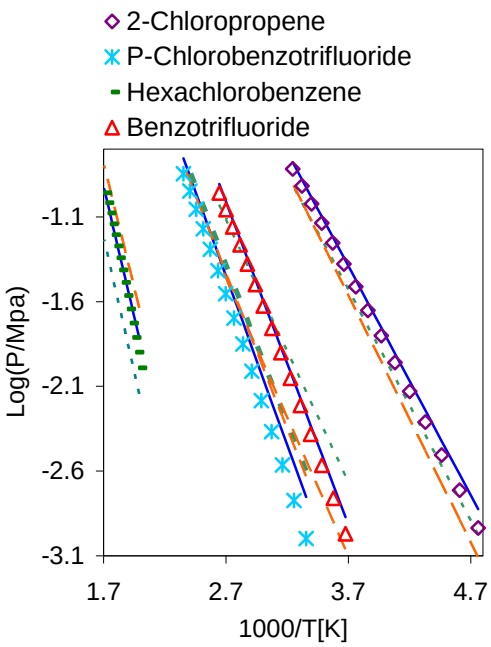


Figure 4. 5 Vapor pressure versus temperature for some halocarbons. Experimental data are shown by points. The solid line, doted line and dashed lines represent for This, Joback and Gani approaches, respectively.

4.5 Conclusions

The proposed method is more accurate than the Joback-Reid or Gani methods. Referring to Table 4.4, for example, this method has an average value of $|\Delta T|$ of 12.2Kwhile Joback-Reid and Gani shows 20.2 K and 16.7 K. Noting that at very high molecular weight the critical pressure would nearly coincide with 10 mmHg, a finite limit for the critical temperature implies a finite intercept for the boiling temperature. The Joback- Reid method has a contradictory asymptotic trend at infinite molecular weight. This suggests that the proposed method may have particular advantages at high molecular

weights. The accuracy of this correlation at 10 mmHg suggests that using the Clausius-Clapeyron equation, boiling temperatures can be accurately predicted at any temperature below 0.2 MPa. Finally, we compared our model with Asher and Pankow[27] for 66 compounds at 10 mmHg. Table 4. 8 reveals that our model predicts the vapor pressures more accurately than the Asher et al. approach except for the alcohols.

These correlations establish a basis for the accuracy that can be achieved with group contribution methods by themselves. The accuracy achieved with the present method is comparable to what was achieved by correlating equation of state parameters[80], but less than the accuracy that is typical of a molecular simulation technique like the SPEADMD method[57]. In future work, we expect to improve the coverage an accuracy of the SPEADMD methodology to the point that group contribution methods become attractive only as preliminary guidelines.

CHAPTER V

CONCLUSIONS

The objectives outlined in the beginning of the thesis were achieved and the following was concluded:

1. In Chapter III, we performed a detailed analysis on the Elliott and Natarajan method and observed a peculiar behavior of the alcohols with multi hydroxyl groups. Presumably, the reason is the intramolecular hydrogen bonding in these kinds of molecules. Moreover, acids show different behavior because of the same reason. Thereby, we decided to delete these two groups of compound from our database and reregress the parameters. By this justification the vapor pressure errors obtained by the Elliott and Natarajan method has been improved from ~81% to ~40% for 878 compounds. Thereafter, the method was implemented for SAFT and PC-SAFT equations of state by the same procedure. A distinctive part of this work to the other already existed is proposing groups for varied associating compounds like alcohols, amines, aldehydes, nitriles, and alcohol-ethers. Finally, we calculated vapor pressures obtained by our approach and compared them to the other existed methods like Tihic et al. approach. We obtained roughly 40% AAD for pressures for both ESD and PC-SAFT and 69% AAD for SAFT. By testing our method against Tihic we obtained

~54% AAD in pressures by Tihic approach and ~28% AAD by our GC-PC-SAFT for ~650 compounds. This approach can easily be used to estimate the thermodynamic behavior of polymers.

2. In Chapter IV, we studied the asymptotic trend of critical temperatures as the infinite molecular weight is approached. Since by increasing the number of carbons the critical pressure coincides with 760mmHg and 10 mmHg at vary high molecular weight, a similar asymptote is expected for boiling temperature curves. Keeping this fact in mind, we have proposed two correlative group contribution formulas for Tb at 760 mmHg and at 10mmHg and one for the critical temperature. The availability of two temperatures enables one to calculate other boiling temperatures via an interpolation by Clausius-Clapeyron equation. We compared our method with Joback-Reid and Gani model. We obtained 3.5 AAD% in temperature and 33 AAD% in pressure for this model. Moreover, Joback method has completely wrong trend as the molecular weight becomes larger. Gani shows almost good results but wrong asymptote for the critical temperature. Finally, we compared the accuracy of our predicted pressures by the ones with Asher and Pankow model for 66 volatile compounds. We obtained more accurate results for the present work compare to Asher and Pankow model.
3. Comparing the EOS approach to the boiling temperature correlation, the two methods provide similar accuracy for vapor pressure. For example, the GC-PC-SAFT model provides 32 *P*AAD% while we estimate the average accuracy from the boiling temperature correlation with the Clausius-Clapeyron equation to be 33%.

Accordingly, the primary advantage of the EOS approach is that it simultaneously provides other properties like density and a straightforward extension to mixtures.

CHAPTER VI

FUTURE RESEARCH

In future research, the EOS methods could be readily extended to mixtures including polymer solutions as demonstrated by Elliott and Natarajan.

1. We hope to address the carboxylic acids and the alcohols with more than one hydroxyl group by GC-ESD and GC-PC-SAFT in the very near future.
2. Predicting other thermodynamic properties such as entropy, speed of sound, and heat capacity can be the subject of future studies.
3. The coverage of the SPEADMD methodology should be extended to include the same compounds that comprised the present database. Then a direct comparison should be made between the molecular simulation approach and these group contribution methods. Preliminary results indicate deviations to be roughly three times smaller for the molecular simulation approach, but molecular simulations have focused on limited families of compounds.

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APPENDICES

APPENDIX A.

THE SAFT AND PC-SAFT EQUATIONS OF STATE AND THEIR DERIVATIONS

A.1. The SAFT Equation of State

At this section we have summarized some quantities in terms of SAFT Eqation of State which are used for the caculations in chapter III.

A.1.1 Compressibility factor

The SAFT equation of state for pure fluids is specified by

$$Z = 1 + Z^{seg} + Z^{chain} + Z^{assoc} \qquad \text{(A.1.1. 1)}$$

$$Z^{seg} = m\left[\frac{4\eta - 2\eta^2}{(1-\eta)^3} + \sum_i \sum_j jD_{ij}\left[\beta u\right]^i \left[\frac{\eta}{\tau}\right]^j\right] \qquad \text{(A.1.1. 2)}$$

where m is a shape factor equal to the number of spherical segments per molecule, $\eta = b\rho$ is the reduced fluid density (segment packing fraction), $b = \tau m \upsilon^{\circ}$ is the molar volume occupied by molecules themselves, $\tau = 0.74048$, υ° is the segment molar volume in a closed-packed arrangement, i.e. the volume occupied by N_{Av} closely packed

segments, in milliliters per mole of segments. By considering the definition of the packing fraction

we can express υ° as

$$\upsilon^{\circ} = \frac{\pi N_{Av}}{6\tau} d^3 \qquad \text{(A.1.1. 3)}$$

Since υ° is implicitly temperature dependent (d is temperature dependent) Huang and Radosz[16] decided to include a corresponding, temperature-independent segment molar volume at zero temperature, $T = 0$, which would be denoted $\upsilon^{\circ\circ}$ and referred to as the *segment volume*:

$$\upsilon^{\circ\circ} = \frac{\pi N_{Av}}{6\tau} \sigma^3 \qquad \text{(A.1.1. 4)}$$

where σ is a temperature-independent segment diameter. Temperature dependence of the segment diameter d is based on the Barker-Henderson approach. Specific equations for d and υ° are given below.

$$d = \sigma\left[1 - C\exp\left(-3\beta u^0\right)\right] \qquad \text{(A.1.1. 5)}$$

$$\upsilon^{\circ} = \upsilon^{\circ\circ}\left[1 - C\exp\left(-3\beta u^0\right)\right]^3 \qquad \text{(A.1.1. 6)}$$

Therefore, we can rewrite the packing fraction as below:

$$\eta = \frac{\pi N_{Av}}{6} \rho m d^3 \qquad \text{(A.1.1. 7)}$$

$$Z^{chain} = (1-m)\left[\frac{\frac{5}{2}\eta - \eta^2}{(1-\eta)(1-\frac{\eta}{2})}\right] \qquad \text{(A.1.1. 8)}$$

$$Z^{assoc} = \frac{-F^2(-\eta^2 + 2\eta + 2)}{(1-\eta)(2-\eta)} \quad \text{(A.1.1. 9)}$$

$$F = 2N_d\alpha^{\frac{1}{2}} / [1 + (1 + 4N_d\alpha)^{\frac{1}{2}}] \quad \text{(A.1.1. 10)}$$

where N_d is the number of segments per molecule possessing hydrogen bonding sites.

$$\alpha = \frac{\rho K^{AD} Y^{HB} (1 - \frac{\eta}{2})}{(1-\eta)^3} \quad \text{(A.1.1. 11)}$$

$$Y^{HB} = \exp(\beta\varepsilon^{HB}) - 1 \quad \text{(A.1.1. 12)}$$

K^{AD} is the hydrogen bonding volume, and ε^{HB} is the energy of hydrogen bonding.

A.1.2 Helmholtz free energy

$$\tilde{A}^{res} = m\left[\frac{4\eta - 3\eta^2}{(1-\eta)^2} + \sum_i \sum_j D_{ij} (\beta u)^i \left(\frac{\eta}{\tau}\right)^j\right] + (1-m)\ln\frac{1-\frac{\eta}{2}}{(1-\eta)^3} + \quad \text{(A.1.2. 1)}$$
$$2N_d \ln(1 - F^2 / N_d) + F^2$$

A.1.3 Solubility parameter

For the association contribution, we use the simplified form of Wertheim's theory developed by Elliott 1996.

$$\frac{\delta^2 V_L^{298}}{298R} = -\frac{U}{298R} \quad \text{(A.1.3. 1)}$$

$$\frac{U}{RT} = \frac{\beta\partial(A/RT)}{\partial\beta} \qquad \text{(A.1.3. 2)}$$

$$\frac{A^{ASSOC}}{RT} = 2N_d \ln(X^A) + N_d(1-X^A) = 2N_d \ln(1-F^2/N_d) + F^2 \qquad \text{(A.1.3. 3)}$$

$$\frac{U^{assoc}}{RT} = \frac{\beta\partial(A^{assoc}/RT)}{\partial\beta} = \left[1 - \frac{2Nd}{Nd-F^2}\right] 2F\beta\frac{\partial F}{\partial\beta} \qquad \text{(A.1.3. 4)}$$

$$\frac{\partial F}{\partial\beta} = \frac{\varepsilon^{HB}\sqrt{\alpha}}{2}\left[\frac{N_d - F^2}{1+2F\sqrt{\alpha}}\right]\frac{\mathrm{Y}^{HB}+1}{\mathrm{Y}^{HB}} \qquad \text{(A.1.3. 5)}$$

$$F\sqrt{\alpha} \equiv \left(\frac{1}{X^A} - 1\right);\ \alpha \equiv g(\sigma)K^{AD}\left[\exp(\varepsilon/kT) - 1\right] \qquad \text{(A.1.3. 6)}$$

The expressions for the solubility parameter, δ, and the molar volume, V_L^{298}, in terms of the SAFT EOS is as follows:

$$\frac{\delta^2 V_L^{298}}{RT} = \frac{9\eta mC\beta u^\circ \exp(-3\beta u^\circ)(2\eta-4)}{(1-\eta)^3\left[1-C\exp(-3\beta u^\circ)\right]} - \frac{m(1+2\beta e)}{1+\beta e}\sum_i\sum_j iD_{ij}\left[\beta u\right]^i\left[\frac{\eta}{\tau}\right]^j -$$

$$\frac{9mC\beta u^\circ \exp(-3\beta u^\circ)}{1-C\exp(-3\beta u^\circ)}\sum_i\sum_j jD_{ij}\left[\beta u\right]^i\left[\frac{\eta}{\tau}\right]^j + \frac{9\eta C\beta u^\circ\left(\eta-\frac{5}{2}\right)(1-m)\exp(-3\beta u^\circ)\left[1-C\exp(-3\beta u^\circ)\right]}{(1-\eta)\left(1-\frac{\eta}{2}\right)} +$$

$$\beta\varepsilon^{HB}\frac{F\sqrt{\alpha}\left(\mathrm{Y}^{HB}+1\right)}{\mathrm{Y}^{HB}}\frac{N_d+F^2}{1+2F\sqrt{\alpha}} \qquad \text{(A.1.3.7)}$$

where, $\beta = 1/kT$ and $T = 298$ K and R is the universal gas constant.

A.1.4 Vapor packing fraction

We can write the vapor phase compressibility factor as below:

$$Z_V^{sat} = P^{sat} b / \eta^V RT = 1 + B_2 \eta^v \qquad \text{(A.1.4. 1)}$$

$$B = \eta^V + B_2 (\eta^V)^2 = \frac{Pb}{RT} \qquad \text{(A.1.4. 2)}$$

or

$$\eta^V = \frac{-1 + \sqrt{1 + 4BB_2}}{2B_2} \qquad \text{(A.1.4. 3)}$$

In order to calculate the second virial coefficient, we have

$$B_2 = \lim_{\eta \to 0} \left(\frac{Z - 1}{\eta} \right) = \left(\frac{dZ}{d\eta} \right)_{\eta = 0} \qquad \text{(A.1.4. 4)}$$

By setting $Z = 1 + B_2\eta$, we can define B_2 for each EOS :

$$B_2 = B_2^{seg} + B_2^{chain} + B_2^{assoc} \qquad \text{(A.1.4. 5)}$$

Where, the derived second Virial coefficient according to above definition is:

$$B_2^{seg} = 4m \qquad \text{(A.1.4. 6)}$$

$$B_2^{chain} = 2.5 \qquad \text{(A.1.4. 7)}$$

B_2^{assoc} is the same for both SAFT and PC-SAFT equations of state and is derived as follows:

$$B_2^{assoc} = -N_d^{\,2} \left[\frac{0.035}{m} \mathrm{Y}^{HB} \right] = -N_d^{\,2} \left[\frac{K^{AD} \mathrm{Y}^{HB}}{b} \right] \qquad \text{(A.1.4. 8)}$$

Another alternative to calculate the η^V is from isofugacity criteria which leads to below relationship:

$$2B_2\eta^V - \ln(\frac{Pb}{\eta^V RT}) = \tilde{A}^{res} + Z_L - 1 - \ln(Z_L) \qquad \text{(A.1.4. 9)}$$

or

$$\eta^v = \eta^L \exp[\tilde{\mu}_L^{res} - \tilde{\mu}_V^{res}] \qquad \text{(A.1.4. 10)}$$

where $\tilde{\mu}^{res} = \beta\mu^{res} / N$ is the reduced chemical potential and the residual chemical potential.

A.2. The PC-SAFT Equation of State

At this section we have summarized some quantities in terms of PC-SAFT Eqation of State which are used for the caculations in chapter III.

A.2.1 Compressibility factor

The PC-SAFT equation of state was derived and described in detail by Gross and Sadowski. In terms of the compressibility factor *Z*, the equation of state is given as the sum of the ideal gas contribution (Z^{id} = 1), the hard-chain term (hc), the dispersive part (disp), and the contribution due to association (assoc) according to

$$Z = 1 + Z^{hc} + Z^{disp} + Z^{assoc} \qquad \text{(A.2.1. 1)}$$

Note that the effect of multiple interactions (such as dipole-dipole and quadrupole-quadrupole forces) is not separately taken into account in eqs 1 and 12. This contribution will be the subject of further investigations.

$$Z^{hc} = mZ^{hs} - (m-1)(g^{hs})^{-1}\rho\frac{\partial g^{hs}}{\partial \rho} \qquad \text{(A.2.1. 2)}$$

where Z^{hs} is the residual contribution of the hard-sphere fluid, ρ is the total number density of molecule given by Gross and Sadowski. g^{hs} is the radial distribution function of the hard-sphere fluid that is

$$g^{hs} = \frac{1}{(1-\xi_3)} + \frac{3d\xi_2}{2(1-\xi_3)^2} + \frac{(\xi_2 d)^2}{2(1-\xi_3)^3} \qquad \text{(A.2.1. 3)}$$

with ξ_n defined as

$$\xi_n = \frac{\pi}{6}\rho m d^n \qquad \text{(A.2.1. 4)}$$
$$n \in \{0,1,2,3\}$$

The temperature-dependent segment diameter d is given by

$$d = \sigma\left[1 - 0.12\exp\left(-3\beta\varepsilon\right)\right] \qquad \text{(A.2.1. 5)}$$

where ε is the disperse attraction energy.

The dispersion contribution to the compressibility factor of the PC-SAFT EOS can be written as

$$Z^{disp} = -2\pi\rho\frac{\partial(\eta I_1)}{\partial\eta}m^2\beta\varepsilon\sigma^3 - \pi\rho m\left[C_1\frac{\partial(\eta I_2)}{\partial\eta} + C_2\eta I_2\right](m\beta\varepsilon)^2\sigma^3 \qquad \text{(A.2.1. 6)}$$

where

$$\frac{\partial(\eta I_1)}{\partial\eta} = \sum_{j=0}^{6} a_j(m)(j+1)\eta^j \qquad \text{(A.2.1. 7)}$$

$$\frac{\partial(\eta I_2)}{\partial \eta} = \sum_{i=0}^{6} b_i(m)(j+1)\eta^i \qquad \text{(A.2.1. 8)}$$

where $a_j(m)$ and $b_i(m)$ are two functions of m that was defined by Gross and Sadowski.

$$C_1 = \left(1 + Z^{hc} + \rho \frac{\partial Z^{hc}}{\partial \rho}\right)^{-1} \qquad \text{(A.2.1. 9)}$$

$$C_2 = \frac{\partial C_1}{\partial \eta} \qquad \text{(A.2.1. 10)}$$

As in the ESD and SAFT equations we can introduce the molecular volume in PC-SAFT as follows

$$b = \frac{\pi}{10} m d^3 \qquad \text{(A.2.1. 11)}$$

And the definition of the association contribution parameters in compressibility factor for PC-SAFT EOS is the same as SAFT equation.

A.2.2 Helmholtz free energy

$$\widetilde{A}^{res} = \frac{m}{\xi_0}\left[\frac{3\xi_1\xi_2}{(1-\xi_3)} + \frac{\xi_2^3}{\xi_3(1-\xi_3)^2} + \left(\frac{\xi_2^3}{\xi_3^2} - \xi_0\right)\ln(1-\xi_3)\right] -$$
$$(m-1)\ln g^{hs}(\sigma) - 2\pi\rho I_1(\eta, m) m^2 \beta\varepsilon\sigma^3 - \pi\rho I_2(\eta, m)(\beta\varepsilon)^2 (m\sigma)^3 + \qquad \text{(A.2.2. 1)}$$
$$2N_d \ln(1 - F^2 / N_d) + F^2$$

A.2.3 Solubility parameter

The expression for the solubility parameter, δ, and the molar volume in terms of the SAFT EOS is as follows:

$$\frac{\delta^2 V_L^{298}}{RT} = T\left[\begin{array}{l} \frac{m}{\xi_0}\left(\begin{array}{l} \frac{3\left(\xi_{1,T}\xi_{2,T}+\xi_1\xi_{2,T}\right)}{(1-\xi_3)}+\frac{3\xi_1\xi_2\xi_{3,T}}{(1-\xi_3)^2}+\frac{3{\xi_2}^2\xi_{2,T}}{\xi_3(1-\xi_3)}+\frac{{\xi_2}^3\xi_{3,T}(3\xi_3-1)}{\xi_3^2(1-\xi_3)}+ \\ \left(\frac{3{\xi_2}^2\xi_{2,T}\xi_3-2\xi_2^3\xi_{3,T}}{\xi_3^3}\right)\ln(1-\xi_3)+\left(\xi_0-\frac{\xi_2^3}{\xi_3^2}\right)\frac{\xi_{3,T}}{(1-\xi_3)} \end{array}\right)- \\ (m-1)(g^{hs})^{-1}\left(\begin{array}{l} \frac{\xi_{3,T}}{(1-\xi_3)^2}+\left(\frac{d_T}{2}\right)\frac{3\xi_2}{(1-\xi_3)}+ \\ \left(\frac{d}{2}\right)\left(\frac{3\xi_{2,T}}{(1-\xi_3)^2}+\frac{6\xi_2\xi_{3,T}}{(1-\xi_3)^3}\right)+\left(\frac{dd_T}{2}\right)\frac{2\xi_2^2}{(1-\xi_3)^3}+ \\ \left(\frac{d}{2}\right)\left(\frac{4\xi_2\xi_{2,T}}{(1-\xi_3)^3}+\frac{6{\xi_2}^2\xi_{3,T}}{(1-\xi_3)^4}\right) \end{array}\right)- \\ 2\pi\rho\left(\frac{\partial I_1}{\partial T}-\frac{I_1}{T}\right)m^2\beta\varepsilon\sigma^3-\pi\rho m\left(\frac{\partial C_1}{\partial T}\mathrm{I}_2+C_1\frac{\partial I_2}{\partial T}-2C_1\frac{I_2}{T}\right)(m\beta\varepsilon)^2\sigma^3 \end{array}\right]+\beta\varepsilon^{HB}\frac{F\sqrt{\alpha}\left(\mathrm{Y}^{HB}+1\right)}{\mathrm{Y}^{HB}}\frac{N_d+F^2}{1+2F\sqrt{\alpha}}$$

(A.2.3. 1)

where, V_L^{298} is the liquid molar volume at 298 K, and R is the universal gas constant. Note that the association term is the same as SAFT EOS.

$$\xi_{n,T}=\frac{\partial\xi_n}{\partial T}=\frac{\pi}{6}\rho mnd_T d^{n-1} \qquad \text{(A.2.3. 2)}$$
$$n\in\{1,2,3\}$$

$$d_T=\frac{\partial d}{\partial T}=\sigma\left(3\frac{\beta\varepsilon}{T}\right)\left[-0.12\exp\left(-3\beta\varepsilon\right)\right] \qquad \text{(A.2.3. 3)}$$

where $T = 298$ K and the number density of molecules, ρ, is calculated from η through

$$\rho = \frac{6}{\pi}\eta(md^3)^{-1} \qquad \text{(A.2.3. 4)}$$

$$\frac{\partial I_1}{\partial T} = \sum_{i=0}^{6} a_i(m) i \xi_{3,T} \eta^{i-1} \qquad \text{(A.2.3. 5)}$$

$$\frac{\partial I_2}{\partial T} = \sum_{i=0}^{6} b_i(m) i \xi_{3,T} \eta^{i-1} \qquad \text{(A.2.3. 6)}$$

$$\frac{\partial C_1}{\partial T} = \xi_{3,T} C_2 \qquad \text{(A.2.3. 7)}$$

A.2.4 Vapor packing fraction

$$B_2 = B_2^{\,hc} + B_2^{\,disp} + B_2^{\,assoc} \qquad \text{(A.2.4. 1)}$$

We can readily derive the second viral coefficient for PC-SAFT EOS according to the definition presented in the previous section as below:

$$B_2^{hc} = \frac{3}{2}m + \frac{5}{2} \qquad \text{(A.2.4. 2)}$$

And,

$$B_2^{disp} = \frac{-12a_0}{md^3} m^2 \beta\varepsilon\sigma^3 \quad - \frac{6b_0}{d^3}(m\beta\varepsilon)^2 \sigma^3 \qquad \text{(A.2.4. 3)}$$

And the association contribution is the same as SAFT EOS.

APPENDIX B.

VAPOR PRESSURES AND THEIR ERRORS CALCULATED BY THE METHODS GIVEN IN CHAPTER III

TableB. 1 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 760 mmHg

	EOS	no. of Occ.	P AAD% 760 mmHg	P Bias% 760 mmHg	$\ln(P^{calc}/P^{exp})$ 760 mmHg
Alcohols	SAFT	77	48.83	37.61	23.37
	PC-SAFT		29.92	11.41	4.35
	ESD		36.39	27.92	18.65
Amines	SAFT	55	53.20	37.37	18.69
	PC-SAFT		37.61	-3.26	-15.63
	ESD		45.10	17.13	1.65
Nitriles	SAFT	10	60.61	58.59	38.27
	PC-SAFT		25.61	-12.59	-20.37
	ESD		28.39	-21.63	-30.13
Silanes	SAFT	10	64.42	64.42	47.73
	PC-SAFT		33.74	26.54	19.89
	ESD		47.23	40.79	28.60
Imines	SAFT	7	105.22	104.30	59.07
(e.g. Acridine)	PC-SAFT		33.12	18.91	10.26
	ESD		55.16	47.26	25.00

Table B.1 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 760 mmHg (Continued)

tert-Ns (e.g. Trimethylamine)	SAFT	6	57.06	99.70	57.11
	PC-SAFT		24.77	-10.39	-18.31
	ESD		22.73	-7.16	-14.99
Nitrates	SAFT	19	43.47	6.63	-10.84
	PC-SAFT		38.10	-15.41	-33.89
	ESD		39.69	-16.06	-35.98
Thiols	SAFT	27	30.07	14.28	8.21
	PC-SAFT		17.83	-2.83	-6.44
	ESD		16.44	5.32	2.08
Aldehydes	SAFT	23	52.81	42.12	25.07
	PC-SAFT		22.21	15.12	10.16
	ESD		23.06	11.01	6.48
Epoxides	SAFT	13	88.27	88.27	51.81
	PC-SAFT		29.26	7.00	1.47
	ESD		47.22	31.17	16.97
Ethers	SAFT	38	40.81	31.52	21.85
	PC-SAFT		27.76	-20.39	-29.38
	ESD		20.45	-0.38	-3.68
Formates	SAFT	16	56.69	43.45	23.12
	PC-SAFT		13.50	-6.21	-7.82
	ESD		10.76	4.72	3.33
Esters	SAFT	92	31.77	1.78	-7.99
	PC-SAFT		22.32	-10.40	-15.31
	ESD		24.98	14.25	9.46
Ketones	SAFT	28	43.72	39.63	26.59
	PC-SAFT		33.84	0.40	-9.59
	ESD		35.77	16.34	3.23
Alcohol-Ethers (e.g. carbitol)	SAFT	18	78.91	65.09	37.02
	PC-SAFT		46.63	-13.79	-32.22
	ESD		52.49	21.42	3.75
Hydrocarbons	SAFT	157	33.44	19.00	11.12
	PC-SAFT		16.41	6.25	3.41
	ESD		22.24	11.76	7.52

Table B.1 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 760 mmHg (Continued)

Cyclic Hydrocarbons	SAFT	41	22.95	20.57	17.40
	PC-SAFT		13.45	3.08	1.52
	ESD		10.40	-0.20	-1.36
Aromatic Hydrocarbons	SAFT	138	39.25	21.15	11.00
	PC-SAFT		39.25	29.61	14.07
	ESD		63.01	57.32	27.98
Halocarbons	SAFT	103	53.38	34.86	7.63
	PC-SAFT		39.80	8.41	-14.11
	ESD		29.88	0.01	-15.90
Total	**SAFT**	**878**	43.36	27.46	13.30
	PC-SAFT		27.95	4.74	-4.35
	ESD		34.29	18.62	6.62

TableB. 2 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 100mmHg

	EOS	no. of occurrence	*P* AAD% 100 mmHg	*P* Bias% 100 mmHg	$100\ln(P^{calc}/P^{exp})$
Alcohols	SAFT	77	71.87	62.23	36.40
	PC-SAFT		31.48	8.09	0.06
	ESD		37.09	23.39	13.09
Amines	SAFT	55	89.05	76.36	35.09
	PC-SAFT		45.52	4.62	-13.28
	ESD		56.39	22.73	-0.12
Nitriles	SAFT	10	129.82	129.82	69.26
	PC-SAFT		39.38	5.45	-4.75
	ESD		36.22	-10.26	-20.23
Silanes	SAFT	10	68.22	68.22	50.34
	PC-SAFT		17.96	-0.24	-2.91
	ESD		27.30	14.67	10.28
Imines (e.g. Acridine)	SAFT	7	172.97	172.97	81.41
	PC-SAFT		30.68	22.60	16.63

Table B.2 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 100mmHg (Continued)

	ESD		53.96	45.03	28.29
tert-Ns	SAFT	6	90.62	2.28	162.95
(e.g.	PC-SAFT		32.55	-22.19	-0.39
Trimethylamine)	ESD		33.31	-22.33	-0.78
Nitrates	SAFT	19	66.00	40.95	11.88
	PC-SAFT		44.61	-3.21	-25.30
	ESD		45.41	-10.86	-35.81
Thiols	SAFT	27	48.13	37.15	23.80
	PC-SAFT		23.53	0.97	-4.40
	ESD		22.52	5.58	0.00
Aldehydes	SAFT	23	87.43	80.95	44.33
	PC-SAFT		31.57	27.16	17.24
	ESD		32.51	17.93	9.19
Epoxides	SAFT	13	158.63	158.63	71.83
	PC-SAFT		50.04	22.32	7.80
	ESD		76.31	53.02	22.05
Ethers	SAFT	38	70.24	65.21	41.84
	PC-SAFT		29.82	-15.43	-24.42
	ESD		25.27	4.79	-0.73
Formates	SAFT	16	93.71	84.19	40.83
	PC-SAFT		16.65	-1.11	-3.76
	ESD		17.74	7.22	4.13
Esters	SAFT	92	42.58	16.87	2.83
	PC-SAFT		25.08	-11.82	-17.96
	ESD		24.72	7.99	2.92
Ketones	SAFT	28	73.82	69.60	38.78
	PC-SAFT		48.90	8.61	-12.60
	ESD		55.52	23.82	-3.61
Alcohol-Ethers	SAFT	18	109.23	96.47	48.38
(e.g. carbitol)	PC-SAFT		53.44	-18.73	-44.39
	ESD		63.33	18.58	-6.35
Hydrocarbons	SAFT	157	49.17	36.22	22.54
	PC-SAFT		18.32	5.84	1.89
	ESD		21.99	8.36	3.23

Table B.2 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 100mmHg (Continued)

Cyclic Hydrocarbons	SAFT	41	39.47	37.26	29.69
	PC-SAFT		13.85	1.69	-0.45
	ESD		12.52	-5.09	-6.71
Aromatic Hydrocarbons	SAFT	138	51.37	33.77	17.93
	PC-SAFT		33.13	19.07	7.76
	ESD		52.04	40.34	17.35
Halocarbons	SAFT	103	73.58	48.71	5.23
	PC-SAFT		45.95	3.88	-34.51
	ESD		36.88	-7.81	-38.29
Total	**SAFT**	**878**	64.76	50.23	24.32
	PC-SAFT		30.33	3.61	-8.15
	ESD		36.46	14.62	-0.20

TableB. 3 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 10mmHg

	EOS	no. of Occ.	*P* AAD% 10 mmHg	*P* Bias% 10 mmHg	$\ln(P^{calc}/P^{exp})$ 10 mmHg
Alcohols	SAFT	77	100.024	89.36	46.67
	PC-SAFT		36.84	5.16	-6.75
	ESD		44.83	18.00	3.64
Amines	SAFT	55	156.51	144.53	52.20
	PC-SAFT		62.54	19.70	-11.36
	ESD		76.16	37.48	-1.71
Nitriles	SAFT	10	261.31	261.31	103.22
	PC-SAFT		64.69	36.17	13.33

Table B.3 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 10mmHg (Continued)

	ESD		55.17	12.20	-6.16
Silanes	SAFT	10	57.24	57.24	42.44
	PC-SAFT		36.49	-23.88	-34.52
	ESD		27.05	-12.85	-18.72
Imines	SAFT	7	297.50	297.50	105.24
(e.g. Acridine)	PC-SAFT		39.91	32.20	24.09
	ESD		57.69	48.46	32.87
tert-Ns	SAFT	6	271.40	58.03	-31.78
(e.g.	PC-SAFT		55.95	-0.85	-26.48
Trimethylamine)	ESD		56.44	-2.58	-28.87
Nitrates	SAFT	19	124.90	105.73	40.71
	PC-SAFT		59.86	17.52	-12.35
	ESD		56.64	1.21	-30.57
Thiols	SAFT	27	81.54	73.10	42.40
	PC-SAFT		34.05	8.41	-1.24
	ESD		35.06	11.59	0.50
Aldehydes	SAFT	23	146.80	144.21	67.44
	PC-SAFT		49.90	47.30	26.67
	ESD		49.31	35.05	16.11
Epoxides	SAFT	13	282.68	282.56	95.09
	PC-SAFT		85.37	50.44	14.38
	ESD		125.32	96.20	29.59
Ethers	SAFT	38	120.64	117.47	63.34
	PC-SAFT		36.34	-6.77	-18.91
	ESD		37.28	15.95	3.99
Formates	SAFT	16	161.00	152.65	59.18
	PC-SAFT		26.16	4.49	-1.38
	ESD		29.88	12.59	4.66
Esters	SAFT	92	62.62	38.31	13.14
	PC-SAFT		32.27	-12.01	-22.73
	ESD		32.90	3.13	-6.45
Ketones	SAFT	28	123.73	118.94	50.73
	PC-SAFT		74.50	26.32	-17.72
	ESD		88.02	45.79	-10.85

Table B.3 Detailed Vapor Pressure Errors for different chemical families for three equations of state SAFT, PC-SAFT and ESD at 10mmHg (Continued)

Alcohol-Ethers (e.g. carbitol)	SAFT	18	144.11	123.95	48.52
	PC-SAFT		61.05	-25.48	-66.32
	ESD		73.05	12.17	-27.49
Hydrocarbons	SAFT	157	70.66	59.21	35.26
	PC-SAFT		21.77	5.98	0.21
	ESD		22.71	6.52	0.07
Cyclic Hydrocarbons	SAFT	41	61.41	59.19	43.35
	PC-SAFT		15.56	-0.01	-3.26
	ESD		15.07	-7.64	-10.16
Aromatic Hydrocarbons	SAFT	138	71.39	51.46	23.69
	PC-SAFT		33.61	10.85	-0.77
	ESD		44.95	21.42	3.22
Halocarbons	SAFT	103	104.59	71.24	-0.82
	PC-SAFT		59.76	5.32	-61.42
	ESD		46.51	-8.40	-59.76
Total	**SAFT**	**878**	99.77	84.53	34.91
	PC-SAFT		38.36	5.55	-13.71
	ESD		44.02	14.19	-7.67

TableB. 4 A Comparison Between the Current Study and FOG of Tihic et al. in Terms of Vapor Pressure Errors

Group		no. of occurrence	*P* AAD% 760 mmHg	*P* AAD% 100 mmHg	*P* AAD% 10 mmHg
Nitriles	Tihic FOG	18	24.71	33.54	48.48
	This Work		36.99	43.89	60.06
Thiols	Tihic FOG	27	73.08	113.30	180.63
	This Work		17.83	23.53	34.05
Epoxides	Tihic FOG	13	80.36	118.44	173.64

Table B.4 A Comparison Between the Current Study and FOG of Tihic et al. in Terms of Vapor Pressure Errors (Continued)

	This Work		29.26	50.04	85.37
Ethers	Tihic FOG	38	25.82	32.64	40.77
	This Work		27.76	29.82	36.34
Formates	Tihic FOG	16	30.62	44.99	68.02
	This Work		13.50	16.65	26.16
Esters	Tihic FOG	92	33.17	43.15	56.15
	This Work		22.32	25.08	32.27
Ketones	Tihic FOG	28	61.00	98.16	165.66
	This Work		33.84	48.90	74.50
Hydrocarbons	Tihic FOG	157	15.94	22.29	30.37
	This Work		16.41	18.32	21.77
Cyclic Hydrocarbons	Tihic FOG	41	59.59	90.11	138.50
	This Work		13.45	13.85	15.56
Aromatics	Tihic FOG	138	18.77	24.09	30.76
	This Work		39.25	33.13	33.61
Halocarbons	Tihic FOG	71	64.93	106.97	197.14
	This Work		27.46	30.95	39.32
Total	**Tihic FOG**	**639**	**34.18**	**50.07**	**76.90**
	This Work		**25.46**	**26.97**	**33.07**

TableB. 5 A Comparison Between the Current Study and SOG of Tihic et al. in Terms of Vapor Pressure Errors

Group		no. of occurrence	*P* AAD% 760 mmHg	*P* AAD% 100 mmHg	*P* AAD% 10 mmHg
Nitriles	Tihic SOG	18	24.71	33.54	48.48
	This Work		36.99	43.89	60.06
Thiols	Tihic SOG	27	66.90	101.70	158.82
	This Work		17.83	23.53	34.05
Aldehydes	Tihic SOG	23	29.26	34.71	41.13

Table B.5 A Comparison Between the Current Study and SOG of Tihic et al. in Terms of Vapor Pressure Errors(Continued)

	This Work		22.21	31.57	49.90
Epoxides	Tihic SOG	13	78.17	115.80	170.65
	This Work		29.26	50.04	85.37
Ethers	Tihic SOG	38	24.07	30.68	38.70
	This Work		27.76	29.82	36.34
Formates	Tihic SOG	16	29.93	44.17	67.11
	This Work		13.50	16.65	26.16
Esters	Tihic SOG	92	39.09	52.61	71.37
	This Work		22.32	25.08	32.27
Ketones	Tihic SOG	27	27.10	36.46	47.49
	This Work		24.05	28.71	33.40
Hydrocarbons	Tihic SOG	157	17.24	24.32	33.35
	This Work		16.41	18.32	21.77
Cyclic Hydrocarbons	Tihic SOG	41	38.01	49.31	64.13
	This Work		13.45	13.85	15.56
Aromatics	Tihic SOG	138	18.51	23.83	30.63
	This Work		39.25	33.13	33.61
Halocarbons	Tihic SOG	71	64.89	107.08	197.22
	This Work		30.44	33.14	40.54
Total	**Tihic SOG**	**661**	**35.57**	**50.73**	**75.57**
	This Work		**24.94**	**26.27**	**31.91**

TableB. 6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State.

Alcohols

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1181	Phenol	C6H6O	0.1733	0.0202	0.0016
1182	O-Cresol	C7H8O	0.1181	0.0118	0.0008
1183	M-Cresol	C7H8O	0.1626	0.0192	0.0016
1176	2,6-Xylenol	C8H10O	0.0874	0.0073	0.0004
1111	2-Mth-2-Butanol	C5H12O	0.0510	0.0064	0.0006
1178	3,5-Xylenol	C8H10O	0.1564	0.0184	0.0015

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1133	2-Octanol	C8H18O	0.0756	0.0093	0.0009
2885	4-Hydroxystyren	C8H8O	0.1427	0.0169	0.0013
1197	P-t-Butylphenol	C10H14O	0.1216	0.0122	0.0009
1172	2,4-Xylenol	C8H10O	0.1155	0.0117	0.0008
1184	P-Cresol	C7H8O	0.1610	0.0191	0.0016
1151	Cyclohexanol	C6H12O	0.0933	0.0131	0.0015
1170	2,3-Xylenol	C8H10O	0.1544	0.0170	0.0012
1187	P-Ethyl Phenol	C8H10O	0.1605	0.0196	0.0016
2859	P-Methoxyphenol	C7H8O2	0.2873	0.0370	0.0037
1121	2-Ethylhexanol	C8H18O	0.0872	0.0113	0.0012
1179	PropargylAlcohol	C3H4O	0.1790	0.0247	0.0024
1123	3-Mth-1-Butanol	C5H12O	0.1096	0.0168	0.0020
2196	P-t-Amylphenol	C11H16O	0.1461	0.0150	0.0010
1174	2,5-Xylenol	C8H10O	0.1160	0.0120	0.0007
1115	2-Hexanol	C6H14O	0.0742	0.0097	0.0009
1152	1-MthCycHexanol	C7H14O	0.0857	0.0079	0.0005
4854	Guaiacol	C7H8O2	0.0954	0.0072	0.0004
1107	Sec-Butanol	C4H10O	0.0809	0.0113	0.0012
1167	Allyl Alcohol	C3H6O	0.1398	0.0205	0.0023
1130	4-Mth-2-Pentanol	C6H14O	0.0614	0.0072	0.0006
1177	3,4-Xylenol	C8H10O	0.1793	0.0221	0.0019
1114	1-Hexanol	C6H14O	0.1176	0.0169	0.0019
1106	Isobutanol	C4H10O	0.1073	0.0167	0.0021
1125	1-Heptanol	C7H16O	0.1125	0.0158	0.0018
1105	N-Butanol	C4H10O	0.1333	0.0201	0.0024
1109	1-Pentanol	C5H12O	0.1228	0.0175	0.0019
1132	1-Octanol	C8H18O	0.1107	0.0153	0.0017
1113	T-Butylcarbinol	C5H12O	0.0764	0.0102	0.0011
1137	1-Undecanol	C11H24O	0.1019	0.0136	0.0014
1108	Tert-Butanol	C4H10O	0.0552	0.0075	0.0008
1103	N-Propanol	C3H8O	0.1497	0.0227	0.0026
1134	1-Nonanol	C9H20O	0.1090	0.0147	0.0016
2195	P-t-Octylphenol	C14H22O	0.1115	0.0110	0.0007
1102	Ethanol	C2H6O	0.1917	0.0288	0.0032
1124	3-Mth-2-Butanol	C5H12O	0.0624	0.0084	0.0010
1136	1-Decanol	C10H22O	0.1077	0.0142	0.0015
1140	Dodecanol	C12H26O	0.1084	0.0139	0.0014
1104	Isopropanol	C3H8O	0.1013	0.0149	0.0017
1110	2-Pentanol	C5H12O	0.0740	0.0103	0.0011
1120	3-Pentanol	C5H12O	0.0655	0.0083	0.0009
1112	2-Mth-1-Butanol	C5H12O	0.1017	0.0155	0.0018
1154	Ts-2-Mth-CycC6OH	C7H14O	0.0821	0.0101	0.0008
1153	Cs-2-Mth-CycC6OH	C7H14O	0.0780	0.0089	0.0007
1156	Ts-3-Mth-CycC6OH	C7H14O	0.1003	0.0146	0.0016
1157	Cs-4-Mth-CycC6OH	C7H14O	0.0922	0.0129	0.0013
2197	P-Cumylphenol	C15H16O	0.1539	0.0167	0.0012

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1180	Benzyl Alcohol	C7H8O	0.1435	0.0193	0.0019
1158	Ts-4-Mth-CycC6OH	C7H14O	0.0931	0.0135	0.0015
1155	Cs-3-Mth-CycC6OH	C7H14O	0.0988	0.0147	0.0016
1168	2-Phn-2-Propanol	C9H12O	0.0567	0.0060	0.0004
1141	1-Tridecanol	C13H28O	0.1103	0.0140	0.0014
1147	2-Eth-1-Butanol	C6H14O	0.0914	0.0117	0.0013
1117	2-Mth-1-Pentanol	C6H14O	0.0965	0.0129	0.0014
2115	2-Phenylethanol	C8H10O	0.1211	0.0173	0.0017
1142	1-Tetradecanol	C14H30O	0.1115	0.0139	0.0014
2118	1-PHN-1-Propanol	C9H12O	0.0791	0.0087	0.0006
2119	1-PHN-2-Propanol	C9H12O	0.0811	0.0091	0.0007
1126	2-Heptanol	C7H16O	0.0728	0.0085	0.0008
1143	1-Pentadecanol	C15H32O	0.1128	0.0141	0.0014
1129	Isoheptanol	C7H16O	0.1058	0.0158	0.0018
2117	2,6-DiMth-4-C7OH	C9H20O	0.0455	0.0058	0.0006
1144	1-Hexadecanol	C16H34O	0.1133	0.0141	0.0014
1145	Heptadecanol	C17H36O	0.1136	0.0141	0.0014
1199	Nonylphenol	C15H24O	0.1239	0.0155	0.0015
1146	1-Octadecanol	C18H38O	0.1151	0.0141	0.0013
1135	2-Nonanol	C9H20O	0.0761	0.0088	0.0008
1149	1-Nonadecanol	C19H40O	0.1122	0.0133	0.0012
1139	Isodecanol	C10H22O	0.0825	0.0120	0.0013
1148	1-Eicosanol	C20H42O	0.1101	0.0131	0.0012
2198	Dinonylphenol	C24H42O	0.3163	0.0445	0.0050
1159	Menthol	C10H20O	0.0669	0.0108	0.0013

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Amines

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1742	Ethyleneimine	C2H5N	0.3173	0.0663	0.0114
1745	Piperidine	C5H11N	0.0630	0.0077	0.0007
1766	Pyrrolidine	C4H9N	0.0868	0.0127	0.0014
1719	Isopropylamine	C3H9N	0.0952	0.0145	0.0018
1711	N-Propylamine	C3H9N	0.0748	0.0108	0.0012
1726	Sec-Butylamine	C4H11N	0.0920	0.0126	0.0013
1704	Ethylamine	C2H7N	0.0831	0.0126	0.0015
1702	Dimethylamine	C2H7N	0.0805	0.0113	0.0012
1710	Diethylamine	C4H11N	0.0465	0.0051	0.0004
1740	Allylamine	C3H7N	0.0999	0.0173	0.0024
1712	N-Butylamine	C4H11N	0.0735	0.0102	0.0011
1794	HexMthyleneimine	C6H13N	0.0710	0.0092	0.001
1729	Cyclohexylamine	C6H13N	0.0819	0.0109	0.0011
1714	Isobutylamine	C4H11N	0.0673	0.0098	0.0011
2853	Acetamide	C2H5NO	0.0953	0.0171	0.0026

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

2731	N-C1-CycC6-Amine	C7H15N	0.0834	0.0109	0.0011
1743	Diisopropylamine	C6H15N	0.0914	0.0091	0.0008
1796	N,N-DiMthAniline	C8H11N	0.0379	0.0033	0.0002
1792	Aniline	C6H7N	0.1001	0.0132	0.0013
1713	N-Pentylamine	C5H13N	0.0716	0.0096	0.001
1733	Benzylamine	C7H9N	0.0878	0.0116	0.0012
1737	M-Toluidine	C7H9N	0.0897	0.011	0.0011
3796	N-Ethylaniline	C8H11N	0.1043	0.0141	0.0015
1878	2-Methacrylamide	C4H7NO	0.0184	0.0023	0.0002
1736	O-Toluidine	C7H9N	0.0827	0.0096	0.0009
2739	Diallylamine	C6H11N	0.0482	0.0071	0.0008
2706	Hexylamine	C6H15N	0.0771	0.0102	0.001
2724	O-Ethylaniline	C8H11N	0.0683	0.0078	0.0006
1707	Dipropylamine	C6H15N	0.0487	0.0054	0.0004
1738	P-Toluidine	C7H9N	0.0831	0.0101	0.0009
1795	N-Methylaniline	C7H9N	0.1709	0.0248	0.0027
1718	Diisobutylamine	C8H19N	0.0400	0.0046	0.0004
1879	Acrylamide	C3H5NO	0.0497	0.0071	0.001
2707	1-Aminoheptane	C7H17N	0.0782	0.01	0.0009
2730	DiCycHexylamine	C12H23N	0.1687	0.0186	0.0016
2787	P-Aminodiphenyl	C12H11N	0.2054	0.0237	0.0018
1744	Dibutylamine	C8H19N	0.0579	0.0065	0.0005
2708	1-Octylamine	C8H19N	0.0801	0.0106	0.001
2791	2,6-DiEthAniline	C10H15N	0.0549	0.0066	0.0005
2709	1-Nonylamine	C9H21N	0.0841	0.0111	0.0011
2710	1-Decylamine	C10H23N	0.0815	0.0107	0.001
3722	Diamylamine	C10H23N	0.0660	0.0087	0.0009
3724	Undecylamine	C11H25N	0.0878	0.0109	0.001
2712	Dodecylamine	C12H27N	0.0887	0.0115	0.0011
1720	Tetradecylamine	C14H31N	0.0901	0.0117	0.0011
2752	Piperazine	C4H10N2	0.0952	0.016	0.0021
1752	Propylenediamine	C3H10N2	0.1464	0.0295	0.0049
1741	Ethylenediamine	C2H8N2	0.1753	0.0368	0.0064
2725	O-Aminoaniline	C6H8N2	0.1068	0.0133	0.0012
2750	P-Aminoaniline	C6H8N2	0.1369	0.0183	0.0018
2727	M-Aminoaniline	C6H8N2	0.2133	0.0289	0.0026
1750	AEP	C6H15N3	0.0801	0.0136	0.0019
1732	Toluene Diamine	C7H10N2	0.1299	0.017	0.0016
1731	hexamethyleneDiamine	C6H16N2	0.0844	0.0127	0.0014
3750	P-Benzidine	C12H12N2	0.2978	0.0407	0.0041

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Nitrilies

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1773	Propionitrile	C3H5N	0.1134	0.0165	0.0019
1782	Butyronitrile	C4H7N	0.0845	0.0117	0.0013
2720	Allyl Cyanide	C4H5N	0.0698	0.0106	0.0013
1783	Valeronitrile	C5H9N	0.0769	0.01	0.001
3874	Benzyl Cyanide	C8H7N	0.0813	0.0106	0.001
1786	Hexanenitrile	C6H11N	0.0730	0.0096	0.0009
1776	Succinonitrile	C4H4N2	0.1236	0.0253	0.0044
1781	Glutaronitrile	C5H6N2	0.1265	0.0217	0.0029
2735	14-2Cyano-2-C4H8	C6H6N2	0.0290	0.0049	0.0007
1777	Adiponitrile	C6H8N2	0.1078	0.0197	0.0028

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Silanes

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
3985	Dimethyl Silane	C2H8Si	0.1213	0.0157	0.0016
3984	Methyl Silane	CH6Si	0.1013	0.0123	0.001
3986	Trimethyl Silane	C3H10Si	0.1031	0.0125	0.0011
1984	TetraMth Silane	C4H12Si	0.0774	0.0088	0.0007
2994	Tetraethyl Si	C8H20Si	0.1517	0.0203	0.0019
1965	HexMthDisiloxane	C6H18OSi2	0.0889	0.0093	0.0006
1966	6C1Cyc3Siloxane	C6H18O3Si3	0.1518	0.0152	0.001
1988	8C1Cyc4Siloxane	C8H24O4Si4	0.1413	0.0128	0.0008
3991	DecaMethcyclpenS	C10H30O5Si5	0.1525	0.0121	0.0006
3992	DodecaMethCyHexS	C12H36O6Si6	0.1930	0.0139	0.0007

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Imines

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1767	N-MthPyrrolidine	C5H11N	0.0949	0.0132	0.0014
2797	3-Methylpyridine	C6H7N	0.1112	0.0159	0.0018
1797	2-Methylpyridine	C6H7N	0.0746	0.0097	0.001
2799	4-Methylpyridine	C6H7N	0.1145	0.0166	0.0019
1753	N,N-DiEthAniline	C10H15N	0.1230	0.0173	0.0018
1754	N-Methylpyrrole	C5H7N	0.0841	0.0159	0.0026
3740	Acridine	C13H9N	0.2410	0.0259	0.0019

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Tert-N

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1703	Trimethylamine	C3H9N	0.0486	0.0064	0.0007
2856	DiMth Acetamide	C4H9NO	0.1886	0.0373	0.006
1706	Triethylamine	C6H15N	0.0955	0.0124	0.0012
2716	Tributylamine	C12H27N	0.0804	0.0109	0.0011
2719	Tripropylamine	C9H21N	0.0833	0.0132	0.0017
3723	Triamylamine	C15H33N	0.0484	0.006	0.0005

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Nitrate

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1761	Nitroethane	C2H5NO2	0.1108	0.014	0.0014
1763	2-Nitropropane	C3H7NO2	0.1012	0.013	0.0013
1762	1-Nitropropane	C3H7NO2	0.0865	0.0101	0.0009
1779	P-Nitrotoluene	C7H7NO2	0.1297	0.0207	0.003
1886	Nitrobenzene	C6H5NO2	0.1133	0.0186	0.0026
1778	O-Nitrotoluene	C7H7NO2	0.0915	0.014	0.0017
1780	M-Nitrotoluene	C7H7NO2	0.1134	0.0178	0.0022
1891	O-Nitroanisole	C7H7NO3	0.2578	0.0451	0.0062
2740	M-Dinitrobenzene	C6H4N2O4	0.0618	0.0095	0.0013
2742	P-Dinitrobenzene	C6H4N2O4	0.0571	0.0085	0.0011
2741	O-Dinitrobenzene	C6H4N2O4	0.0847	0.0131	0.0018
2749	3,5-DiNitToluene	C7H6N2O4	0.0662	0.0105	0.0012
2743	DNT	C7H6N2O4	0.0691	0.0099	0.0011
2745	3,4-DiNitToluene	C7H6N2O4	0.0992	0.0154	0.0017
2744	2,6-DiNitToluene	C7H6N2O4	0.0360	0.0045	0.0004
2748	2,5-DiNitToluene	C7H6N2O4	0.0688	0.0099	0.001
2746	1,3,5-TrinitroBz	C6H3N3O6	0.0204	0.0026	0.0003
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	0.0424	0.0057	0.0006
2747	Trinitrotoluene	C7H5N3O6	0.0186	0.0021	0.0002

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Thiols

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1802	Ethyl Mercaptan	C2H6S	0.1084	0.0161	0.0019
1820	Dimethyl Sulfide	C2H6S	0.1043	0.0138	0.0014
1843	Thiacyclopentane	C4H8S	0.1632	0.0236	0.0026
1803	1-Propanethiol	C3H8S	0.1055	0.0153	0.0017
1805	Isobut Mercaptan	C4H10S	0.0948	0.0139	0.0016
6860	Ethylenedithiol	C2H6S2	0.1272	0.0228	0.0033
1811	Cyclohexanethiol	C6H12S	0.0846	0.0108	0.0011
1828	DiMth Disulfide	C2H6S2	0.0498	0.0068	0.0008
1841	Butanethiol	C4H10S	0.1065	0.0149	0.0016
1814	Methylproylsulf	C4H10S	0.0985	0.0137	0.0015
2816	ETHYLtBUTYL SUL	C6H14S	0.0775	0.0091	0.0008
1818	Diethyl Sulfide	C4H10S	0.1035	0.0127	0.0011
1812	Benzyl Mercaptan	C7H8S	0.1082	0.014	0.0014
1838	T-OctylMercaptan	C8H18S	0.0464	0.0048	0.0003
1827	1-Pentanethiol	C5H12S	0.1085	0.0152	0.0017
2815	METHnBUTYL SULFD	C5H12S	0.1000	0.0127	0.0012
1824	DiethylDisulfide	C4H10S2	0.0790	0.0089	0.0007
1807	N-Hexylmercaptan	C6H14S	0.1099	0.0152	0.0016
6857	Dimercaptoethyl	C4H10OS2	0.0620	0.0103	0.0014
1839	1-Heptanethiol	C7H16S	0.1126	0.0156	0.0017
1829	DiProp Disulfide	C6H14S2	0.0772	0.0086	0.0006
1809	1-Octanethiol	C8H18S	0.1129	0.0154	0.0016
1808	N-Nonanethiol	C9H20S	0.1131	0.0155	0.0017
1826	1-Decanethiol	C10H22S	0.1141	0.0157	0.0017
2838	tertDodecanThiol	C12H26S	0.0622	0.0078	0.0007
1825	1-Undecanethiol	C11H24S	0.1138	0.0156	0.0017
1837	Dodecylthiol	C12H26S	0.1147	0.0145	0.0015

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Aldehydes

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1037	Methacrolein	C4H6O	0.1070	0.0155	0.0017
1002	Acetaldehyde	C2H4O	0.1917	0.0284	0.0035
1003	Propionaldehyde	C3H6O	0.1380	0.0201	0.0022
1041	Benzaldehyde	C7H6O	0.1134	0.0141	0.0013
1034	Acrolein	C3H4O	0.1862	0.0304	0.0039

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1005	N-Butyraldehyde	C4H8O	0.1152	0.0158	0.0017
1036	Trans-2-Butenal	C4H6O	0.2375	0.0462	0.0073
1007	Valeraldehyde	C5H10O	0.1108	0.0152	0.0016
1006	Isobutyraldehyde	C4H8O	0.1064	0.0169	0.0021
1009	1-Hexanal	C6H12O	0.1054	0.0144	0.0015
1040	P-Tolualdehyde	C8H8O	0.1169	0.0159	0.0016
1016	2-Methylhexanal	C7H14O	0.0881	0.0127	0.0014
1017	3-Methylhexanal	C7H14O	0.0924	0.0128	0.0013
1008	1-Heptanal	C7H14O	0.1052	0.0141	0.0014
1013	2-Ethylhexanal	C8H16O	0.0777	0.0109	0.0012
1010	1-Octanal	C8H16O	0.1000	0.0136	0.0014
1011	1-Nonanal	C9H18O	0.0991	0.013	0.0014
1020	1-Decanal	C10H20O	0.0985	0.013	0.0014
1021	1-Undecanal	C11H22O	0.0978	0.0125	0.0014
1025	Dodecanal	C12H24O	0.0969	0.0126	0.0013
1026	1-Tridecanal	C13H26O	0.0962	0.0125	0.0013
1014	1,2-Ethanedione	C2H2O2	0.0840	0.0136	0.0017
1044	1,4BenzDicarboxAldehy	C8H6O2	0.1186	0.0159	0.0016

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Epoxides

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1440	ISOBUTYLENE OXID	C4H8O	0.2061	0.0378	0.0056
1479	Tetrahydrofuran	C4H8O	0.1419	0.0237	0.0032
1477	2,5-Dihydrofuran	C4H6O	0.1015	0.0156	0.0018
1408	1-Methoxypropane	C4H10O	0.0763	0.0082	0.0006
1411	2-Methoxypropane	C4H10O	0.0805	0.0094	0.0008
1421	1,4-Dioxane	C4H8O2	0.1300	0.0236	0.0034
2422	1,3-DIOXANE	C4H8O2	0.1419	0.0273	0.0044
1426	2-Methoxybutane	C5H12O	0.0794	0.0093	0.0008
1413	1-Methoxybutane	C5H12O	0.0874	0.0098	0.0008
1461	Methoxybenzene	C7H8O	0.1255	0.0148	0.0013
1448	1-Ethoxybutane	C6H14O	0.0776	0.0103	0.001
1429	1-MethoxyPentane	C6H14O	0.0948	0.0131	0.0014
6885	Ethyl-3-Ethoxypr	C7H14O3	0.0667	0.0093	0.001

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Ether

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1401	Dimethyl Ether	C2H6O	0.0684	0.0071	0.0005
1407	MethylEthylEther	C3H8O	0.1080	0.0174	0.0023
1470	VinylMethylEther	C3H6O	0.0903	0.0117	0.0011
1405	MTBE	C5H12O	0.0969	0.0118	0.001
1445	VinylEthyl Ether	C4H8O	0.0968	0.0158	0.0021
1402	Diethyl Ether	C4H10O	0.0823	0.0114	0.0013
1431	Methylal	C3H8O2	0.0716	0.0074	0.0006
1428	T-But EthylEther	C6H14O	0.0707	0.0099	0.0011
1427	TAME	C6H14O	0.1076	0.0132	0.0012
1410	Mth Isobut Ether	C5H12O	0.0777	0.009	0.0008
1430	Eth-t-Pent-Ether	C7H16O	0.0718	0.0096	0.0009
1403	DiisopropylEther	C6H14O	0.0855	0.0116	0.0011
1415	Eth Propyl Ether	C5H12O	0.0774	0.0101	0.0011
1455	Dimethyl Acetal	C4H10O2	0.1167	0.0216	0.0033
1446	Dipropyl Ether	C6H14O	0.0727	0.0092	0.0009
1447	Butyl VinylEther	C6H12O	0.0809	0.0124	0.0015
1462	EthylPhenylEther	C8H10O	0.0850	0.0109	0.0011
1406	Di-sec-But Ether	C8H18O	0.0817	0.0109	0.0011
1432	Acetal	C6H14O2	0.0421	0.0059	0.0006
1460	BenzylEthylEther	C9H12O	0.0726	0.0105	0.0012
1050	Paraldehyde	C6H12O3	0.1154	0.0212	0.0032
1404	Di-n-Butyl Ether	C8H18O	0.0748	0.0097	0.001
1420	Anethole	C10H12O	0.1668	0.0197	0.0017
1456	DimethylCarbitol	C6H14O3	0.1321	0.0192	0.0021
1463	Dibenzyl Ether	C14H14O	0.0576	0.0088	0.001
1425	Di-n-PentylEther	C10H22O	0.0799	0.0102	0.0009
1458	Diethyl Carbitol	C8H18O3	0.0408	0.0061	0.0007
1412	Dihexyl Ether	C12H26O	0.0820	0.0116	0.0013
1454	Triglyme	C8H18O4	0.0851	0.0136	0.0017
1459	Dibutyl Carbitol	C12H26O3	0.0382	0.0048	0.0004
1424	Di-n-Octyl Ether	C16H34O	0.0768	0.0109	0.0012
1457	Tetraglyme	C10H22O5	0.0154	0.0025	0.0003
1418	Dinonyl Ether	C18H38O	0.0837	0.0119	0.0013
2432	ETHYLAL	C5H12O2	0.0537	0.0074	0.0008
2405	DIISOBUTYL ETHER	C8H18O	0.0556	0.0074	0.0008
2456	Ethyl Glyme	C6H14O2	0.0653	0.0102	0.0013
2417	ETHYLHEXYL ETHER	C8H18O	0.0809	0.0112	0.0012
2415	ETHYLISOPROPETH	C5H12O	0.1047	0.0146	0.0015

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Formate

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1301	Methyl Formate	C2H4O2	0.15216	0.0251	0.0033
1311	Vinyl Formate	C3H4O2	0.0949	0.016	0.0021
1302	Ethyl Formate	C3H6O2	0.10714	0.0154	0.0017
2306	t-Butyl Formate	C5H10O2	0.07102	0.0092	0.0009
1303	Propyl Formate	C4H8O2	0.0968	0.0135	0.0015
2305	sec-ButylFormate	C5H10O2	0.0749	0.0103	0.0011
2311	CYCLOHEXL FORMAT	C7H12O2	0.0835	0.011	0.0011
1304	N-Butyl Formate	C5H10O2	0.0912	0.0122	0.0012
1305	Isobutyl Formate	C5H10O2	0.0853	0.0121	0.0012
2350	Benzyl Formate	C8H8O2	0.1038	0.0133	0.0013
2307	n-Hexyl Formate	C7H14O2	0.0932	0.0129	0.0014
1306	N-Pentyl Formate	C6H12O2	0.0939	0.0124	0.0013
2308	n-Heptyl Formate	C8H16O2	0.0965	0.0122	0.0011
1308	N-Octyl Formate	C9H18O2	0.0972	0.0115	0.0009
1309	n-Nonyl Formate	C10H20O2	0.0881	0.0116	0.0011
1310	n-Decyl Formate	C11H22O2	0.0909	0.0123	0.0012

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Ester

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1351	Mth Methacrylate	C5H8O2	0.0982	0.0119	0.0011
1312	Methyl Acetate	C3H6O2	0.1206	0.0149	0.0013
1331	Vinyl Propionate	C5H8O2	0.0978	0.0151	0.0018
1321	Vinyl Acetate	C4H6O2	0.0907	0.0112	0.001
1352	Eth MthAcrylate	C6H10O2	0.0868	0.0117	0.0012
1322	MethylPropionate	C4H8O2	0.1012	0.0119	0.001
1341	Methyl Acrylate	C4H6O2	0.1336	0.0219	0.0028
1313	Ethyl Acetate	C4H8O2	0.1331	0.0206	0.0025
1319	IsopropylAcetate	C5H10O2	0.0728	0.0081	0.0006
1332	Methyl Butyrate	C5H10O2	0.1195	0.0174	0.002
1342	Ethyl Acrylate	C5H8O2	0.0961	0.0148	0.0017
1318	Allyl Acetate	C5H8O2	0.1067	0.0123	0.001
1314	N-Propyl Acetate	C5H10O2	0.0910	0.0103	0.0009
1323	Ethyl Propionate	C5H10O2	0.1084	0.0155	0.0017
1360	I-But I-Butyrate	C8H16O2	0.0588	0.0076	0.0008
1320	Sec-ButylAcetate	C6H12O2	0.0713	0.0079	0.0006

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1336	PropylI-Butyrate	C7H14O2	0.0721	0.0102	0.0011
1353	N-C3-Mthacrylate	C7H12O2	0.0925	0.0127	0.0014
1333	Ethyl Butyrate	C6H12O2	0.0957	0.0121	0.0011
1347	EthylIsovalerate	C7H14O2	0.0791	0.0108	0.0011
1315	N-Butyl Acetate	C6H12O2	0.0947	0.0107	0.0009
1390	Methyl Benzoate	C8H8O2	0.1303	0.0143	0.0012
1388	Isobutyl Mthacr	C8H14O2	0.0626	0.0081	0.0008
1343	1-PropylAcrylate	C6H10O2	0.0884	0.0133	0.0016
1316	Isobutyl Acetate	C6H12O2	0.0827	0.0096	0.0008
1344	N-Butyl Acrylate	C7H12O2	0.0898	0.0118	0.0011
1357	Pentyl Acetate	C7H14O2	0.0942	0.0102	0.0008
1327	N-PropN-Butyrate	C7H14O2	0.0886	0.0114	0.0011
1324	N-PropPropionate	C6H12O2	0.0986	0.0134	0.0014
1291	Acetic Anhydride	C4H6O3	0.1133	0.0149	0.0015
1389	N-ButMthacrylate	C8H14O2	0.0721	0.0098	0.001
1359	Benzyl Acetate	C9H10O2	0.1263	0.017	0.0017
1326	N-But Propionate	C7H14O2	0.0940	0.0129	0.0013
1391	Ethyl Benzoate	C9H10O2	0.0942	0.0112	0.0009
1897	CH3OC3H600CH3	C6H12O3	0.0992	0.0119	0.001
1392	DiethylCarbonate	C5H10O3	0.0900	0.013	0.0016
1385	N-But N-Butyrate	C8H16O2	0.0884	0.011	0.001
1317	IsopentylAcetate	C7H14O2	0.0898	0.0097	0.0008
1363	N-Hexyl Acetate	C8H16O2	0.0940	0.0128	0.0013
1387	Ethylene Acetate	C6H10O4	0.1643	0.0221	0.0028
1393	Diethyl Oxalate	C6H10O4	0.1339	0.0215	0.0028
1365	Butyl Benzoate	C11H14O2	0.0936	0.0114	0.001
1361	I-C5 I-Valerate	C10H20O2	0.0727	0.0088	0.0007
1367	Heptyl Acetate	C9H18O2	0.0946	0.013	0.0013
1346	N-Butyl Valerate	C9H18O2	0.0894	0.0121	0.0012
1358	2-C2-C6 Acetate	C10H20O2	0.0868	0.0094	0.0007
1394	Diethyl Malonate	C7H12O4	0.0974	0.0151	0.0017
1292	Propionyl Oxide	C6H10O3	0.0743	0.0098	0.001
1364	Benzyl Benzoate	C14H12O2	0.0945	0.0109	0.0011
1381	2Mth p-Phthalate	C10H10O4	0.2121	0.02	0.0011
1368	n-Octyl Acetate	C10H20O2	0.0929	0.0126	0.0013
1377	DiMthI-Phthalate	C10H10O4	0.1170	0.0111	0.0008
1896	Ethylene DiAcr	C8H10O4	0.0780	0.0129	0.0016
1386	2-Ethylhexyl Acr	C11H20O2	0.0611	0.0081	0.0007
1395	Methyl Decanoate	C11H22O2	0.1069	0.0146	0.0015
1369	n-Nonyl Acetate	C11H22O2	0.0808	0.011	0.0012
1370	n-Decyl Acetate	C12H24O2	0.0873	0.0114	0.0012
1345	N-ButylNonanoate	C13H26O2	0.0677	0.006	0.0004
1375	DiProp Phthalate	C14H18O4	0.0725	0.0077	0.0006
1376	Diisobutyl Phtha	C16H22O4	0.0409	0.0044	0.0004
1396	IsopropMyristate	C17H34O2	0.0802	0.0103	0.001

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1383	Butyl Stearate	C22H44O2	0.0507	0.0053	0.0004
1362	Methyl Oleate	C19H36O2	0.0772	0.0108	0.0012
1355	Diisooctyl Phtha	C24H38O4	0.0651	0.0071	0.0006
1382	DioctylTerephtha	C24H38O4	0.0789	0.0083	0.0006
1384	Dibutyl Sebacate	C18H34O4	0.0685	0.0097	0.001
1371	Diisodecyl Phtha	C28H46O4	0.0860	0.0075	0.0004
1354	DioctylPhthalate	C24H38O4	0.0279	0.0028	0.0002
2375	DiethylPhthalate	C12H14O4	0.0896	0.0106	0.0009
2388	Dipropyl Maleate	C10H16O4	0.0588	0.0089	0.0011
2381	Diallyl Maleate	C10H12O4	0.0435	0.0072	0.001
2370	Glyceryl Triacet	C9H14O6	0.1108	0.0137	0.0013
2382	Dibutyl Maleate	C12H20O4	0.0591	0.0091	0.0011
2376	DibutylPhthalate	C16H22O4	0.0694	0.0076	0.0006
2353	CetylMthacrylate	C20H38O2	0.0993	0.0127	0.001
2379	Dihexyl Adipate	C18H34O4	0.0661	0.0089	0.0009
2321	T-Butyl Acetate	C6H12O2	0.0607	0.0083	0.0009
2332	Methl.I-butyrate	C5H10O2	0.0937	0.0139	0.0016
2354	AllylMthacrylate	C7H10O2	0.0636	0.0094	0.0011
2364	Cyclohexl Acetat	C8H14O2	0.0744	0.0102	0.001
2337	EthylIsobutyrate	C6H12O2	0.0709	0.0093	0.0009
2384	IsobutylAcrylate	C7H12O2	0.0700	0.0102	0.0011
2380	1,1-Diacetoxy C2	C6H10O4	0.0737	0.0113	0.0014
2392	n-PropylBenzoate	C10H12O2	0.0908	0.0103	0.0009
2377	DiMth Phthalate	C10H10O4	0.1940	0.0211	0.0015
2386	Diethyl Maleate	C8H12O4	0.0807	0.0122	0.0013
2385	Mth Dodecanoate	C13H26O2	0.1095	0.0147	0.0015
3379	Dioctyl Adipate	C22H42O4	0.0855	0.0082	0.0004
5886	Mth Acetoacetate	C5H8O3	0.1361	0.0227	0.003
5884	Ethoxy Acetate	C6H12O3	0.1045	0.0143	0.0015
5887	EthAcetoAcetate	C6H10O3	0.0965	0.0142	0.0015
5885	Carbitol Acetate	C8H16O4	0.0807	0.0107	0.001

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

	Ketone				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1096	Methyl Isopropen	C5H8O	0.0814	0.0109	0.0011
1079	Cyclopentanone	C5H8O	0.1492	0.0212	0.0023
1051	Acetone	C3H6O	0.1322	0.0191	0.0021
1052	MEK	C4H8O	0.1026	0.0137	0.0014
1065	Mesityl Oxide	C6H10O	0.0873	0.0118	0.0012

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1066	T-But Mth Ketone	C6H12O	0.0677	0.0084	0.0008
1060	2-Pentanone	C5H10O	0.0871	0.0111	0.0011
1061	Mth iC3 Ketone	C5H10O	0.0813	0.0107	0.001
1053	Diethyl Ketone	C5H10O	0.0933	0.0115	0.001
1059	3-Hexanone	C6H12O	0.0840	0.0101	0.0009
1099	Diketene	C4H4O2	0.4034	0.0925	0.0171
1055	Sec-ButMthKetone	C6H12O	0.0746	0.0095	0.0009
1054	MIBK	C6H12O	0.0713	0.0088	0.0009
1095	EthIsopropKetone	C6H12O	0.0728	0.0093	0.0009
1063	2-Heptanone	C7H14O	0.0866	0.0108	0.001
1064	5-Mth-2-Hexanone	C7H14O	0.0805	0.0105	0.001
1058	4-Heptanone	C7H14O	0.0779	0.0089	0.0007
1057	3-Heptanone	C7H14O	0.0847	0.0105	0.001
1076	2,4-Pentanedione	C5H8O2	0.0451	0.0034	0.0002
1068	DiisobutylKetone	C9H18O	0.0550	0.0064	0.0006
1097	2-CycC6 CycC6one	C12H20O	0.0782	0.0099	0.0011
1083	2-Octanone	C8H16O	0.0867	0.0109	0.001
1073	Dibutyl Ketone	C9H18O	0.0832	0.0098	0.0009
1062	2-Hexanone	C6H12O	0.0869	0.0109	0.001
1077	Isophorone	C9H14O	0.1666	0.0229	0.0022
1090	Acetophenone	C8H8O	0.1061	0.0129	0.0011
1080	Cyclohexanone	C6H10O	0.1349	0.0179	0.0018
1074	2-Nonanone	C9H18O	0.0881	0.0112	0.001

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Alcohol-Ethers

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
2862	2-Butoxyethanol	C6H14O2	0.0734	0.0083	0.0007
4857	butyl carbitol	C8H18O3	0.0587	0.0068	0.0006
2898	2-Chloroethanol	C2H5ClO	0.1355	0.0179	0.0015
2864	Carbitol	C6H14O3	0.0673	0.0086	0.0008
3854	Methyl propasol	C4H10O2	0.0786	0.0076	0.0005
2860	2-Methoxyethanol	C3H8O2	0.1688	0.0189	0.0015
2854	DiacetoneAlcohol	C6H12O2	0.0490	0.0047	0.0003
2861	2-Ethoxyethanol	C4H10O2	0.0859	0.0097	0.0008
2889	HydroxyAcetone	C3H6O2	0.1320	0.0152	0.0012
3856	1tButoxy2Propnol	C7H16O2	0.0209	0.0024	0.0002
3858	PROPGLYC2tBUTYL	C7H16O2	0.0481	0.0061	0.0006
4855	2-Propoxyethanol	C5H12O2	0.0740	0.0077	0.0006

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

4849	Acetovanillone	C9H10O3	0.1804	0.0212	0.0017
5883	Ethyl Lactate	C5H10O3	0.0549	0.0052	0.0003
6883	2-HydroxyEth Acr	C5H8O3	0.1893	0.0351	0.0048
2863	Methyl Carbitol	C5H12O3	0.0873	0.0123	0.0013
3855	Dowanol DPM	C7H16O3	0.0430	0.004	0.0002
3857	TriPropGlymEthlE	C10H22O4	0.0254	0.0032	0.0003

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Hydrocarbons

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
404	DiMth-Acetylene	C4H6	0.1062	0.0142	0.0014
202	Propylene	C3H6	0.0600	0.007	0.0006
412	2-Pentyne	C5H8	0.0140	0.0009	0
207	2-Methylpropene	C4H8	0.0808	0.0101	0.001
204	1-Butene	C4H8	0.0749	0.0091	0.0008
205	Cis-2-Butene	C4H8	0.1015	0.014	0.0015
402	Propyne	C3H4	0.1103	0.0178	0.0023
406	3-Hexyne	C6H10	0.0894	0.0106	0.0009
206	Trans-2-Butene	C4H8	0.0913	0.012	0.0012
407	2-Hexyne	C6H10	0.0986	0.012	0.0011
231	33-2Mth-1-Butene	C6H12	0.0839	0.0111	0.0012
230	23-2Mth-1-Butene	C6H12	0.0993	0.0137	0.0015
229	2-Ethyl-1-Butene	C6H12	0.1004	0.0134	0.0013
8	I-Pentane	C5H12	0.0898	0.0107	0.0009
14	2,2-DiMth-Butane	C6H14	0.0958	0.0116	0.0011
232	23-2Mth-2-Butene	C6H12	0.1202	0.016	0.0016
213	3-Mth-1-Butene	C5H10	0.0847	0.0111	0.0011
212	2-Mth-1-Butene	C5H10	0.0940	0.0123	0.0012
211	Trans-2-Pentene	C5H10	0.0955	0.0127	0.0013
210	Cis-2-Pentene	C5H10	0.0974	0.0131	0.0014
223	4-Mth-1-Pentene	C6H12	0.0875	0.0114	0.0011
221	2-Mth-1-Pentene	C6H12	0.0929	0.0119	0.0012
248	2-t-Butylpropene	C7H14	0.1051	0.0146	0.0016
227	Cs-4-Mth-2-C5H10	C6H12	0.0870	0.0118	0.0013
224	2-Mth-2-Pentene	C6H12	0.0990	0.0129	0.0013
403	1-Butyne	C4H6	0.0884	0.0129	0.0015
15	2,3-DiMth-Butane	C6H14	0.1178	0.0161	0.0017
214	2-Mth-2-Butene	C5H10	0.1060	0.014	0.0014
228	Ts-4-Mth-2-C5H10	C6H12	0.0935	0.0131	0.0014

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

225	Cs-3-Mth-2-C5H10	C6H12	0.1002	0.0129	0.0012
218	Trans-2-Hexene	C6H12	0.0966	0.0128	0.0013
2226	3-METH-Tr-2Pente	C6H12	0.1093	0.0147	0.0015
222	3-Mth-1-Pentene	C6H12	0.0887	0.0114	0.0011
257	2-Diisobutylene	C8H16	0.0932	0.0125	0.0013
256	1-Diisobutylene	C8H16	0.0910	0.0117	0.0012
217	Cis-2-Hexene	C6H12	0.0997	0.0132	0.0013
2414	1-Heptyne	C7H12	0.0898	0.0119	0.0012
13	3-Methylpentane	C6H14	0.1052	0.0133	0.0013
219	Cis-3-Hexene	C6H12	0.0924	0.012	0.0012
12	2-Methylpentane	C6H14	0.0955	0.0118	0.0011
220	Trans-3-Hexene	C6H12	0.0943	0.0124	0.0012
405	1-Pentyne	C5H8	0.0851	0.0113	0.0012
209	1-Pentene	C5H10	0.0829	0.0102	0.0009
11	N-Hexane	C6H14	0.0961	0.0113	0.001
235	Cis-2-Heptene	C7H14	0.1025	0.0132	0.0013
249	Cis-3-Heptene	C7H14	0.0949	0.012	0.0012
216	1-Hexene	C6H12	0.0906	0.0115	0.0011
239	3-Eth-1-Pentene	C7H14	0.0886	0.012	0.0012
226	4-Mth-1-Hexene	C7H14	0.0959	0.0133	0.0014
240	3-Mth-1-Hexene	C7H14	0.0881	0.0119	0.0013
419	3-Mth-1-Butyne	C5H8	0.0813	0.0116	0.0013
233	2-Eth-1-Pentene	C7H14	0.1023	0.0131	0.0013
238	2-Mth-1-Hexene	C7H14	0.0965	0.0124	0.0012
416	1-Octyne	C8H14	0.0914	0.0122	0.0012
289	2,3Dimeth Hexene	C8H16	0.0902	0.0122	0.0013
234	1-Heptene	C7H14	0.0964	0.0123	0.0012
413	1-Hexyne	C6H10	0.0875	0.0116	0.0012
237	Trans-3-Heptene	C7H14	0.0943	0.0121	0.0012
236	Trans-2-Heptene	C7H14	0.1008	0.013	0.0013
251	Trans-2-Octene	C8H16	0.1030	0.013	0.0012
279	Trans-4-Octene	C8H16	0.0955	0.0119	0.0011
277	Trans-3-Octene	C8H16	0.0985	0.0123	0.0012
2252	2Methl-1-Heptene	C8H16	0.0989	0.0124	0.0011
250	1-Octene	C8H16	0.1002	0.0129	0.0013
258	2-Ethyl-1-Hexene	C8H16	0.1008	0.0129	0.0012
280	3-Octene	C8H16	0.0971	0.0121	0.0011
278	4-Octene	C8H16	0.0965	0.0121	0.0011
276	2-Octene	C8H16	0.1051	0.0133	0.0012
259	1-Nonene	C9H18	0.1037	0.0135	0.0013
262	1-Dodecene	C12H24	0.1113	0.0147	0.0015
263	1-Tridecene	C13H26	0.1129	0.015	0.0015
264	1-Tetradecene	C14H28	0.1150	0.0152	0.0016
265	1-Pentadecene	C15H30	0.1166	0.0154	0.0016
266	1-Hexadecene	C16H32	0.1183	0.0156	0.0016

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

267	1-Octadecene	C18H36	0.1191	0.0156	0.0016
281	1-Heptadecene	C17H34	0.1185	0.0154	0.0016
284	1-Eicosene	C20H40	0.1226	0.0162	0.0017
283	1-Nonadecene	C19H38	0.1205	0.0158	0.0017
3	Propane	C3H8	0.0440	0.004	0.0003
4	I-Butane	C4H10	0.0689	0.0077	0.0007
9	Neopentane	C5H12	0.0699	0.0076	0.0006
5	N-Butane	C4H10	0.0670	0.0069	0.0005
7	pentane	C5H12	0.0840	0.0094	0.0008
44	Hexamethylethane	C8H18	0.1517	0.0224	0.0025
25	223-TriMthButane	C7H16	0.1284	0.0177	0.0019
24	3,3-DiMthPentane	C7H16	0.1193	0.0152	0.0014
51	2,2,3,3-4Mth-C5	C9H20	0.1766	0.0264	0.0031
21	2,2-DiMthPentane	C7H16	0.0969	0.0118	0.0011
42	2,3,3-TriMth-C5	C8H18	0.1465	0.0207	0.0022
22	2,3-DiMthPentane	C7H16	0.1233	0.0171	0.0018
40	2,2,3-TriMth-C5	C8H18	0.1285	0.0177	0.0019
23	2,4-DiMthPentane	C7H16	0.0936	0.0121	0.0012
41	2,2,4-TriMth-C5	C8H18	0.0953	0.012	0.0011
39	3-Mth-3-Eth-C5	C8H18	0.1366	0.0179	0.0018
20	3-Ethylpentane	C7H16	0.1111	0.0142	0.0014
52	2,2,3,4-4Mth-C5	C9H20	0.1341	0.0194	0.0022
54	2334TetrMethPent	C9H20	0.1650	0.0254	0.003
53	2,2,4,4-4Mth-C5	C9H20	0.1118	0.0146	0.0014
43	2,3,4-TriMth-C5	C8H18	0.1293	0.0189	0.0021
36	3,3-DiMth-Hexane	C8H18	0.1147	0.0146	0.0014
19	3-Methylhexane	C7H16	0.1057	0.0135	0.0013
18	2-Methylhexane	C7H16	0.1001	0.0126	0.0012
38	2-Mth-3-Eth-C5	C8H18	0.1170	0.0158	0.0016
190	2,2-2C1-3-C2-C5	C9H20	0.1201	0.0165	0.0017
32	2,2-DiMth-Hexane	C8H18	0.0989	0.0123	0.0012
37	3,4-DiMth-Hexane	C8H18	0.1237	0.0171	0.0018
50	3,3-DiEthPentane	C9H20	0.1454	0.019	0.0018
34	2,4-DiMth-Hexane	C8H18	0.0983	0.0128	0.0013
33	2,3-DiMth-Hexane	C8H18	0.1166	0.0159	0.0017
17	N-Heptane	C7H16	0.1051	0.0129	0.0012
49	244TriMethHexane	C9H20	0.1106	0.0145	0.0014
192	2,4-2C1-3-C2-C5	C9H20	0.1175	0.0166	0.0018
47	2,2,5-TriMth-C6	C9H20	0.0930	0.0118	0.0011
35	2,5-DiMth-Hexane	C8H18	0.0976	0.0127	0.0013
31	3-Ethylhexane	C8H18	0.1076	0.0137	0.0013
30	4-Methylheptane	C8H18	0.1052	0.0134	0.0013
29	3-Methylheptane	C8H18	0.1092	0.014	0.0014
28	2-Methylheptane	C8H18	0.1049	0.0134	0.0013
96	2,2-DiMthHeptane	C9H20	0.1019	0.0126	0.0012

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

176	2,6-DiMthHeptane	C9H20	0.0999	0.0134	0.0014
27	N-Octane	C8H18	0.1124	0.014	0.0013
94	3-Ethylheptane	C9H20	0.1079	0.0138	0.0013
92	3-Methyloctane	C9H20	0.1117	0.0144	0.0014
93	4-Methyloctane	C9H20	0.1066	0.0135	0.0013
91	2-Methyloctane	C9H20	0.1091	0.0141	0.0014
72	2,2-DiMthOctane	C10H22	0.1046	0.0134	0.0013
2095	2,3Dimethloctane	C10H22	0.1153	0.0155	0.0016
2096	2,4Dimethloctane	C10H22	0.0925	0.0121	0.0012
2098	2,6DimethlOctane	C10H22	0.1044	0.014	0.0014
2097	2,5Dimethloctane	C10H22	0.0994	0.013	0.0013
2099	2,7DimethlOctane	C10H22	0.1033	0.0137	0.0014
46	N-Nonane	C9H20	0.1175	0.0149	0.0014
88	5-Methylnonane	C10H22	0.1067	0.0135	0.0013
85	3-Methylnonane	C10H22	0.1145	0.015	0.0015
87	4-Methylnonane	C10H22	0.1084	0.0139	0.0013
86	2-Methylnonane	C10H22	0.1123	0.0147	0.0015
56	N-Decane	C10H22	0.1230	0.0159	0.0015
63	N-Undecane	C11H24	0.1263	0.0164	0.0016
64	N-Dodecane	C12H26	0.1296	0.0169	0.0017
65	N-Tridecane	C13H28	0.1316	0.0174	0.0018
66	N-Tetradecane	C14H30	0.1343	0.0178	0.0018
67	N-Pentadecane	C15H32	0.1363	0.0182	0.0018
68	N-Hexadecane	C16H34	0.1384	0.0183	0.0019
69	N-Heptadecane	C17H36	0.1412	0.0189	0.0019
70	N-Octadecane	C18H38	0.1401	0.0188	0.0019
71	N-Nonadecane	C19H40	0.1412	0.0188	0.0019
73	N-Eicosane	C20H42	0.1445	0.0192	0.002
74	n-HENEICOSANE	C21H44	0.1453	0.0191	0.002
75	n-DOCOSANE	C22H46	0.1455	0.0187	0.0019
76	n-TRICOSANE	C23H48	0.1450	0.0193	0.002
77	n-Tetracosane	C24H50	0.1457	0.0195	0.002
78	n-PENTACOSANE	C25H52	0.1466	0.0192	0.002
79	n-HEXACOSANE	C26H54	0.1470	0.0195	0.002
81	n-Octacosane	C28H58	0.1479	0.0194	0.002
2081	n-TRICONTANE	C30H62	0.1506	0.0191	0.0019
2082	n-Dotriacontane	C32H66	0.1480	0.0186	0.0018
2086	Hexatriacontane	C36H74	0.1536	0.0187	0.0017

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Cyclic Hydrocarbons

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
269	Cyclopentene	C5H8	0.08058	0.0107	0.0011
270	Cyclohexene	C6H10	0.09371	0.0128	0.0014
287	3MthCyclopentene	C6H10	0.08504	0.0119	0.0013
286	1-MthCyclPentene	C6H10	0.08465	0.011	0.0011
288	4MthCyclopenten	C6H10	0.0881	0.0125	0.0014
273	Cycloheptene	C7H12	0.0955	0.0131	0.0013
274	Cyclooctene	C8H14	0.0947	0.013	0.0013
101	Cyclopropane	C3H6	0.0492	0.0051	0.0004
810	ADAMANTANE	C10H16	0.1256	0.0158	0.0014
102	Cyclobutane	C4H8	0.0747	0.0086	0.0007
104	Cyclopentane	C5H10	0.0834	0.01	0.0009
137	Cyclohexane	C6H12	0.0839	0.01	0.0009
105	MthCyclopentane	C6H12	0.0980	0.0125	0.0011
146	Cs-1,4-2C1-CycC6	C8H16	0.1168	0.0154	0.0015
142	Cs-1,2-2C1-CycC6	C8H16	0.1347	0.0184	0.0019
141	1,1-2C1-CycC6	C8H16	0.1064	0.013	0.0012
145	Ts-1,3-2C1-CycC6	C8H16	0.1173	0.0155	0.0016
144	Cs-1,3-2C1-CycC6	C8H16	0.1042	0.0132	0.0013
147	Ts-1,4-2C1-CycC6	C8H16	0.1021	0.0127	0.0012
143	Ts-1,2-2C1-CycC6	C8H16	0.1141	0.0146	0.0014
138	MthCyclohexane	C7H14	0.0938	0.0115	0.0011
159	Cycloheptane	C7H14	0.1083	0.0137	0.0013
140	Ethylcyclohexane	C8H16	0.1069	0.0135	0.0013
154	Trans-Decalin	C10H18	0.1038	0.0132	0.0013
149	N-PropylCyc-C6	C9H18	0.1082	0.0137	0.0013
109	Cs-1,2-2C1-CycC5	C7H14	0.1338	0.0187	0.002
110	Ts-1,2-2C1-CycC5	C7H14	0.1076	0.0142	0.0014
112	Ts-1,3-2C1-CycC5	C7H14	0.1074	0.0141	0.0014
107	Eth-Cyclopentane	C7H14	0.1067	0.0137	0.0013
114	N-PropCycPentane	C8H16	0.1101	0.0143	0.0014
108	1,1-DiMthCycC5	C7H14	0.0981	0.012	0.0011
111	Cs-1,3-2C1-CycC5	C7H14	0.1052	0.0138	0.0013
152	N-ButylCycHexane	C10H20	0.1123	0.0144	0.0014
160	Cyclooctane	C8H16	0.1220	0.0159	0.0016
153	Cis-Decalin	C10H18	0.1275	0.0173	0.0018
115	ISOPROPYLCYCLOPENTANE	C8H16	0.1106	0.015	0.0015
150	Isopropyl-CycC6	C9H18	0.1118	0.015	0.0015
116	1-C1-1-C2-CycC5	C8H16	0.1180	0.0152	0.0015
122	Butylcyclpentane	C9H18	0.1129	0.0149	0.0015
155	1,1-Bicyclohexyl	C12H22	0.1144	0.015	0.0015
158	N-Decylcyclo-C6	C16H32	0.1306	0.0172	0.0017

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Aromatic Hydrocarbons

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
307	1,4-Pentadiene	C5H8	0.0867	0.0124	0.0014
306	1-ts3-Pentadiene	C5H8	0.1323	0.0216	0.0029
414	2-Methyl-1-Butenyne	C5H6	0.0806	0.0109	0.0011
305	Cs1,3-Pentadiene	C5H8	0.1408	0.0237	0.0033
309	Isoprene	C5H8	0.1228	0.0193	0.0024
421	1-Pentene-4-yne	C5H6	0.1040	0.0149	0.0017
303	1,3-Butadiene	C4H6	0.1114	0.0174	0.0022
332	1,4-CyclHexadien	C6H8	0.1022	0.0177	0.0025
501	Benzene	C6H6	0.1032	0.0155	0.0019
315	Cyclopentadiene	C5H6	0.0777	0.0102	0.0009
319	Diisopropenyl	C6H10	0.1313	0.0207	0.0026
615	Ethynylbezene	C8H6	0.0716	0.0076	0.0006
601	Styrene	C8H8	0.0969	0.0115	0.001
331	1,3-CycHexadiene	C6H8	0.0841	0.0126	0.0015
310	1,5-Hexadiene	C6H10	0.0871	0.0116	0.0012
312	MthCycPentadiene	C6H8	0.0873	0.0128	0.0015
420	1-Pentene-3-yne	C5H6	0.1246	0.0166	0.0018
502	Toluene	C7H8	0.0950	0.0131	0.0014
521	T-Butylbenzene	C10H14	0.0767	0.0082	0.0006
320	Dipropylene	C6H10	0.1469	0.0246	0.0033
520	Sec-Butylbenzene	C10H14	0.0995	0.0127	0.0013
313	1,4-Hexadiene	C6H10	0.0951	0.0136	0.0015
314	Dipropylene	C6H10	0.1409	0.0234	0.0032
316	DiCycPentadiene	C10H12	0.0457	0.0065	0.0007
333	1,5-CycOctadiene	C8H12	0.0999	0.0157	0.002
701	Naphthalene	C10H8	0.1386	0.0145	0.0011
504	Ethylbenzene	C8H10	0.1006	0.0136	0.0014
820	Indan	C9H10	0.1182	0.016	0.0016
505	O-Xylene	C8H10	0.1050	0.0144	0.0015
612	P-Methylstyrene	C9H10	0.1008	0.0118	0.001
330	DIISOCROTYL	C8H14	0.1377	0.0217	0.0028
507	P-Xylene	C8H10	0.0898	0.0117	0.0012
329	DIISOBUTENYL	C8H14	0.0895	0.0123	0.0013
506	M-Xylene	C8H10	0.0916	0.0121	0.0012
603	Methylstyrene	C9H10	0.0973	0.0116	0.001
613	Alpha-MthStyrene	C9H10	0.0930	0.011	0.0009
510	Isopropylbenzene	C9H12	0.1059	0.0143	0.0015
724	2-Methylindene	C10H10	0.1151	0.0134	0.0011
285	Vinylcyclohexene	C8H12	0.0826	0.0115	0.0013
803	Indene	C9H8	0.0943	0.0084	0.0006
706	Tetralin	C10H12	0.1307	0.0181	0.0019
511	O-Ethyltoluene	C9H12	0.1046	0.014	0.0014
723	1-Methylindene	C10H10	0.0580	0.0091	0.0012

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

738	Fluorene	C13H10	0.2139	0.0221	0.0016
619	Tr-1PropenylBz	C9H10	0.1157	0.0148	0.0014
525	O-Diethylbenzene	C10H14	0.1015	0.0132	0.0013
618	Propenyl Bz(cis)	C9H10	0.1179	0.0146	0.0013
602	O-Methylstyrene	C9H10	0.0937	0.0112	0.001
702	1-MthNaphthalene	C11H10	0.1588	0.0175	0.0013
509	N-Propylbenzene	C9H12	0.0962	0.0126	0.0013
526	M-Diethylbenzene	C10H14	0.0965	0.0122	0.0012
583	Cs-2-PhnButene-2	C10H12	0.1086	0.013	0.0011
543	M-DiisopropylBz	C12H18	0.0937	0.0118	0.0011
584	Ts-2-PhnButene-2	C10H12	0.0629	0.0065	0.0005
580	1,2-DiC1-3C2-Bz	C10H14	0.1144	0.0154	0.0016
704	1-EthNaphthalene	C12H12	0.1542	0.017	0.0013
512	M-Ethyltoluene	C9H12	0.0944	0.0124	0.0012
522	1-Mth-2-iC3-Benz	C10H14	0.1049	0.0137	0.0013
513	P-Ethyltoluene	C9H12	0.0967	0.0124	0.0012
514	1,2,3-Mesitylene	C9H12	0.1182	0.0163	0.0017
614	M-Divinylbenzene	C10H10	0.1040	0.0109	0.0008
524	1-Mth-4-iC3-Benz	C10H14	0.1013	0.013	0.0013
822	Gamma-Terpinene	C10H16	0.1123	0.0168	0.0019
821	Alpha-Terpinene	C10H16	0.0912	0.0126	0.0013
523	1-Mth-3-iC3-Benz	C10H14	0.0970	0.0124	0.0012
703	2-MthNaphthalene	C11H10	0.1485	0.0154	0.0012
557	CycHexylBenzene	C12H16	0.1051	0.0154	0.0018
515	1,2,4-Mesitylene	C9H12	0.1003	0.0132	0.0013
519	Isobutylbenzene	C10H14	0.0799	0.0105	0.001
424	DiPhnAcetylene	C14H10	0.1298	0.0134	0.001
544	P-DiisopropylBz	C12H18	0.1096	0.0147	0.0015
518	N-Butylbenzene	C10H14	0.0994	0.0131	0.0013
516	1,3,5-Mesitylene	C9H12	0.0886	0.0115	0.0011
809	Acenaphthalene	C12H8	0.1626	0.0144	0.0008
725	123-TriMthIndene	C12H14	0.1087	0.012	0.0009
527	1,4-DiEthBenzene	C10H14	0.1022	0.0132	0.0013
558	Diphenyl	C12H10	0.1267	0.0144	0.0012
576	2-Ethyl-m-Xylene	C10H14	0.1041	0.0136	0.0013
620	p-ISOPROPENYLSTY	C11H12	0.1848	0.0177	0.0013
585	o-PropylToluene	C10H14	0.0972	0.0123	0.0012
577	2-Ethyl-p-Xylene	C10H14	0.0965	0.0125	0.0012
579	4-Ethyl-o-Xylene	C10H14	0.1032	0.0135	0.0013
586	m-Propyltoluene	C10H14	0.0900	0.0114	0.0011
587	p-Propyltoluene	C10H14	0.0933	0.0119	0.0011
578	4-Ethyl-m-Xylene	C10H14	0.1004	0.0131	0.0012
575	5-Ethyl-m-Xylene	C10H14	0.0890	0.011	0.001
530	Prehnitene	C10H14	0.1300	0.0181	0.002
709	2,6-2Mth-Naphtha	C12H12	0.1536	0.0168	0.0012

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

715	2,7-2Mth-Naphtha	C12H12	0.1574	0.0175	0.0013
719	2-ETHYLNAPHTHALENE	C12H12	0.1548	0.016	0.0012
621	p-tert-BUTYLSTY	C12H16	0.1046	0.0101	0.0007
532	1,2,4,5-TetMthBz	C10H14	0.1068	0.0142	0.0014
531	1,2,3,5-TetMthBz	C10H14	0.1103	0.0148	0.0015
533	p-tert-BUTYL ET	C12H18	0.0763	0.0068	0.0004
567	N-Pentylbenzene	C11H16	0.1012	0.0132	0.0013
718	1-n-PROPYLNAPHTH	C13H14	0.1464	0.0129	0.0008
562	1,1-DiPhnEthane	C14H14	0.0991	0.012	0.0011
616	4-ISOBUTYLSTYRE	C12H16	0.1650	0.0195	0.0017
260	1-Decene	C10H20	0.1065	0.0141	0.0014
735	Cis-Stilbene	C14H12	0.0876	0.0093	0.0007
568	Hexylbenzene	C12H18	0.1028	0.0134	0.0014
563	Diphenylmethane	C13H12	0.1005	0.0123	0.0011
564	1,2-DiPhnEthane	C14H14	0.0815	0.011	0.0011
804	Anthracene	C14H10	0.3838	0.0391	0.0026
736	Trans-Stilbene	C14H12	0.1555	0.0213	0.0021
805	Phenanthrene	C14H10	0.3481	0.0366	0.0026
713	1-ButNaphthalene	C14H16	0.1483	0.0165	0.0013
807	Pyrene	C16H10	0.6883	0.0625	0.0039
261	1-Undecene	C11H22	0.1091	0.0144	0.0015
581	23-2C1-23-2PhnC4	C18H22	0.0753	0.0073	0.0005
549	N-Heptylbenzene	C13H20	0.1064	0.0134	0.0013
710	1-PhnNaphthalene	C16H12	0.1646	0.016	0.0011
566	2,4-Diphenyl-4-M	C18H20	0.1041	0.0113	0.0009
561	O-Terphenyl	C18H14	0.0873	0.0072	0.0004
569	N-Octylbenzene	C14H22	0.1067	0.0137	0.0014
565	Triphenylmethane	C19H16	0.0933	0.0094	0.0007
714	N-C6-Naphthalene	C16H20	0.1593	0.0186	0.0016
717	Fluoranthene	C16H10	0.5338	0.0435	0.0022
716	1-Hexyl-Tetralin	C16H24	0.1250	0.0133	0.001
731	TriPhnEthylene	C20H16	0.1410	0.0156	0.0012
806	Chrysene	C18H12	0.9946	0.1132	0.0104
588	1,1,2TriPhenEth	C20H18	0.0567	0.005	0.0003
711	1-n-NonylNaphtha	C19H26	0.1776	0.0191	0.0015
570	N-Nonylbenzene	C15H24	0.1101	0.014	0.0014
712	1-Decyl Naphtha	C20H28	0.1818	0.0195	0.0015
559	P-Terphenyl	C18H14	0.2403	0.0296	0.0026
560	M-Terphenyl	C18H14	0.2060	0.0229	0.0018
589	TetraPhenylMetha	C25H20	0.1860	0.0206	0.0016
554	Decylbenzene	C16H26	0.1096	0.0143	0.0015
732	TetraPhnEthylene	C26H20	0.2075	0.023	0.0018
574	N-Dodecylbenzene	C18H30	0.1099	0.0147	0.0015
571	N-Undecylbenzene	C17H28	0.1107	0.0142	0.0015
572	Tridecylbenzene	C19H32	0.1112	0.0148	0.0015

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

573	n-TETRADECYLBENZ	C20H34	0.1263	0.0153	0.0014
2575	n-PENTADECYLBENZ	C21H36	0.1280	0.0157	0.0014
2576	n-HEXADECYLBENZ	C22H38	0.1292	0.0162	0.0015
2577	n-HEPTADECYLBENZ	C23H40	0.1292	0.0156	0.0014
2578	n-OCTADECYLBENZE	C24H42	0.1299	0.0155	0.0014

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

Halocarbons

Dip ID	**Name**	**Formula**	$P_{760\,nnHg}^{calc}$	$P_{100\,nnHg}^{calc}$	$P_{10\,nnHg}^{calc}$
1544	Allyl Chloride	C3H5Cl	0.10345	0.0148	0.0017
1595	2-Chloropropene	C3H5Cl	0.11476	0.0153	0.0015
1531	3-Chloropropyne	C3H3Cl	0.10821	0.0156	0.0017
1561	6Cl-1,3Butadiene	C4Cl6	0.1406	0.0165	0.0015
1535	T-Butyl Chloride	C4H9Cl	0.12143	0.0153	0.0014
1583	Chloroprene	C4H5Cl	0.13657	0.0208	0.0025
1530	Isopropyl Cl	C3H7Cl	0.12049	0.0162	0.0016
1572	O-DiCl-Benzene	C6H4Cl2	0.10747	0.0153	0.0017
1585	Propyl Chloride	C3H7Cl	0.09578	0.0124	0.0012
1684	Isopropyl Iodide	C3H7I	0.09029	0.0129	0.0014
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	0.11096	0.0162	0.0019
1651	2-Bromopropane	C3H7Br	0.11616	0.0164	0.0018
1691	Iodobenzene	C6H5I	0.07568	0.0086	0.0007
1860	Fluorobenzene	C6H5F	0.12142	0.0183	0.0021
1571	Chlorobenzene	C6H5Cl	0.10257	0.0147	0.0016
1680	Bromobenzene	C6H5Br	0.07372	0.0076	0.0006
1526	1,2-DiCl-Propane	C3H6Cl2	0.08816	0.0111	0.001
1683	Propyl Iodide	C3H7I	0.11269	0.0158	0.0017
1576	Benzotrichloride	C7H5Cl3	0.18445	0.014	0.0006
1536	2,3-DICHLOROBUT	C4H8Cl2	0.14181	0.0201	0.0022
2638	2-Bromobutane	C4H9Br	0.1188	0.0179	0.0021
1586	1-Chlorobutane	C4H9Cl	0.1004	0.0129	0.0013
1573	M-DiCl-Benzene	C6H4Cl2	0.0899	0.012	0.0012
2634	Benzotrifluoride	C7H5F3	0.1426	0.0114	0.0006
1574	P-DiCl-Benzene	C6H4Cl2	0.0925	0.0127	0.0013
1650	1-Bromopropane	C3H7Br	0.1297	0.0176	0.0018
1587	2-Chlorobutane	C4H9Cl	0.1234	0.0159	0.0015
2653	8F-2-Butene	C4F8	0.0099	0.0001	0
1678	M-Dibromobenzene	C6H4Br2	0.0715	0.0058	0.0003
1537	1,2-DiCl-Butane	C4H8Cl2	0.0789	0.0094	0.0008

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1597	34-DiCl-1-Butene	C4H6Cl2	0.0652	0.0094	0.0011
1577	O-Chlorotoluene	C7H7Cl	0.0986	0.0135	0.0014
1532	123-3Cl-Propane	C3H5Cl3	0.0773	0.01	0.001
1578	P-Chlorotoluene	C7H7Cl	0.1072	0.0152	0.0017
1562	Benzyl Chloride	C7H7Cl	0.1045	0.0126	0.0011
2661	P-Bromotoluene	C7H7Br	0.0838	0.0089	0.0006
1508	1,4-DiCl-Butane	C4H8Cl2	0.1315	0.0195	0.0022
1655	1-Bromobutane	C4H9Br	0.1342	0.0177	0.0018
1599	BenzylDichloride	C7H6Cl2	0.1320	0.0147	0.0011
2652	Perfluoropropane	C3F8	0.0161	0.0003	0
1505	2-Butylene DiCl	C4H6Cl2	0.1087	0.018	0.0024
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	0.0974	0.015	0.0018
1588	1-Chloropentane	C5H11Cl	0.1067	0.0131	0.0012
1592	1,2,4-TriCl-Bz	C6H3Cl3	0.0868	0.0113	0.001
1579	2,4-2Cl-Toluene	C7H6Cl2	0.0983	0.0137	0.0014
2593	1,3,5-TriCl-BZ	C6H3Cl3	0.0780	0.0098	0.0009
1697	1-Br-Naphthalene	C10H7Br	0.1726	0.0175	0.0012
1622	Perfluorobutane	C4F10	0.1196	0.0045	0.0001
1857	P-Cl-Benzo-TriF	C7H4ClF3	0.1645	0.0141	0.0008
1509	1,5-DiCl-Pentane	C5H10Cl2	0.1426	0.0215	0.0025
1589	1-Cl-Naphthalene	C10H7Cl	0.1707	0.0186	0.0015
1582	6ClCycPentadiene	C5Cl6	0.1004	0.0121	0.0011
1864	Perfluorobenzene	C6F6	0.0937	0.0122	0.0012
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	0.2124	0.0206	0.0013
1667	1-Bromoheptane	C7H15Br	0.1365	0.0186	0.0019
1575	HexaCl-Benzene	C6Cl6	0.0727	0.0122	0.0018
2640	Freon 123B1	C2HBrClF3	0.0709	0.0049	0.0002
1504	Vinyl Chloride	C2H3Cl	0.0509	0.0059	0.0005
1672	1,1-DiBr-Ethane	C2H4Br2	0.0867	0.0135	0.0017
1580	Acetylene DiCl	C2H2Cl2	0.1013	0.0137	0.0015
1692	Diiodomethane	CH2I2	0.0989	0.0167	0.0024
1698	Bromoform	CHBr3	0.0545	0.007	0.0007
2687	Freon 13B1	CBrF3	0.0024	0	0
2690	Br-3F-Ethylene	C2BrF3	0.0584	0.0035	0.0001
1649	Tetrabromoethane	C2H2Br4	0.0441	0.0061	0.0007
2686	Freon 12B1	CBrClF2	0.0492	0.0036	0.0002
1503	Ethyl Chloride	C2H5Cl	0.0928	0.012	0.0012
2641	Br-TriCl-Methane	CBrCl3	0.0663	0.0041	0.0001
1641	Methyl Bromide	CH3Br	0.1376	0.0197	0.0022
2688	Freon 12B2	CBr2F2	0.0483	0.0035	0.0002
2545	2,3-DiCl-Propene	C3H4Cl2	0.1037	0.0153	0.0019
1673	1,2-DiBr-Ethane	C2H4Br2	0.1483	0.0212	0.0022
2637	Dibromomethane	CH2Br2	0.1318	0.0201	0.0024
1542	TetraCl-Ethylene	C2Cl4	0.0711	0.0077	0.0006
1541	TriCl-Ethylene	C2HCl3	0.0876	0.0107	0.0009

Table B.6 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-PC-SAFT Equation of State (Continued)

1527	111-TriCl-Ethane	C2H3Cl3	0.0775	0.005	0.0002
1612	Cl-2F-Ethylene	C2HClF2	0.1592	0.0182	0.0014
2639	Br-Cl-Methane	CH2BrCl	0.0869	0.0122	0.0013
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	0.0662	0.0079	0.0008
1682	Ethyl Iodide	C2H5I	0.1151	0.017	0.0019
1522	1,1-DiCl-Ethane	C2H4Cl2	0.1192	0.0166	0.0017
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	0.1339	0.0224	0.0031
1525	Hexachloroethane	C2Cl6	0.2496	0.0178	0.0008
1528	1112-4Cl-Ethane	C2H2Cl4	0.1107	0.0088	0.0005
1590	Penta-Cl-Ethane	C2HCl5	0.1410	0.011	0.0006
1529	1122-4Cl-Ethane	C2H2Cl4	0.0878	0.0116	0.0011
2693	Perfluoroethane	C2F6	0.0005	0	0
2692	Cl-PentaF-Ethane	C2ClF5	0.0204	0.001	0
2655	122-3Cl-112-3FC2	C2Cl3F3	0.0601	0.0083	0.0009
1609	12-2Cl-1122-4FC2	C2Cl2F4	0.0290	0.0041	0.0005
2526	1,1-DiCl-Propane	C3H6Cl2	0.1208	0.0163	0.0017
1645	Ethyl Bromide	C2H5Br	0.1292	0.018	0.002
2658	1112-4Cl-22-2FC2	C2Cl4F2	0.0473	0.0033	0.0001
1619	111-3F-Ethane	C2H3F3	0.0535	0.003	0.0001
1524	1,1,2-3Cl-Ethane	C2H3Cl3	0.0824	0.0106	0.001
2691	Genetron 1113	C2ClF3	0.0475	0.0028	0.0001
1591	Vinylidene DiCl	C2H2Cl2	0.1072	0.012	0.001
1614	Difluoromethane	CH2F2	0.3469	0.0385	0.003
2694	Vinyl Bromide	C2H3Br	0.0703	0.0088	0.0008
1694	Refrigerant 123	C2HCl2F3	0.0670	0.0045	0.0002
1523	1,2-DiCl-Ethane	C2H4Cl2	0.0857	0.0116	0.0012
2656	1122-4Cl-12-2FC2	C2Cl4F2	0.1261	0.0183	0.0021
2527	1,3-DiCl-Propane	C3H6Cl2	0.1071	0.0146	0.0016

TableB. 7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State.

Alcohols

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1181	Phenol	C6H6O	0.21837	0.0316	0.0032
1182	O-Cresol	C7H8O	0.14149	0.0176	0.0015
1183	M-Cresol	C7H8O	0.19031	0.0276	0.0028
1176	2,6-Xylenol	C8H10O	0.10095	0.0105	0.0007
1111	2-Mth-2-Butanol	C5H12O	0.10761	0.0163	0.0018
1178	3,5-Xylenol	C8H10O	0.17124	0.0245	0.0025
1133	2-Octanol	C8H18O	0.09866	0.0148	0.0018
2885	4-HYDROXYSTYREN	C8H8O	0.152	0.0216	0.0021
1197	P-t-Butylphenol	C10H14O	0.12282	0.015	0.0014
1172	2,4-Xylenol	C8H10O	0.12996	0.0162	0.0014
1184	P-Cresol	C7H8O	0.18861	0.0274	0.0029
1151	Cyclohexanol	C6H12O	0.1559	0.0265	0.0036
1170	2,3-Xylenol	C8H10O	0.13441	0.0176	0.0015
1187	P-Ethyl Phenol	C8H10O	0.13907	0.02	0.0019
2859	P-Methoxyphenol	C7H8O2	0.2778	0.0433	0.0053
1121	2-Ethylhexanol	C8H18O	0.11225	0.0176	0.0023
1179	PropargylAlcohol	C3H4O	0.39013	0.0644	0.0072
1123	3-Mth-1-Butanol	C5H12O	0.19364	0.0358	0.005
2196	P-t-Amylphenol	C11H16O	0.13798	0.0171	0.0014
1174	2,5-Xylenol	C8H10O	0.13054	0.0165	0.0013
1115	2-Hexanol	C6H14O	0.121	0.0192	0.0022
1152	1-MthCycHexanol	C7H14O	0.11671	0.0133	0.0011
4854	Guaiacol	C7H8O2	0.10396	0.0098	0.0007
1107	Sec-Butanol	C4H10O	0.16781	0.0279	0.0035
1167	Allyl Alcohol	C3H6O	0.29114	0.0496	0.0063
1130	4-Mth-2-Pentanol	C6H14O	0.12906	0.019	0.0019
1177	3,4-Xylenol	C8H10O	0.19377	0.0289	0.003
1114	1-Hexanol	C6H14O	0.14886	0.0257	0.0034
1106	Isobutanol	C4H10O	0.21619	0.0399	0.0057
1125	1-Heptanol	C7H16O	0.13006	0.0218	0.003
1105	N-Butanol	C4H10O	0.2092	0.0375	0.0051
1109	1-Pentanol	C5H12O	0.17246	0.0295	0.0038
1132	1-Octanol	C8H18O	0.1157	0.019	0.0025
1113	T-Butylcarbinol	C5H12O	0.15427	0.025	0.0031
1137	1-Undecanol	C11H24O	0.08348	0.0128	0.0016
1108	Tert-Butanol	C4H10O	0.13109	0.0209	0.0026
1103	N-Propanol	C3H8O	0.26239	0.0464	0.006
1134	1-Nonanol	C9H20O	0.10526	0.0167	0.0022
2195	P-t-Octylphenol	C14H22O	0.10914	0.013	0.0011
1102	Ethanol	C2H6O	0.36952	0.0635	0.0077
1124	3-Mth-2-Butanol	C5H12O	0.14911	0.0246	0.0034
1136	1-Decanol	C10H22O	0.09591	0.0148	0.0019
1140	Dodecanol	C12H26O	0.08078	0.0119	0.0014
1104	Isopropanol	C3H8O	0.23451	0.0399	0.0049

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

1110	2-Pentanol	C5H12O	0.13641	0.0228	0.0029
1120	3-Pentanol	C5H12O	0.12231	0.0187	0.0022
1112	2-Mth-1-Butanol	C5H12O	0.18108	0.0332	0.0045
1154	Ts-2-Mth-CycC6OH	C7H14O	0.11224	0.0167	0.0016
1153	Cs-2-Mth-CycC6OH	C7H14O	0.10746	0.0148	0.0014
1156	Ts-3-Mth-CycC6OH	C7H14O	0.13445	0.0233	0.003
1157	Cs-4-Mth-CycC6OH	C7H14O	0.12461	0.0209	0.0026
2197	P-Cumylphenol	C15H16O	0.13298	0.0171	0.0015
1180	Benzyl Alcohol	C7H8O	0.18914	0.031	0.0037
1158	Ts-4-Mth-CycC6OH	C7H14O	0.1257	0.0217	0.0028
1155	Cs-3-Mth-CycC6OH	C7H14O	0.13268	0.0236	0.0031
1168	2-Phn-2-Propanol	C9H12O	0.08843	0.0117	0.001
1141	1-Tridecanol	C13H28O	0.07925	0.0114	0.0013
1147	2-Eth-1-Butanol	C6H14O	0.14556	0.0229	0.003
1117	2-Mth-1-Pentanol	C6H14O	0.15271	0.025	0.0032
2115	2-Phenylethanol	C8H10O	0.14665	0.0249	0.0029
1142	1-Tetradecanol	C14H30O	0.07484	0.0105	0.0012
2118	1-PHN-1-PROPANOL	C9H12O	0.11151	0.0152	0.0013
2119	1-PHN-2-PROPANOL	C9H12O	0.11257	0.0156	0.0014
1126	2-Heptanol	C7H16O	0.10611	0.0152	0.0017
1143	1-Pentadecanol	C15H32O	0.07088	0.0099	0.0011
1129	Isoheptanol	C7H16O	0.14817	0.0268	0.0036
2117	2,6-DiMth-4-C7OH	C9H20O	0.08539	0.0137	0.0016
1144	1-Hexadecanol	C16H34O	0.06797	0.0093	0.001
1145	Heptadecanol	C17H36O	0.06327	0.0086	0.0009
1199	Nonylphenol	C15H24O	0.0712	0.0098	0.001
1146	1-Octadecanol	C18H38O	0.06161	0.0082	0.0008
1135	2-Nonanol	C9H20O	0.09036	0.0127	0.0014
1149	1-Nonadecanol	C19H40O	0.05729	0.0073	0.0007
1139	Isodecanol	C10H22O	0.08864	0.0153	0.002
1148	1-Eicosanol	C20H42O	0.05251	0.0067	0.0007
2198	Dinonylphenol	C24H42O	0.08865	0.0136	0.0015
1159	Menthol	C10H20O	0.08846	0.0149	0.0019

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Amines

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1742	Ethyleneimine	C2H5N	0.50149	0.1164	0.0224
1745	Piperidine	C5H11N	0.10397	0.0148	0.0015
1766	Pyrrolidine	C4H9N	0.14368	0.0242	0.0032

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

1719	Isopropylamine	C3H9N	0.12575	0.0219	0.0031
1711	N-Propylamine	C3H9N	0.12607	0.0208	0.0026
1726	Sec-Butylamine	C4H11N	0.11299	0.0178	0.0021
1704	Ethylamine	C2H7N	0.14688	0.025	0.0033
1702	Dimethylamine	C2H7N	0.12178	0.0196	0.0025
1710	Diethylamine	C4H11N	0.08278	0.0107	0.001
1740	Allylamine	C3H7N	0.19278	0.0377	0.0058
1712	N-Butylamine	C4H11N	0.11525	0.0184	0.0023
1794	HexMthyleneimine	C6H13N	0.11269	0.017	0.0021
1729	Cyclohexylamine	C6H13N	0.08962	0.0137	0.0016
1714	Isobutylamine	C4H11N	0.13008	0.0217	0.0028
2853	Acetamide	C2H5NO	0.4001	0.0887	0.0166
2731	N-C1-CycC6-Amine	C7H15N	0.08361	0.0125	0.0014
1743	Diisopropylamine	C6H15N	0.13551	0.0162	0.0018
1796	N,N-DiMthAniline	C8H11N	0.04871	0.0049	0.0003
1792	Aniline	C6H7N	0.13602	0.0207	0.0024
1713	N-Pentylamine	C5H13N	0.10385	0.0162	0.0019
1733	Benzylamine	C7H9N	0.13242	0.0203	0.0024
1737	M-Toluidine	C7H9N	0.11555	0.0164	0.0018
3796	N-Ethylaniline	C8H11N	0.16083	0.0254	0.0032
1878	2-Methacrylamide	C4H7NO	0.10071	0.0162	0.002
1736	O-Toluidine	C7H9N	0.10721	0.0145	0.0015
2739	Diallylamine	C6H11N	0.09368	0.016	0.0022
2706	Hexylamine	C6H15N	0.10279	0.0157	0.0018
2724	O-Ethylaniline	C8H11N	0.06197	0.008	0.0008
1707	Dipropylamine	C6H15N	0.07525	0.0098	0.0009
1738	P-Toluidine	C7H9N	0.10738	0.0151	0.0016
1795	N-Methylaniline	C7H9N	0.20966	0.0349	0.0044
1718	Diisobutylamine	C8H19N	0.07932	0.0109	0.0011
1879	Acrylamide	C3H5NO	0.30368	0.0576	0.0104
2707	1-Aminoheptane	C7H17N	0.09654	0.0143	0.0016
2730	DiCycHexylAmine	C12H23N	0.16148	0.0207	0.002
2787	P-Aminodiphenyl	C12H11N	0.18729	0.0252	0.0022
1744	Dibutylamine	C8H19N	0.07656	0.0101	0.001
2708	1-Octylamine	C8H19N	0.09147	0.0138	0.0016
2791	2,6-DiEthAniline	C10H15N	0.03287	0.0043	0.0004
2709	1-Nonylamine	C9H21N	0.0891	0.0133	0.0015
2710	1-Decylamine	C10H23N	0.08068	0.0119	0.0014
3722	Diamylamine	C10H23N	0.07539	0.0114	0.0014
3724	Undecylamine	C11H25N	0.08091	0.0113	0.0012
2712	Dodecylamine	C12H27N	0.07636	0.011	0.0012
1720	Tetradecylamine	C14H31N	0.06836	0.0098	0.0011
2752	Piperazine	C4H10N2	0.17739	0.0329	0.0048
1752	Propylenediamine	C3H10N2	0.2043	0.0438	0.0076
1741	Ethylenediamine	C2H8N2	0.32814	0.0735	0.0134

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

2725	O-Aminoaniline	C6H8N2	0.12078	0.0171	0.0017
2750	P-Aminoaniline	C6H8N2	0.15213	0.023	0.0026
2727	M-Aminoaniline	C6H8N2	0.22928	0.0353	0.0037
1750	AEP	C6H15N3	0.16413	0.0316	0.0049
1732	Toluene Diamine	C7H10N2	0.13844	0.0205	0.0022
1731	hexamethyleneDiamine	C6H16N2	0.12559	0.0211	0.0025
3750	P-Benzidine	C12H12N2	0.23397	0.0375	0.0044

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Nitrilies

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1773	Propionitrile	C3H5N	0.19569	0.0331	0.0044
1782	Butyronitrile	C4H7N	0.13119	0.0211	0.0027
2720	Allyl Cyanide	C4H5N	0.14965	0.0266	0.0037
1783	Valeronitrile	C5H9N	0.10659	0.0162	0.0019
3874	Benzyl Cyanide	C8H7N	0.10518	0.0158	0.0017
1786	Hexanenitrile	C6H11N	0.0911	0.0138	0.0015
1776	Succinonitrile	C4H4N2	0.30941	0.0741	0.0151
1781	Glutaronitrile	C5H6N2	0.2436	0.0486	0.0076
2735	14-2Cyano-2-C4H8	C6H6N2	0.10363	0.0216	0.0038
1777	Adiponitrile	C6H8N2	0.17092	0.0356	0.0059

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Silanes

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
3985	Dimethyl Silane	C2H8Si	0.16322	0.0247	0.003
3984	Methyl Silane	CH6Si	0.14424	0.0208	0.0021
3986	Trimethyl Silane	C3H10Si	0.14229	0.0201	0.0021
1984	TetraMth Silane	C4H12Si	0.11233	0.0151	0.0015
2994	TETRAETHYL Si	C8H20Si	0.16386	0.0255	0.0028
1965	HexMthDisiloxane	C6H18OSi2	0.1321	0.0169	0.0015
1966	6C1Cyc3Siloxane	C6H18O3Si3	0.21024	0.0274	0.0024
1988	8C1Cyc4Siloxane	C8H24O4Si4	0.19124	0.0241	0.0021
3991	DecaMethcyclpenS	C10H30O5Si5	0.19332	0.0234	0.0016
3992	DodecaMethCyHexS	C12H36O6Si6	0.2131	0.0264	0.0019

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Imines

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1767	N-MthPyrrolidine	C5H11N	0.14819	0.0238	0.0029
2797	3-Methylpyridine	C6H7N	0.14203	0.0234	0.0031
1797	2-Methylpyridine	C6H7N	0.09805	0.0148	0.0018
2799	4-Methylpyridine	C6H7N	0.146	0.0243	0.0032
1753	N,N-DiEthAniline	C10H15N	0.17548	0.029	0.0036
1754	N-Methylpyrrole	C5H7N	0.45381	0.1015	0.0191
3740	Acridine	C13H9N	0.28547	0.038	0.0034

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Tert-N

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1703	Trimethylamine	C3H9N	0.14979	0.0208	0.0023
2856	DiMth Acetamide	C4H9NO	0.74982	0.1772	0.034
1706	Triethylamine	C6H15N	0.15218	0.023	0.0026
2716	Tributylamine	C12H27N	0.08622	0.0135	0.0016
2719	Tripropylamine	C9H21N	0.10888	0.0199	0.0029
3723	Triamylamine	C15H33N	0.04441	0.0062	0.0007

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Nitrate

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1761	Nitroethane	C2H5NO2	0.15199	0.0224	0.0026
1763	2-Nitropropane	C3H7NO2	0.12872	0.0192	0.0022
1762	1-Nitropropane	C3H7NO2	0.11192	0.0152	0.0015
1779	P-Nitrotoluene	C7H7NO2	0.16229	0.0299	0.005
1886	Nitrobenzene	C6H5NO2	0.17097	0.0328	0.0053
1778	O-Nitrotoluene	C7H7NO2	0.11809	0.0209	0.003
1780	M-Nitrotoluene	C7H7NO2	0.14368	0.026	0.0037
1891	O-Nitroanisole	C7H7NO3	0.24546	0.0478	0.0074
2740	M-Dinitrobenzene	C6H4N2O4	0.08225	0.015	0.0024

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

2742	P-Dinitrobenzene	C6H4N2O4	0.07767	0.0137	0.0021
2741	O-Dinitrobenzene	C6H4N2O4	0.11119	0.0203	0.0033
2749	3,5-DiNitToluene	C7H6N2O4	0.06536	0.0117	0.0016
2743	DNT	C7H6N2O4	0.06827	0.0111	0.0014
2745	3,4-DiNitToluene	C7H6N2O4	0.09549	0.0167	0.0022
2744	2,6-DiNitToluene	C7H6N2O4	0.03703	0.0053	0.0006
2748	2,5-DiNitToluene	C7H6N2O4	0.06785	0.011	0.0013
2746	1,3,5-TrinitroBz	C6H3N3O6	0.15122	0.0287	0.0055
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	0.05265	0.008	0.0009
2747	Trinitrotoluene	C7H5N3O6	0.01069	0.0011	0.0001

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Thiols

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1802	Ethyl Mercaptan	C2H6S	0.15322	0.026	0.0034
1820	Dimethyl Sulfide	C2H6S	0.1506	0.0229	0.0027
1843	Thiacyclopentane	C4H8S	0.21501	0.0358	0.0047
1803	1-Propanethiol	C3H8S	0.13612	0.0227	0.003
1805	Isobut Mercaptan	C4H10S	0.13977	0.0236	0.0032
6860	Ethylenedithiol	C2H6S2	0.1858	0.0381	0.0064
1811	Cyclohexanethiol	C6H12S	0.09905	0.0147	0.0017
1828	DiMth Disulfide	C2H6S2	0.07838	0.0125	0.0016
1841	Butanethiol	C4H10S	0.12481	0.0201	0.0026
1814	Methylproylsulf	C4H10S	0.11594	0.0186	0.0024
2816	ETHYLtBUTYL SUL	C6H14S	0.12725	0.0177	0.0019
1818	Diethyl Sulfide	C4H10S	0.15038	0.0216	0.0022
1812	Benzyl Mercaptan	C7H8S	0.12056	0.0179	0.0021
1838	T-OctylMercaptan	C8H18S	0.05425	0.0065	0.0006
1827	1-Pentanethiol	C5H12S	0.11557	0.0186	0.0024
2815	METHnBUTYL SULFD	C5H12S	0.11365	0.0166	0.0019
1824	DiethylDisulfide	C4H10S2	0.13244	0.0178	0.0018
1807	N-Hexylmercaptan	C6H14S	0.10745	0.0169	0.0021
6857	Dimercaptoethyl	C4H10OS2	0.12995	0.026	0.0043
1839	1-Heptanethiol	C7H16S	0.10085	0.0157	0.002
1829	DiProp Disulfide	C6H14S2	0.11068	0.0146	0.0013
1809	1-Octanethiol	C8H18S	0.09369	0.0143	0.0017
1808	N-Nonanethiol	C9H20S	0.08733	0.0133	0.0017
1826	1-Decanethiol	C10H22S	0.08234	0.0125	0.0015

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

2838	tertDodecanThiol	C12H26S	0.05224	0.0073	0.0008
1825	1-Undecanethiol	C11H24S	0.07669	0.0115	0.0014
1837	Dodecylthiol	C12H26S	0.07251	0.01	0.0011

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Aldehydes

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1037	Methacrolein	C4H6O	0.16339	0.0271	0.0034
1002	Acetaldehyde	C2H4O	0.28061	0.0472	0.0065
1003	Propionaldehyde	C3H6O	0.19435	0.0325	0.0042
1041	Benzaldehyde	C7H6O	0.14746	0.0212	0.0023
1034	Acrolein	C3H4O	0.29554	0.0543	0.0079
1005	N-Butyraldehyde	C4H8O	0.15265	0.0242	0.003
1036	Trans-2-Butenal	C4H6O	0.35366	0.0777	0.0139
1007	Valeraldehyde	C5H10O	0.13564	0.0215	0.0027
1006	Isobutyraldehyde	C4H8O	0.17006	0.0308	0.0044
1009	1-Hexanal	C6H12O	0.11986	0.0188	0.0024
1040	P-Tolualdehyde	C8H8O	0.14027	0.0218	0.0026
1016	2-Methylhexanal	C7H14O	0.11275	0.0186	0.0024
1017	3-Methylhexanal	C7H14O	0.11838	0.0188	0.0022
1008	1-Heptanal	C7H14O	0.11049	0.0169	0.002
1013	2-Ethylhexanal	C8H16O	0.09321	0.0149	0.0019
1010	1-Octanal	C8H16O	0.09785	0.0151	0.0018
1011	1-Nonanal	C9H18O	0.09226	0.0136	0.0017
1020	1-Decanal	C10H20O	0.08441	0.0124	0.0015
1021	1-Undecanal	C11H22O	0.07705	0.011	0.0014
1025	Dodecanal	C12H24O	0.07245	0.0104	0.0012
1026	1-Tridecanal	C13H26O	0.06745	0.0096	0.0011
1014	1,2-Ethanedione	C2H2O2	0.11182	0.0186	0.0024
1044	1,4BenzDicarboxAldehy	C8H6O2	0.12041	0.018	0.002

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Epoxides

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1440	ISOBUTYLENE OXID	C4H8O	0.39306	0.08	0.013

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

1479	Tetrahydrofuran	C4H8O	0.13297	0.0205	0.0024
1477	2,5-Dihydrofuran	C4H6O	0.2885	0.0618	0.0106
1408	1-Methoxypropane	C4H10O	0.10798	0.0137	0.0013
1411	2-Methoxypropane	C4H10O	0.13024	0.0177	0.0018
1421	1,4-Dioxane	C4H8O2	0.31182	0.0653	0.0108
2422	1,3-DIOXANE	C4H8O2	0.33671	0.0744	0.0135
1426	2-Methoxybutane	C5H12O	0.12126	0.0166	0.0017
1413	1-Methoxybutane	C5H12O	0.11425	0.0151	0.0015
1461	Methoxybenzene	C7H8O	0.16729	0.0232	0.0024
1448	1-Ethoxybutane	C6H14O	0.11863	0.0183	0.0022
1429	1-MethoxyPentane	C6H14O	0.1439	0.023	0.0029
6885	Ethyl-3-Ethoxypr	C7H14O3	0.11344	0.0185	0.0024

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Ether

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1401	Dimethyl Ether	C2H6O	0.10869	0.0131	0.0011
1407	MethylEthylEther	C3H8O	0.19581	0.0348	0.005
1470	VinylMethylEther	C3H6O	0.14012	0.0209	0.0023
1405	MTBE	C5H12O	0.15451	0.022	0.0023
1445	VinylEthyl Ether	C4H8O	0.19338	0.0352	0.0051
1402	Diethyl Ether	C4H10O	0.14561	0.023	0.0029
1431	Methylal	C3H8O2	0.11399	0.014	0.0013
1428	T-But EthylEther	C6H14O	0.14373	0.0233	0.0029
1427	TAME	C6H14O	0.16018	0.023	0.0025
1410	Mth Isobut Ether	C5H12O	0.11904	0.0162	0.0016
1430	Eth-t-Pent-Ether	C7H16O	0.13524	0.0211	0.0025
1403	DiisopropylEther	C6H14O	0.12899	0.0202	0.0023
1415	Eth Propyl Ether	C5H12O	0.12867	0.0194	0.0024
1455	Dimethyl Acetal	C4H10O2	0.31152	0.0657	0.0113
1446	Dipropyl Ether	C6H14O	0.11237	0.0166	0.0019
1447	Butyl VinylEther	C6H12O	0.13868	0.0245	0.0035
1462	EthylPhenylEther	C8H10O	0.13753	0.0207	0.0024
1406	Di-sec-But Ether	C8H18O	0.10669	0.0164	0.002
1432	Acetal	C6H14O2	0.13341	0.0221	0.0028
1460	BenzylEthylEther	C9H12O	0.10507	0.0177	0.0023
1050	Paraldehyde	C6H12O3	0.15199	0.0317	0.0055
1404	Di-n-Butyl Ether	C8H18O	0.09945	0.015	0.0017
1420	Anethole	C10H12O	0.17098	0.0237	0.0024

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

1456	DimethylCarbitol	C6H14O3	0.21388	0.0367	0.0049
1463	Dibenzyl Ether	C14H14O	0.06609	0.0114	0.0015
1425	Di-n-PentylEther	C10H22O	0.09123	0.0134	0.0014
1458	Diethyl Carbitol	C8H18O3	0.12791	0.0234	0.0032
1412	Dihexyl Ether	C12H26O	0.0811	0.013	0.0016
1454	Triglyme	C8H18O4	0.16687	0.0316	0.0048
1459	Dibutyl Carbitol	C12H26O3	0.07638	0.0116	0.0012
1424	Di-n-Octyl Ether	C16H34O	0.0591	0.0093	0.0012
1457	Tetraglyme	C10H22O5	0.13816	0.0298	0.005
1418	Dinonyl Ether	C18H38O	0.05706	0.0089	0.0011
2432	ETHYLAL	C5H12O2	0.13921	0.0225	0.0028
2405	DIISOBUTYL ETHER	C8H18O	0.11296	0.0178	0.0022
2456	Ethyl Glyme	C6H14O2	0.15058	0.0275	0.0041
2417	ETHYLHEXYL ETHER	C8H18O	0.10686	0.0171	0.0022
2415	ETHYLISOPROPETH	C5H12O	0.14087	0.0227	0.0028

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Formate

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1301	Methyl Formate	C2H4O2	0.18943	0.0356	0.0054
1311	Vinyl Formate	C3H4O2	0.12319	0.0235	0.0036
1302	Ethyl Formate	C3H6O2	0.12537	0.0207	0.0027
2306	t-Butyl Formate	C5H10O2	0.09443	0.0142	0.0016
1303	Propyl Formate	C4H8O2	0.10467	0.0168	0.0022
2305	sec-ButylFormate	C5H10O2	0.09165	0.0145	0.0018
2311	CYCLOHEXL FORMAT	C7H12O2	0.08262	0.0125	0.0015
1304	N-Butyl Formate	C5H10O2	0.09142	0.0141	0.0017
1305	Isobutyl Formate	C5H10O2	0.10347	0.0169	0.002
2350	Benzyl Formate	C8H8O2	0.0997	0.0145	0.0016
2307	n-Hexyl Formate	C7H14O2	0.07941	0.0124	0.0015
1306	N-Pentyl Formate	C6H12O2	0.08647	0.013	0.0016
2308	n-Heptyl Formate	C8H16O2	0.07667	0.0109	0.0011
1308	N-Octyl Formate	C9H18O2	0.07172	0.0095	0.0009
1309	n-Nonyl Formate	C10H20O2	0.0611	0.0089	0.0009
1310	n-Decyl Formate	C11H22O2	0.05913	0.0087	0.0009

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Ester

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1351	Mth Methacrylate	C5H8O2	0.1332	0.0189	0.0021
1312	Methyl Acetate	C3H6O2	0.17375	0.0252	0.0027
1331	Vinyl Propionate	C5H8O2	0.1172	0.0206	0.0029
1321	Vinyl Acetate	C4H6O2	0.13079	0.0188	0.002
1352	Eth MthAcrylate	C6H10O2	0.09731	0.0151	0.0018
1322	MethylPropionate	C4H8O2	0.13883	0.0193	0.002
1341	Methyl Acrylate	C4H6O2	0.2134	0.04	0.006
1313	Ethyl Acetate	C4H8O2	0.1569	0.0278	0.0039
1319	IsopropylAcetate	C5H10O2	0.11129	0.0146	0.0014
1332	Methyl Butyrate	C5H10O2	0.1303	0.0218	0.0029
1342	Ethyl Acrylate	C5H8O2	0.14402	0.0255	0.0035
1318	Allyl Acetate	C5H8O2	0.14158	0.0192	0.0018
1314	N-Propyl Acetate	C5H10O2	0.11797	0.0157	0.0016
1323	Ethyl Propionate	C5H10O2	0.1192	0.0196	0.0026
1360	I-But I-Butyrate	C8H16O2	0.09565	0.0123	0.0012
1320	Sec-ButylAcetate	C6H12O2	0.10216	0.0134	0.0012
1336	PropylI-Butyrate	C7H14O2	0.10496	0.0171	0.0022
1353	N-C3-Mthacrylate	C7H12O2	0.09004	0.014	0.0018
1333	Ethyl Butyrate	C6H12O2	0.09787	0.0142	0.0015
1347	EthylIsovalerate	C7H14O2	0.09121	0.0143	0.0017
1315	N-Butyl Acetate	C6H12O2	0.11298	0.015	0.0015
1390	Methyl Benzoate	C8H8O2	0.15824	0.0206	0.002
1388	ISOBUTYL MTHACR	C8H14O2	0.09457	0.0143	0.0017
1343	1-PropylAcrylate	C6H10O2	0.09707	0.0166	0.0023
1316	Isobutyl Acetate	C6H12O2	0.11696	0.016	0.0016
1344	N-Butyl Acrylate	C7H12O2	0.07994	0.012	0.0013
1357	Pentyl Acetate	C7H14O2	0.10595	0.0135	0.0013
1327	N-PropN-Butyrate	C7H14O2	0.08447	0.0124	0.0014
1324	N-PropPropionate	C6H12O2	0.10058	0.0157	0.0019
1291	Acetic Anhydride	C4H6O3	0.18052	0.0279	0.0033
1389	N-ButMthacrylate	C8H14O2	0.08719	0.0136	0.0017
1359	Benzyl Acetate	C9H10O2	0.12494	0.0191	0.0022
1326	N-But Propionate	C7H14O2	0.08909	0.0139	0.0017
1391	Ethyl Benzoate	C9H10O2	0.11741	0.0163	0.0016
1897	CH3OC3H600CH3	C6H12O3	0.14599	0.0209	0.0022
1392	DiethylCarbonate	C5H10O3	0.14205	0.0238	0.0035
1385	N-But N-Butyrate	C8H16O2	0.07799	0.011	0.0012
1317	IsopentylAcetate	C7H14O2	0.11799	0.0151	0.0015
1363	N-Hexyl Acetate	C8H16O2	0.10294	0.016	0.0019
1387	Ethylene Acetate	C6H10O4	0.19757	0.0315	0.0047
1393	Diethyl Oxalate	C6H10O4	0.12039	0.0217	0.0032
1365	Butyl Benzoate	C11H14O2	0.10118	0.0142	0.0014
1361	I-C5 I-Valerate	C10H20O2	0.08133	0.0113	0.0011
1367	Heptyl Acetate	C9H18O2	0.09674	0.0151	0.0018

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

1346	N-Butyl Valerate	C9H18O2	0.07327	0.0111	0.0013
1358	2-C2-C6 Acetate	C10H20O2	0.09385	0.0119	0.0011
1394	Diethyl Malonate	C7H12O4	0.10516	0.0183	0.0025
1292	Propionyl Oxide	C6H10O3	0.09563	0.0146	0.0017
1364	Benzyl Benzoate	C14H12O2	0.0879	0.0113	0.0013
1381	2Mth p-Phthalate	C10H10O4	0.20534	0.024	0.0016
1368	n-Octyl Acetate	C10H20O2	0.08718	0.0134	0.0016
1377	DiMthI-Phthalate	C10H10O4	0.13031	0.0147	0.0012
1896	Ethylene DiAcr	C8H10O4	0.12228	0.0233	0.0034
1386	2-Ethylhexyl Acr	C11H20O2	0.07026	0.0106	0.0011
1395	Methyl Decanoate	C11H22O2	0.07426	0.0112	0.0013
1369	n-Nonyl Acetate	C11H22O2	0.07277	0.0112	0.0013
1370	n-Decyl Acetate	C12H24O2	0.07328	0.0107	0.0013
1345	N-ButylNonanoate	C13H26O2	0.04283	0.0042	0.0003
1375	DiProp Phthalate	C14H18O4	0.0665	0.0081	0.0007
1376	Diisobutyl Phtha	C16H22O4	0.04718	0.006	0.0006
1396	IsopropMyristate	C17H34O2	0.05931	0.0084	0.0009
1383	Butyl Stearate	C22H44O2	0.02007	0.0022	0.0002
1362	Methyl Oleate	C19H36O2	0.03675	0.0054	0.0006
1355	Diisooctyl Phtha	C24H38O4	0.04637	0.0057	0.0005
1382	DioctylTerephtha	C24H38O4	0.04151	0.0049	0.0004
1384	DIBUTYL SEBACATE	C18H34O4	0.02989	0.0044	0.0005
1371	Diisodecyl Phtha	C28H46O4	0.04921	0.0049	0.0003
1354	DioctylPhthalate	C24H38O4	0.02101	0.0023	0.0002
2375	DiethylPhthalate	C12H14O4	0.06137	0.008	0.0008
2388	Dipropyl Maleate	C10H16O4	0.07376	0.0127	0.0018
2381	Diallyl Maleate	C10H12O4	0.03994	0.0073	0.0011
2370	Glyceryl Triacet	C9H14O6	0.13736	0.0206	0.0023
2382	Dibutyl Maleate	C12H20O4	0.06338	0.0109	0.0015
2376	DibutylPhthalate	C16H22O4	0.05697	0.0071	0.0006
2353	CetylMthacrylate	C20H38O2	0.05394	0.0074	0.0007
2379	Dihexyl Adipate	C18H34O4	0.02888	0.004	0.0004
2321	T-Butyl Acetate	C6H12O2	0.10309	0.0165	0.0022
2332	Methl.I-butyrate	C5H10O2	0.15665	0.0269	0.0037
2354	AllylMthacrylate	C7H10O2	0.09501	0.0162	0.0023
2364	CYCLOHEXL ACETAT	C8H14O2	0.09957	0.0157	0.0019
2337	EthylIsobutyrate	C6H12O2	0.11138	0.0171	0.002
2384	IsobutylAcrylate	C7H12O2	0.11205	0.0189	0.0025
2380	1,1-Diacetoxy C2	C6H10O4	0.13761	0.0247	0.0036
2392	n-PropylBenzoate	C10H12O2	0.10526	0.0139	0.0014
2377	DiMth Phthalate	C10H10O4	0.18945	0.0252	0.0022
2386	Diethyl Maleate	C8H12O4	0.11772	0.0205	0.0027
2385	Mth Dodecanoate	C13H26O2	0.06868	0.01	0.0011
3379	Dioctyl Adipate	C22H42O4	0.07187	0.0079	0.0005
5886	Mth Acetoacetate	C5H8O3	0.17919	0.034	0.0053

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

5884	Ethoxy Acetate	C6H12O3	0.16217	0.0261	0.0033
5887	EthAcetoAcetate	C6H10O3	0.11958	0.0201	0.0025
5885	Carbitol Acetate	C8H16O4	0.14931	0.0237	0.0027

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

	Ketone				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1096	Methyl Isopropen	C5H8O	0.13404	0.0208	0.0025
1079	Cyclopentanone	C5H8O	0.19952	0.0327	0.0041
1051	Acetone	C3H6O	0.2183	0.0362	0.0046
1052	MEK	C4H8O	0.15969	0.0247	0.0029
1065	Mesityl Oxide	C6H10O	0.17214	0.0274	0.0033
1066	T-But Mth Ketone	C6H12O	0.12168	0.0177	0.002
1060	2-Pentanone	C5H10O	0.12691	0.0189	0.0021
1061	Mth iC3 Ketone	C5H10O	0.14451	0.0221	0.0025
1053	Diethyl Ketone	C5H10O	0.13798	0.0199	0.002
1059	3-Hexanone	C6H12O	0.1166	0.0163	0.0018
1099	Diketene	C4H4O2	0.40941	0.1039	0.0216
1055	Sec-ButMthKetone	C6H12O	0.12298	0.0184	0.002
1054	MIBK	C6H12O	0.11817	0.0172	0.002
1095	EthIsopropKetone	C6H12O	0.12247	0.0183	0.002
1063	2-Heptanone	C7H14O	0.10829	0.0157	0.0018
1064	5-Mth-2-Hexanone	C7H14O	0.12204	0.0185	0.0022
1058	4-Heptanone	C7H14O	0.10086	0.0134	0.0013
1057	3-Heptanone	C7H14O	0.10892	0.0158	0.0018
1076	2,4-Pentanedione	C5H8O2	0.08551	0.0079	0.0005
1068	DiisobutylKetone	C9H18O	0.09085	0.0125	0.0013
1097	2-CycC6 CycC6one	C12H20O	0.08537	0.0123	0.0016
1083	2-Octanone	C8H16O	0.10055	0.0146	0.0016
1073	Dibutyl Ketone	C9H18O	0.09335	0.0127	0.0013
1062	2-Hexanone	C6H12O	0.1172	0.0171	0.0019
1077	Isophorone	C9H14O	0.22573	0.0361	0.0041
1090	Acetophenone	C8H8O	0.14784	0.0211	0.0022
1080	Cyclohexanone	C6H10O	0.17581	0.0271	0.0032
1074	2-Nonanone	C9H18O	0.09472	0.0138	0.0015

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Alcohol-Ethers

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
2862	2-Butoxyethanol	C6H14O2	0.13505	0.0194	0.002
4857	butyl carbitol	C8H18O3	0.12496	0.0189	0.0023
2898	2-Chloroethanol	C2H5ClO	0.24843	0.0394	0.004
2864	Carbitol	C6H14O3	0.18705	0.0317	0.004
3854	Methyl propasol	C4H10O2	0.15354	0.0188	0.0014
2860	2-Methoxyethanol	C3H8O2	0.27752	0.0387	0.0037
2854	DiacetoneAlcohol	C6H12O2	0.10608	0.0133	0.001
2861	2-Ethoxyethanol	C4H10O2	0.2064	0.0296	0.003
2889	HydroxyAcetone	C3H6O2	0.26911	0.0395	0.0037
3856	1tButoxy2Propnol	C7H16O2	0.07441	0.0111	0.0012
3858	PROPGLYC2tBUTYL	C7H16O2	0.09273	0.0147	0.0017
4855	2-Propoxyethanol	C5H12O2	0.15554	0.0208	0.0021
4849	Acetovanillone	C9H10O3	0.16394	0.0232	0.0023
5883	Ethyl Lactate	C5H10O3	0.09519	0.0112	0.0007
6883	2-HydroxyEth Acr	C5H8O3	0.3255	0.0735	0.0124
2863	Methyl Carbitol	C5H12O3	0.27727	0.052	0.007
3855	Dowanol DPM	C7H16O3	0.072	0.0085	0.0006
3857	TriPropGlymEthlE	C10H22O4	0.04633	0.0072	0.0008

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Hydrocarbons

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
404	DiMth-Acetylene	C4H6	0.22746	0.0343	0.0038
202	Propylene	C3H6	0.09146	0.0119	0.0012
412	2-Pentyne	C5H8	0.03103	0.0026	0.0002
207	2-Methylpropene	C4H8	0.11639	0.0168	0.0019
204	1-Butene	C4H8	0.10659	0.0149	0.0016
205	Cis-2-Butene	C4H8	0.14669	0.0231	0.0028
402	Propyne	C3H4	0.17035	0.0303	0.0042
406	3-Hexyne	C6H10	0.17953	0.0251	0.0025
206	Trans-2-Butene	C4H8	0.13293	0.0199	0.0023
407	2-Hexyne	C6H10	0.19619	0.0283	0.0031
231	33-2Mth-1-Butene	C6H12	0.06678	0.0074	0.0006
230	23-2Mth-1-Butene	C6H12	0.10893	0.0143	0.0014
229	2-Ethyl-1-Butene	C6H12	0.12144	0.0188	0.0022
8	I-Pentane	C5H12	0.12933	0.018	0.0019

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

14	2,2-DiMth-Butane	C6H14	0.13663	0.0192	0.0021
232	23-2Mth-2-Butene	C6H12	0.1489	0.023	0.0027
213	3-Mth-1-Butene	C5H10	0.13154	0.0197	0.0023
212	2-Mth-1-Butene	C5H10	0.12412	0.0189	0.0022
211	Trans-2-Pentene	C5H10	0.12924	0.0199	0.0024
210	Cis-2-Pentene	C5H10	0.13117	0.0204	0.0025
223	4-Mth-1-Pentene	C6H12	0.12719	0.0192	0.0023
221	2-Mth-1-Pentene	C6H12	0.11302	0.0169	0.002
248	2-t-Butylpropene	C7H14	0.15194	0.0244	0.0031
227	Cs-4-Mth-2-C5H10	C6H12	0.13174	0.0206	0.0026
224	2-Mth-2-Pentene	C6H12	0.15564	0.0236	0.0027
403	1-Butyne	C4H6	0.13159	0.0218	0.0029
15	2,3-DiMth-Butane	C6H14	0.18337	0.0288	0.0035
214	2-Mth-2-Butene	C5H10	0.17642	0.0267	0.0031
228	Ts-4-Mth-2-C5H10	C6H12	0.14081	0.0227	0.0029
225	Cs-3-Mth-2-C5H10	C6H12	0.15758	0.0236	0.0027
218	Trans-2-Hexene	C6H12	0.12051	0.0185	0.0022
2226	3-METH-Tr-2Pente	C6H12	0.17037	0.0265	0.0032
222	3-Mth-1-Pentene	C6H12	0.12773	0.0191	0.0022
257	2-Diisobutylene	C8H16	0.16409	0.0258	0.0032
256	1-Diisobutylene	C8H16	0.12315	0.0185	0.0022
217	Cis-2-Hexene	C6H12	0.12357	0.019	0.0022
2414	1-Heptyne	C7H12	0.10657	0.0163	0.0019
13	3-Methylpentane	C6H14	0.13966	0.0206	0.0023
219	Cis-3-Hexene	C6H12	0.15187	0.0225	0.0025
12	2-Methylpentane	C6H14	0.12753	0.0184	0.002
220	Trans-3-Hexene	C6H12	0.1553	0.0234	0.0027
405	1-Pentyne	C5H8	0.11809	0.0182	0.0022
209	1-Pentene	C5H10	0.1085	0.0155	0.0017
11	N-Hexane	C6H14	0.10912	0.015	0.0016
235	Cis-2-Heptene	C7H14	0.11689	0.0174	0.002
249	Cis-3-Heptene	C7H14	0.1104	0.0161	0.0018
216	1-Hexene	C6H12	0.10859	0.016	0.0018
239	3-Eth-1-Pentene	C7H14	0.11791	0.0185	0.0023
226	4-Mth-1-Hexene	C7H14	0.12699	0.0203	0.0025
240	3-Mth-1-Hexene	C7H14	0.11725	0.0183	0.0023
419	3-Mth-1-Butyne	C5H8	0.13616	0.022	0.0029
233	2-Eth-1-Pentene	C7H14	0.11433	0.017	0.002
238	2-Mth-1-Hexene	C7H14	0.1082	0.0161	0.0018
416	1-Octyne	C8H14	0.10029	0.0154	0.0018
289	2,3Dimeth Hexene	C8H16	0.11286	0.0176	0.0021
234	1-Heptene	C7H14	0.10568	0.0156	0.0018
413	1-Hexyne	C6H10	0.11135	0.0171	0.0021
237	Trans-3-Heptene	C7H14	0.10804	0.0161	0.0018
236	Trans-2-Heptene	C7H14	0.11556	0.0173	0.002

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

251	Trans-2-Octene	C8H16	0.10837	0.0158	0.0018
279	Trans-4-Octene	C8H16	0.10142	0.0146	0.0016
277	Trans-3-Octene	C8H16	0.10413	0.015	0.0017
2252	2Methl-1-Heptene	C8H16	0.10178	0.0147	0.0016
250	1-Octene	C8H16	0.10112	0.015	0.0017
258	2-Ethyl-1-Hexene	C8H16	0.10412	0.0154	0.0017
280	3-Octene	C8H16	0.10277	0.0148	0.0016
278	4-Octene	C8H16	0.10252	0.0148	0.0016
276	2-Octene	C8H16	0.11	0.0161	0.0018
259	1-Nonene	C9H18	0.09677	0.0144	0.0017
262	1-Dodecene	C12H24	0.08383	0.0124	0.0014
263	1-Tridecene	C13H26	0.07963	0.0117	0.0014
264	1-Tetradecene	C14H28	0.07614	0.0111	0.0013
265	1-Pentadecene	C15H30	0.07266	0.0105	0.0012
266	1-Hexadecene	C16H32	0.06944	0.01	0.0011
267	1-Octadecene	C18H36	0.06251	0.0088	0.001
281	1-Heptadecene	C17H34	0.06573	0.0092	0.001
284	1-Eicosene	C20H40	0.05771	0.0081	0.0009
283	1-Nonadecene	C19H38	0.05991	0.0084	0.001
3	Propane	C3H8	0.06661	0.0072	0.0006
4	I-Butane	C4H10	0.10758	0.0139	0.0014
9	Neopentane	C5H12	0.10825	0.0137	0.0012
5	N-Butane	C4H10	0.09131	0.0112	0.001
7	pentane	C5H12	0.10404	0.0138	0.0014
44	Hexamethylethane	C8H18	0.23196	0.0395	0.0052
25	223-TriMthButane	C7H16	0.19912	0.0317	0.0039
24	3,3-DiMthPentane	C7H16	0.15645	0.0232	0.0026
51	2,2,3,3-4Mth-C5	C9H20	0.24856	0.0431	0.0058
21	2,2-DiMthPentane	C7H16	0.12914	0.0184	0.002
42	2,3,3-TriMth-C5	C8H18	0.2097	0.0344	0.0044
22	2,3-DiMthPentane	C7H16	0.17935	0.0288	0.0036
40	2,2,3-TriMth-C5	C8H18	0.18602	0.0298	0.0037
23	2,4-DiMthPentane	C7H16	0.1389	0.0208	0.0024
41	2,2,4-TriMth-C5	C8H18	0.1411	0.0208	0.0024
39	3-Mth-3-Eth-C5	C8H18	0.16506	0.0251	0.0029
20	3-Ethylpentane	C7H16	0.13673	0.0204	0.0023
52	2,2,3,4-4Mth-C5	C9H20	0.21535	0.0363	0.0048
54	2334TetrMethPent	C9H20	0.26251	0.0467	0.0066
53	2,2,4,4-4Mth-C5	C9H20	0.16343	0.025	0.0029
43	2,3,4-TriMth-C5	C8H18	0.20901	0.0354	0.0047
36	3,3-DiMth-Hexane	C8H18	0.14045	0.0207	0.0024
19	3-Methylhexane	C7H16	0.1308	0.0195	0.0022
18	2-Methylhexane	C7H16	0.12422	0.0182	0.002
38	2-Mth-3-Eth-C5	C8H18	0.15855	0.0249	0.003
190	2,2-2C1-3-C2-C5	C9H20	0.16271	0.0259	0.0032

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

32	2,2-DiMth-Hexane	C8H18	0.12254	0.0178	0.002
37	3,4-DiMth-Hexane	C8H18	0.1669	0.0267	0.0033
50	3,3-DiEthPentane	C9H20	0.16298	0.0247	0.0028
34	2,4-DiMth-Hexane	C8H18	0.13267	0.0201	0.0024
33	2,3-DiMth-Hexane	C8H18	0.15817	0.0251	0.0031
17	N-Heptane	C7H16	0.11005	0.0156	0.0017
49	244TriMethHexane	C9H20	0.15063	0.0229	0.0027
192	2,4-2C1-3-C2-C5	C9H20	0.17788	0.0292	0.0037
47	2,2,5-TriMth-C6	C9H20	0.12766	0.0189	0.0022
35	2,5-DiMth-Hexane	C8H18	0.13402	0.0203	0.0024
31	3-Ethylhexane	C8H18	0.1235	0.0182	0.0021
30	4-Methylheptane	C8H18	0.1208	0.0178	0.002
29	3-Methylheptane	C8H18	0.12506	0.0186	0.0021
28	2-Methylheptane	C8H18	0.12062	0.0178	0.002
96	2,2-DiMthHeptane	C9H20	0.11754	0.0168	0.0019
176	2,6-DiMthHeptane	C9H20	0.12575	0.0195	0.0023
27	N-Octane	C8H18	0.10893	0.0157	0.0017
94	3-Ethylheptane	C9H20	0.11534	0.017	0.0019
92	3-Methyloctane	C9H20	0.11889	0.0177	0.002
93	4-Methyloctane	C9H20	0.11407	0.0167	0.0019
91	2-Methyloctane	C9H20	0.1163	0.0174	0.002
72	2,2-DiMthOctane	C10H22	0.11168	0.0165	0.0018
2095	2,3Dimethloctane	C10H22	0.13557	0.021	0.0025
2096	2,4Dimethloctane	C10H22	0.11079	0.0167	0.002
2098	2,6DimethlOctane	C10H22	0.12344	0.0191	0.0023
2097	2,5Dimethloctane	C10H22	0.11811	0.0178	0.0021
2099	2,7DimethlOctane	C10H22	0.12242	0.0187	0.0022
46	N-Nonane	C9H20	0.10578	0.0154	0.0017
88	5-Methylnonane	C10H22	0.1063	0.0154	0.0018
85	3-Methylnonane	C10H22	0.11537	0.0172	0.002
87	4-Methylnonane	C10H22	0.10776	0.0159	0.0018
86	2-Methylnonane	C10H22	0.11244	0.0168	0.002
56	N-Decane	C10H22	0.10298	0.0151	0.0017
63	N-Undecane	C11H24	0.09881	0.0144	0.0016
64	N-Dodecane	C12H26	0.09504	0.0139	0.0016
65	N-Tridecane	C13H28	0.09055	0.0133	0.0015
66	N-Tetradecane	C14H30	0.08693	0.0127	0.0014
67	N-Pentadecane	C15H32	0.08327	0.0122	0.0014
68	N-Hexadecane	C16H34	0.07967	0.0115	0.0013
69	N-Heptadecane	C17H36	0.07681	0.0112	0.0013
70	N-Octadecane	C18H38	0.0723	0.0105	0.0012
71	N-Nonadecane	C19H40	0.06917	0.0099	0.0011
73	N-Eicosane	C20H42	0.0671	0.0096	0.001
74	n-HENEICOSANE	C21H44	0.06416	0.009	0.001
75	n-DOCOSANE	C22H46	0.06116	0.0084	0.0009

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

76	n-TRICOSANE	C23H48	0.05806	0.0082	0.0009
77	n-Tetracosane	C24H50	0.05557	0.0079	0.0008
78	n-PENTACOSANE	C25H52	0.05339	0.0074	0.0008
79	n-HEXACOSANE	C26H54	0.0511	0.0071	0.0008
81	n-Octacosane	C28H58	0.04585	0.0064	0.0007
2081	n-TRICONTANE	C30H62	0.04423	0.0059	0.0006
2082	n-Dotriacontane	C32H66	0.04012	0.0053	0.0005
2086	Hexatriacontane	C36H74	0.03486	0.0044	0.0004

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Cyclic Hydrocarbons

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
269	Cyclopentene	C5H8	0.10773	0.0165	0.002
270	Cyclohexene	C6H10	0.11767	0.0185	0.0023
287	3MthCyclopentene	C6H10	0.11357	0.0184	0.0023
286	1-MthCyclPentene	C6H10	0.12889	0.0195	0.0022
288	4MthCyclopenten	C6H10	0.11785	0.0192	0.0024
273	Cycloheptene	C7H12	0.11489	0.0182	0.0022
274	Cyclooctene	C8H14	0.10921	0.0173	0.0021
101	Cyclopropane	C3H6	0.07005	0.0084	0.0007
810	ADAMANTANE	C10H16	0.12724	0.0184	0.002
102	Cyclobutane	C4H8	0.09939	0.0133	0.0013
104	Cyclopentane	C5H10	0.10451	0.0146	0.0015
137	Cyclohexane	C6H12	0.1015	0.0141	0.0015
105	MthCyclopentane	C6H12	0.12378	0.0183	0.002
146	Cs-1,4-2C1-CycC6	C8H16	0.14367	0.0218	0.0026
142	Cs-1,2-2C1-CycC6	C8H16	0.16405	0.0258	0.0032
141	1,1-2C1-CycC6	C8H16	0.10913	0.0153	0.0017
145	Ts-1,3-2C1-CycC6	C8H16	0.14426	0.0221	0.0026
144	Cs-1,3-2C1-CycC6	C8H16	0.12967	0.019	0.0022
147	Ts-1,4-2C1-CycC6	C8H16	0.12679	0.0183	0.002
143	Ts-1,2-2C1-CycC6	C8H16	0.14099	0.0209	0.0024
138	MthCyclohexane	C7H14	0.11472	0.0163	0.0018
159	Cycloheptane	C7H14	0.12465	0.0183	0.0021
140	Ethylcyclohexane	C8H16	0.11945	0.0174	0.0019
154	Trans-Decalin	C10H18	0.10652	0.0155	0.0018
149	N-PropylCyc-C6	C9H18	0.11216	0.0163	0.0018
109	Cs-1,2-2C1-CycC5	C7H14	0.16812	0.0272	0.0035
110	Ts-1,2-2C1-CycC5	C7H14	0.13739	0.021	0.0025

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

112	Ts-1,3-2C1-CycC5	C7H14	0.13881	0.021	0.0025
107	Eth-Cyclopentane	C7H14	0.12315	0.0183	0.0021
114	N-PropCycPentane	C8H16	0.11707	0.0175	0.002
108	1,1-DiMthCycC5	C7H14	0.10342	0.0148	0.0017
111	Cs-1,3-2C1-CycC5	C7H14	0.13603	0.0206	0.0024
152	N-ButylCycHexane	C10H20	0.10779	0.0157	0.0018
160	Cyclooctane	C8H16	0.13453	0.0202	0.0023
153	Cis-Decalin	C10H18	0.1292	0.0199	0.0025
115	Isopropylcyclopentane	C8H16	0.15172	0.0238	0.0029
150	Isopropyl-CycC6	C9H18	0.14852	0.0231	0.0028
116	1-C1-1-C2-CycC5	C8H16	0.13426	0.0202	0.0024
122	Butylcyclpentane	C9H18	0.11111	0.0167	0.002
155	1,1-Bicyclohexyl	C12H22	0.11039	0.0163	0.0019
158	N-Decylcyclo-C6	C16H32	0.08499	0.0122	0.0014

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Aromatic Hydrocarbons

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
307	1,4-Pentadiene	C5H8	0.12425	0.0203	0.0026
306	1-ts3-Pentadiene	C5H8	0.19491	0.036	0.0053
414	2-Methyl-1-Butenyne	C5H6	0.1295	0.0198	0.0024
305	Cs1,3-Pentadiene	C5H8	0.20617	0.0391	0.006
309	Isoprene	C5H8	0.17529	0.0311	0.0044
421	1-Pentene-4-yne	C5H6	0.15688	0.0256	0.0033
303	1,3-Butadiene	C4H6	0.16905	0.0292	0.0041
332	1,4-CyclHexadien	C6H8	0.14489	0.0285	0.0045
501	Benzene	C6H6	0.17852	0.0309	0.0043
315	Cyclopentadiene	C5H6	0.11945	0.0179	0.0019
319	Diisopropenyl	C6H10	0.17438	0.0314	0.0046
615	Ethynylbezene	C8H6	0.09794	0.0123	0.0011
601	Styrene	C8H8	0.11978	0.0165	0.0018
331	1,3-CycHexadiene	C6H8	0.12118	0.0209	0.0029
310	1,5-Hexadiene	C6H10	0.11356	0.0175	0.0021
312	MthCycPentadiene	C6H8	0.13486	0.0228	0.003
420	1-Pentene-3-yne	C5H6	0.27905	0.0428	0.0052
502	Toluene	C7H8	0.14981	0.0239	0.003
521	T-Butylbenzene	C10H14	0.10183	0.0128	0.0012
320	Dipropylene	C6H10	0.20673	0.0395	0.0061
520	Sec-Butylbenzene	C10H14	0.12765	0.0189	0.0023

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

313	1,4-Hexadiene	C6H10	0.13081	0.0215	0.0028
314	Dipropylene	C6H10	0.19916	0.0378	0.006
316	DiCycPentadiene	C10H12	0.08407	0.0148	0.0021
333	1,5-CycOctadiene	C8H12	0.12465	0.0225	0.0033
701	Naphthalene	C10H8	0.1398	0.017	0.0015
504	Ethylbenzene	C8H10	0.10448	0.0162	0.002
820	Indan	C9H10	0.06298	0.0093	0.0011
505	O-Xylene	C8H10	0.15061	0.0239	0.003
612	P-Methylstyrene	C9H10	0.11442	0.0156	0.0016
330	DIISOCROTYL	C8H14	0.26206	0.0482	0.0072
507	P-Xylene	C8H10	0.13005	0.0197	0.0023
329	DIISOBUTENYL	C8H14	0.10117	0.016	0.002
506	M-Xylene	C8H10	0.13265	0.0204	0.0024
603	Methylstyrene	C9H10	0.11324	0.0156	0.0016
613	Alpha-MthStyrene	C9H10	0.10902	0.0149	0.0015
510	Isopropylbenzene	C9H12	0.1485	0.0233	0.0029
724	2-Methylindene	C10H10	0.08361	0.0108	0.0011
285	Vinylcyclohexene	C8H12	0.11354	0.0183	0.0024
803	Indene	C9H8	0.09398	0.0097	0.0008
706	Tetralin	C10H12	0.06773	0.0102	0.0012
511	O-Ethyltoluene	C9H12	0.10019	0.0152	0.0018
723	1-Methylindene	C10H10	0.15125	0.0291	0.0046
738	Fluorene	C13H10	0.11749	0.0134	0.0011
619	Tr-1PropenylBz	C9H10	0.13742	0.0203	0.0023
525	O-Diethylbenzene	C10H14	0.06464	0.0093	0.001
618	Propenyl Bz(cis)	C9H10	0.13924	0.02	0.0021
602	O-Methylstyrene	C9H10	0.10925	0.0152	0.0016
702	1-MthNaphthalene	C11H10	0.1504	0.0192	0.0017
509	N-Propylbenzene	C9H12	0.09156	0.0137	0.0016
526	M-Diethylbenzene	C10H14	0.06167	0.0087	0.0009
583	Cs-2-PhnButene-2	C10H12	0.15508	0.0219	0.0023
543	M-DiisopropylBz	C12H18	0.11495	0.0168	0.0018
584	Ts-2-PhnButene-2	C10H12	0.09387	0.0116	0.001
580	1,2-DiC1-3C2-Bz	C10H14	0.10214	0.0155	0.0018
704	1-EthNaphthalene	C12H12	0.10476	0.0129	0.0012
512	M-Ethyltoluene	C9H12	0.09127	0.0136	0.0015
522	1-Mth-2-iC3-Benz	C10H14	0.13735	0.0209	0.0023
513	P-Ethyltoluene	C9H12	0.0933	0.0136	0.0016
514	1,2,3-Mesitylene	C9H12	0.15585	0.0249	0.003
614	M-Divinylbenzene	C10H10	0.10189	0.0123	0.001
524	1-Mth-4-iC3-Benz	C10H14	0.1328	0.0199	0.0023
822	Gamma-Terpinene	C10H16	0.19817	0.0347	0.0048
821	Alpha-Terpinene	C10H16	0.16399	0.0266	0.0034
523	1-Mth-3-iC3-Benz	C10H14	0.12792	0.0191	0.0021
703	2-MthNaphthalene	C11H10	0.14156	0.0171	0.0015

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

557	CycHexylBenzene	C12H16	0.11954	0.0199	0.0026
515	1,2,4-Mesitylene	C9H12	0.134	0.0204	0.0024
519	Isobutylbenzene	C10H14	0.08711	0.0131	0.0015
424	DiPhnAcetylene	C14H10	0.2108	0.0272	0.0024
544	P-DiisopropylBz	C12H18	0.13296	0.0207	0.0025
518	N-Butylbenzene	C10H14	0.0866	0.0129	0.0015
516	1,3,5-Mesitylene	C9H12	0.11923	0.0179	0.002
809	Acenaphthalene	C12H8	0.11694	0.0124	0.0009
725	123-TriMthIndene	C12H14	0.10397	0.0132	0.0011
527	1,4-DiEthBenzene	C10H14	0.06521	0.0093	0.001
558	Diphenyl	C12H10	0.13366	0.0176	0.0017
576	2-Ethyl-m-Xylene	C10H14	0.09398	0.0138	0.0016
620	p-ISOPROPENYLSTY	C11H12	0.16711	0.0186	0.0016
585	o-PropylToluene	C10H14	0.0865	0.0124	0.0014
577	2-Ethyl-p-Xylene	C10H14	0.08724	0.0128	0.0014
579	4-Ethyl-o-Xylene	C10H14	0.09218	0.0136	0.0016
586	m-Propyltoluene	C10H14	0.08036	0.0115	0.0013
587	p-Propyltoluene	C10H14	0.08281	0.0119	0.0013
578	4-Ethyl-m-Xylene	C10H14	0.09078	0.0133	0.0015
575	5-Ethyl-m-Xylene	C10H14	0.07913	0.0111	0.0012
530	Prehnitene	C10H14	0.15924	0.0255	0.0032
709	2,6-2Mth-Naphtha	C12H12	0.13949	0.0176	0.0015
715	2,7-2Mth-Naphtha	C12H12	0.14269	0.0183	0.0016
719	2-ETHYLNAPHTHALENE	C12H12	0.12786	0.0148	0.0012
621	p-tert-BUTYLSTY	C12H16	0.05491	0.0042	0.0002
532	1,2,4,5-TetMthBz	C10H14	0.13259	0.0203	0.0024
531	1,2,3,5-TetMthBz	C10H14	0.13679	0.0212	0.0025
533	p-tert-BUTYL ET	C12H18	0.07878	0.0083	0.0006
567	N-Pentylbenzene	C11H16	0.08148	0.0119	0.0014
718	1-n-PROPYLNAPHTH	C13H14	0.11194	0.0115	0.0008
562	1,1-DiPhnEthane	C14H14	0.11613	0.0163	0.0017
616	4-ISOBUTYLSTYRE	C12H16	0.15591	0.0214	0.0021
260	1-Decene	C10H20	0.09246	0.0138	0.0016
735	Cis-Stilbene	C14H12	0.08977	0.011	0.001
568	Hexylbenzene	C12H18	0.07675	0.0111	0.0013
563	Diphenylmethane	C13H12	0.08631	0.0118	0.0012
564	1,2-DiPhnEthane	C14H14	0.05566	0.0082	0.0009
804	Anthracene	C14H10	0.2577	0.0312	0.0024
736	Trans-Stilbene	C14H12	0.1537	0.024	0.0028
805	Phenanthrene	C14H10	0.23549	0.0292	0.0024
713	1-ButNaphthalene	C14H16	0.09003	0.011	0.001
807	Pyrene	C16H10	0.31274	0.0361	0.0026
261	1-Undecene	C11H22	0.08805	0.0131	0.0015
581	23-2C1-23-2PhnC4	C18H22	0.0857	0.0099	0.0008
549	N-Heptylbenzene	C13H20	0.07382	0.0102	0.0011

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

710	1-PhnNaphthalene	C16H12	0.12289	0.014	0.0011
566	2,4-Diphenyl-4-M	C18H20	0.10059	0.0126	0.0012
561	O-Terphenyl	C18H14	0.07098	0.0068	0.0005
569	N-Octylbenzene	C14H22	0.06917	0.0097	0.0011
565	Triphenylmethane	C19H16	0.09065	0.0107	0.0009
714	N-C6-Naphthalene	C16H20	0.08623	0.0109	0.001
717	Fluoranthene	C16H10	0.25594	0.026	0.0015
716	1-Hexyl-Tetralin	C16H24	0.08161	0.0097	0.0008
731	TriPhnEthylene	C20H16	0.14453	0.019	0.0018
806	Chrysene	C18H12	0.42194	0.0648	0.0068
588	1,1,2TriPhenEth	C20H18	0.0536	0.0054	0.0004
711	1-n-NonylNaphtha	C19H26	0.08171	0.0095	0.0008
570	N-Nonylbenzene	C15H24	0.06692	0.0092	0.001
712	1-Decyl Naphtha	C20H28	0.07953	0.0092	0.0007
559	P-Terphenyl	C18H14	0.17898	0.0259	0.0027
560	M-Terphenyl	C18H14	0.1551	0.0203	0.0018
589	TetraPhenylMetha	C25H20	0.14923	0.0197	0.0018
554	Decylbenzene	C16H26	0.06265	0.0087	0.001
732	TetraPhnEthylene	C26H20	0.14018	0.0183	0.0017
574	N-Dodecylbenzene	C18H30	0.05592	0.0079	0.0009
571	N-Undecylbenzene	C17H28	0.0596	0.0082	0.0009
572	Tridecylbenzene	C19H32	0.0535	0.0075	0.0008
573	n-TETRADECYLBENZ	C20H34	0.06992	0.0093	0.0009
2575	n-PENTADECYLBENZ	C21H36	0.06722	0.009	0.0009
2576	n-HEXADECYLBENZ	C22H38	0.06446	0.0087	0.0009
2577	n-HEPTADECYLBENZ	C23H40	0.0613	0.008	0.0008
2578	n-OCTADECYLBENZE	C24H42	0.05865	0.0076	0.0007

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

Halocarbons

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1544	Allyl Chloride	C3H5Cl	0.15032	0.0245	0.0031
1595	2-Chloropropene	C3H5Cl	0.17366	0.0264	0.003
1531	3-Chloropropyne	C3H3Cl	0.1695	0.028	0.0035
1561	6Cl-1,3Butadiene	C4Cl6	0.16302	0.0223	0.0023
1535	T-Butyl Chloride	C4H9Cl	0.18158	0.0266	0.0029
1583	Chloroprene	C4H5Cl	0.06416	0.0078	0.0007
1530	Isopropyl Cl	C3H7Cl	0.17547	0.0273	0.0032
1572	O-DiCl-Benzene	C6H4Cl2	0.11543	0.0188	0.0024

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

1585	Propyl Chloride	C3H7Cl	0.12478	0.0187	0.0022
1684	Isopropyl Iodide	C3H7I	0.13968	0.023	0.003
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	0.19576	0.0332	0.0047
1651	2-Bromopropane	C3H7Br	0.18696	0.0302	0.0038
1691	Iodobenzene	C6H5I	0.08509	0.0111	0.0011
1860	Fluorobenzene	C6H5F	0.19251	0.0334	0.0045
1571	Chlorobenzene	C6H5Cl	0.14215	0.0236	0.003
1680	Bromobenzene	C6H5Br	0.09736	0.0118	0.001
1526	1,2-DiCl-Propane	C3H6Cl2	0.12351	0.0181	0.002
1683	Propyl Iodide	C3H7I	0.13188	0.0213	0.0026
1576	Benzotrichloride	C7H5Cl3	0.19403	0.0186	0.0011
1536	2,3-DICHLOROBUT	C4H8Cl2	0.11486	0.0168	0.0019
2638	2-Bromobutane	C4H9Br	0.17599	0.0305	0.0041
1586	1-Chlorobutane	C4H9Cl	0.11993	0.0179	0.0021
1573	M-DiCl-Benzene	C6H4Cl2	0.0974	0.015	0.0017
2634	Benzotrifluoride	C7H5F3	0.12623	0.0124	0.0008
1574	P-DiCl-Benzene	C6H4Cl2	0.10035	0.0158	0.002
1650	1-Bromopropane	C3H7Br	0.17047	0.0267	0.0033
1587	2-Chlorobutane	C4H9Cl	0.16764	0.0251	0.0028
2653	8F-2-Butene	C4F8	0.00056	0	0
1678	M-Dibromobenzene	C6H4Br2	0.07636	0.0073	0.0005
1537	1,2-DiCl-Butane	C4H8Cl2	0.17964	0.0279	0.0034
1597	34-DiCl-1-Butene	C4H6Cl2	0.09614	0.0161	0.0022
1577	O-Chlorotoluene	C7H7Cl	0.12322	0.0195	0.0024
1532	123-3Cl-Propane	C3H5Cl3	0.1023	0.0154	0.0018
1578	P-Chlorotoluene	C7H7Cl	0.13118	0.0214	0.0028
1562	Benzyl Chloride	C7H7Cl	0.11985	0.0167	0.0017
2661	P-Bromotoluene	C7H7Br	0.10283	0.0128	0.0011
1508	1,4-DiCl-Butane	C4H8Cl2	0.14008	0.0236	0.0031
1655	1-Bromobutane	C4H9Br	0.16298	0.0248	0.003
1599	BenzylDichloride	C7H6Cl2	0.17354	0.0227	0.002
2652	Perfluoropropane	C3F8	0.02874	0.0009	0
1505	2-Butylene DiCl	C4H6Cl2	0.1641	0.0316	0.0049
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	0.12986	0.0231	0.0033
1588	1-Chloropentane	C5H11Cl	0.11627	0.0166	0.0018
1592	1,2,4-TriCl-Bz	C6H3Cl3	0.0718	0.0105	0.0011
1579	2,4-2Cl-Toluene	C7H6Cl2	0.09596	0.0151	0.0018
2593	1,3,5-TriCl-BZ	C6H3Cl3	0.06499	0.0092	0.0009
1697	1-Br-Naphthalene	C10H7Br	0.14622	0.0171	0.0014
1622	Perfluorobutane	C4F10	0.15999	0.0099	0.0003
1857	P-Cl-Benzo-TriF	C7H4ClF3	0.12069	0.0125	0.0008
1509	1,5-DiCl-Pentane	C5H10Cl2	0.13787	0.0235	0.0031
1589	1-Cl-Naphthalene	C10H7Cl	0.14212	0.0174	0.0016
1582	6ClCycPentadiene	C5Cl6	0.1226	0.017	0.0017
1864	Perfluorobenzene	C6F6	0.12539	0.0191	0.0022

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	0.1272	0.0144	0.0011
1667	1-Bromoheptane	C7H15Br	0.13048	0.0202	0.0024
1575	HexaCl-Benzene	C6Cl6	0.02525	0.0043	0.0007
2640	Freon 123B1	C2HBrClF3	0.11611	0.0114	0.0008
1504	Vinyl Chloride	C2H3Cl	0.0717	0.0096	0.001
1672	1,1-DiBr-Ethane	C2H4Br2	0.15957	0.0288	0.0041
1580	Acetylene DiCl	C2H2Cl2	0.14478	0.0226	0.0028
1692	Diiodomethane	CH2I2	0.14863	0.0292	0.005
1698	Bromoform	CHBr3	0.12213	0.0188	0.0022
2687	Freon 13B1	CBrF3	0.00408	0.0001	0
2690	Br-3F-Ethylene	C2BrF3	0.01371	0.0013	0.0001
1649	Tetrabromoethane	C2H2Br4	0.12448	0.0214	0.0029
2686	Freon 12B1	CBrClF2	0.08738	0.0076	0.0004
1503	Ethyl Chloride	C2H5Cl	0.13199	0.0197	0.0022
2641	Br-TriCl-Methane	CBrCl3	0.09011	0.007	0.0003
1641	Methyl Bromide	CH3Br	0.20947	0.0339	0.0043
2688	Freon 12B2	CBr2F2	0.08454	0.0075	0.0005
2545	2,3-DiCl-Propene	C3H4Cl2	0.13007	0.022	0.0032
1673	1,2-DiBr-Ethane	C2H4Br2	0.20363	0.0336	0.0041
2637	Dibromomethane	CH2Br2	0.20228	0.0355	0.005
1542	TetraCl-Ethylene	C2Cl4	0.12756	0.0164	0.0015
1541	TriCl-Ethylene	C2HCl3	0.19572	0.0283	0.0029
1527	111-TriCl-Ethane	C2H3Cl3	0.10378	0.0085	0.0004
1612	Cl-2F-Ethylene	C2HClF2	0.23369	0.0312	0.0029
2639	Br-Cl-Methane	CH2BrCl	0.13398	0.0216	0.0027
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	0.09721	0.0134	0.0015
1682	Ethyl Iodide	C2H5I	0.15046	0.0256	0.0033
1522	1,1-DiCl-Ethane	C2H4Cl2	0.18876	0.0303	0.0037
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	0.30174	0.0519	0.007
1525	Hexachloroethane	C2Cl6	0.25246	0.0242	0.0015
1528	1112-4Cl-Ethane	C2H2Cl4	0.13206	0.0129	0.0009
1590	Penta-Cl-Ethane	C2HCl5	0.18402	0.0181	0.0012
1529	1122-4Cl-Ethane	C2H2Cl4	0.1563	0.0243	0.0028
2693	Perfluoroethane	C2F6	0.00145	0	0
2692	Cl-PentaF-Ethane	C2ClF5	0.03428	0.002	0.0001
2655	122-3Cl-112-3FC2	C2Cl3F3	0.1487	0.0232	0.0028
1609	12-2Cl-1122-4FC2	C2Cl2F4	0.15851	0.0219	0.0022
2526	1,1-DiCl-Propane	C3H6Cl2	0.17779	0.0279	0.0034
1645	Ethyl Bromide	C2H5Br	0.18405	0.0294	0.0037
2658	1112-4Cl-22-2FC2	C2Cl4F2	0.10183	0.0089	0.0005
1619	111-3F-Ethane	C2H3F3	0.0812	0.0065	0.0003
1524	1,1,2-3Cl-Ethane	C2H3Cl3	0.12772	0.0192	0.0022
2691	Genetron 1113	C2ClF3	0.01936	0.002	0.0001
1591	Vinylidene DiCl	C2H2Cl2	0.13411	0.0178	0.0019
1614	Difluoromethane	CH2F2	0.84732	0.129	0.0147

Table B.7 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-SAFT Equation of State (Continued)

2694	Vinyl Bromide	C2H3Br	0.11742	0.0167	0.0017
1694	Refrigerant 123	C2HCl2F3	0.07716	0.0066	0.0004
1523	1,2-DiCl-Ethane	C2H4Cl2	0.1157	0.0181	0.0022
2656	1122-4Cl-12-2FC2	C2Cl4F2	0.11955	0.0199	0.0027
2527	1,3-DiCl-Propane	C3H6Cl2	0.1279	0.0202	0.0025

TableB. 8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State.

Alcohols

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1181	Phenol	C6H6O	0.18643	0.0216	0.0017
1182	O-Cresol	C7H8O	0.12869	0.0126	0.0008
1183	M-Cresol	C7H8O	0.17893	0.0208	0.0017
1176	2,6-Xylenol	C8H10O	0.09854	0.008	0.0004
1111	2-Mth-2-Butanol	C5H12O	0.06933	0.0089	0.0009
1178	3,5-Xylenol	C8H10O	0.17693	0.0205	0.0017
1133	2-Octanol	C8H18O	0.08561	0.0104	0.001
2885	4-HYDROXYSTYREN	C8H8O	0.17101	0.0198	0.0015
1197	P-t-Butylphenol	C10H14O	0.14428	0.0142	0.001
1172	2,4-Xylenol	C8H10O	0.13037	0.0129	0.0008
1184	P-Cresol	C7H8O	0.17715	0.0207	0.0017
1151	Cyclohexanol	C6H12O	0.11166	0.0158	0.0018
1170	2,3-Xylenol	C8H10O	0.15406	0.0164	0.0011
1187	P-Ethyl Phenol	C8H10O	0.15992	0.0189	0.0014
2859	P-Methoxyphenol	C7H8O2	0.33332	0.043	0.0041
1121	2-Ethylhexanol	C8H18O	0.09879	0.0127	0.0014
1179	PropargylAlcohol	C3H4O	0.2453	0.0349	0.0035
1123	3-Mth-1-Butanol	C5H12O	0.13937	0.0218	0.0026
2196	P-t-Amylphenol	C11H16O	0.17511	0.0176	0.0011
1174	2,5-Xylenol	C8H10O	0.13103	0.0132	0.0008
1115	2-Hexanol	C6H14O	0.0903	0.0119	0.0012
1152	1-MthCycHexanol	C7H14O	0.09084	0.0083	0.0005
4854	Guaiacol	C7H8O2	0.11297	0.0082	0.0004
1107	Sec-Butanol	C4H10O	0.10951	0.0157	0.0017
1167	Allyl Alcohol	C3H6O	0.18958	0.0285	0.0033
1130	4-Mth-2-Pentanol	C6H14O	0.08581	0.0104	0.0009
1177	3,4-Xylenol	C8H10O	0.20284	0.0246	0.002
1114	1-Hexanol	C6H14O	0.12784	0.0185	0.0021
1106	Isobutanol	C4H10O	0.14459	0.023	0.0029
1125	1-Heptanol	C7H16O	0.1199	0.0167	0.0019
1105	N-Butanol	C4H10O	0.15686	0.0241	0.0029
1109	1-Pentanol	C5H12O	0.13804	0.0199	0.0022
1132	1-Octanol	C8H18O	0.11453	0.0156	0.0017
1113	T-Butylcarbinol	C5H12O	0.10307	0.0142	0.0015
1137	1-Undecanol	C11H24O	0.10157	0.0129	0.0013
1108	Tert-Butanol	C4H10O	0.07987	0.0111	0.0013
1103	N-Propanol	C3H8O	0.18539	0.0287	0.0033
1134	1-Nonanol	C9H20O	0.11196	0.0147	0.0016
2195	P-t-Octylphenol	C14H22O	0.14458	0.0139	0.0009
1102	Ethanol	C2H6O	0.24987	0.0384	0.0043
1124	3-Mth-2-Butanol	C5H12O	0.09237	0.0129	0.0016
1136	1-Decanol	C10H22O	0.10943	0.0139	0.0014
1140	Dodecanol	C12H26O	0.10568	0.0129	0.0013

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1104	Isopropanol	C3H8O	0.14645	0.022	0.0025
1110	2-Pentanol	C5H12O	0.09463	0.0134	0.0015
1120	3-Pentanol	C5H12O	0.0839	0.0108	0.0011
1112	2-Mth-1-Butanol	C5H12O	0.1294	0.0201	0.0024
1154	Ts-2-Mth-CycC6OH	C7H14O	0.08699	0.0107	0.0008
1153	Cs-2-Mth-CycC6OH	C7H14O	0.0829	0.0094	0.0007
1156	Ts-3-Mth-CycC6OH	C7H14O	0.10626	0.0154	0.0016
1157	Cs-4-Mth-CycC6OH	C7H14O	0.09767	0.0136	0.0014
2197	P-Cumylphenol	C15H16O	0.20583	0.0218	0.0015
1180	Benzyl Alcohol	C7H8O	0.16825	0.0225	0.0022
1158	Ts-4-Mth-CycC6OH	C7H14O	0.09862	0.0142	0.0015
1155	Cs-3-Mth-CycC6OH	C7H14O	0.1047	0.0156	0.0017
1168	2-Phn-2-Propanol	C9H12O	0.07266	0.0076	0.0005
1141	1-Tridecanol	C13H28O	0.11144	0.0133	0.0012
1147	2-Eth-1-Butanol	C6H14O	0.11085	0.0145	0.0016
1117	2-Mth-1-Pentanol	C6H14O	0.1169	0.0159	0.0017
2115	2-Phenylethanol	C8H10O	0.13122	0.0185	0.0018
1142	1-Tetradecanol	C14H30O	0.11254	0.0132	0.0012
2118	1-PHN-1-PROPANOL	C9H12O	0.09921	0.0107	0.0007
2119	1-PHN-2-PROPANOL	C9H12O	0.10026	0.0111	0.0008
1126	2-Heptanol	C7H16O	0.08515	0.01	0.0009
1143	1-Pentadecanol	C15H32O	0.11385	0.0133	0.0012
1129	Isoheptanol	C7H16O	0.12337	0.0186	0.0021
2117	2,6-DiMth-4-C7OH	C9H20O	0.06248	0.0081	0.0008
1144	1-Hexadecanol	C16H34O	0.11659	0.0134	0.0012
1145	Heptadecanol	C17H36O	0.11547	0.0133	0.0011
1199	Nonylphenol	C15H24O	0.12632	0.0148	0.0012
1146	1-Octadecanol	C18H38O	0.1199	0.0136	0.0011
1135	2-Nonanol	C9H20O	0.0845	0.0096	0.0008
1149	1-Nonadecanol	C19H40O	0.11837	0.013	0.001
1139	Isodecanol	C10H22O	0.08984	0.0128	0.0013
1148	1-Eicosanol	C20H42O	0.11499	0.0126	0.001
2198	Dinonylphenol	C24H42O	0.31682	0.0462	0.0047
1159	Menthol	C10H20O	0.0697	0.0095	0.0009

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Amines

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1742	Ethyleneimine	C2H5N	0.43101	0.0892	0.0154
1745	Piperidine	C5H11N	0.09142	0.0109	0.001

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1766	Pyrrolidine	C4H9N	0.12403	0.0179	0.0021
1719	Isopropylamine	C3H9N	0.08961	0.0138	0.0018
1711	N-Propylamine	C3H9N	0.07847	0.0113	0.0013
1726	Sec-Butylamine	C4H11N	0.08676	0.0118	0.0012
1704	Ethylamine	C2H7N	0.08732	0.0134	0.0017
1702	Dimethylamine	C2H7N	0.07512	0.0109	0.0013
1710	Diethylamine	C4H11N	0.05882	0.0064	0.0005
1740	Allylamine	C3H7N	0.11054	0.0191	0.0027
1712	N-Butylamine	C4H11N	0.0765	0.0105	0.0011
1794	HexMthyleneimine	C6H13N	0.10459	0.0132	0.0014
1729	Cyclohexylamine	C6H13N	0.08662	0.0111	0.0011
1714	Isobutylamine	C4H11N	0.07797	0.0112	0.0013
2853	Acetamide	C2H5NO	0.13962	0.0244	0.0036
2731	N-C1-CycC6-Amine	C7H15N	0.08502	0.0106	0.001
1743	Diisopropylamine	C6H15N	0.0922	0.0091	0.0008
1796	N,N-DiMthAniline	C8H11N	0.04473	0.0035	0.0002
1792	Aniline	C6H7N	0.11093	0.0137	0.0013
1713	N-Pentylamine	C5H13N	0.07389	0.0097	0.001
1733	Benzylamine	C7H9N	0.10418	0.013	0.0013
1737	M-Toluidine	C7H9N	0.10407	0.012	0.0011
3796	N-Ethylaniline	C8H11N	0.15207	0.0197	0.002
1878	2-Methacrylamide	C4H7NO	0.03284	0.004	0.0004
1736	O-Toluidine	C7H9N	0.09577	0.0104	0.0009
2739	Diallylamine	C6H11N	0.06826	0.0099	0.0011
2706	Hexylamine	C6H15N	0.07938	0.0101	0.001
2724	O-Ethylaniline	C8H11N	0.07081	0.0075	0.0006
1707	Dipropylamine	C6H15N	0.06133	0.0066	0.0005
1738	P-Toluidine	C7H9N	0.09594	0.0109	0.0009
1795	N-Methylaniline	C7H9N	0.17797	0.0243	0.0025
1718	Diisobutylamine	C8H19N	0.06072	0.0069	0.0005
1879	Acrylamide	C3H5NO	0.09899	0.0142	0.002
2707	1-Aminoheptane	C7H17N	0.0806	0.0098	0.0009
2730	DiCycHexylAmine	C12H23N	0.18189	0.0188	0.0014
2787	P-Aminodiphenyl	C12H11N	0.28471	0.0315	0.0021
1744	Dibutylamine	C8H19N	0.07303	0.0079	0.0006
2708	1-Octylamine	C8H19N	0.08262	0.0102	0.0009
2791	2,6-DiEthAniline	C10H15N	0.05368	0.0059	0.0004
2709	1-Nonylamine	C9H21N	0.08725	0.0107	0.001
2710	1-Decylamine	C10H23N	0.08492	0.0103	0.0009
3722	Diamylamine	C10H23N	0.08394	0.0106	0.001
3724	Undecylamine	C11H25N	0.09236	0.0105	0.0009
2712	Dodecylamine	C12H27N	0.09383	0.0111	0.001
1720	Tetradecylamine	C14H31N	0.09694	0.0115	0.001
2752	Piperazine	C4H10N2	0.1733	0.0283	0.0036
1752	Propylenediamine	C3H10N2	0.14292	0.0278	0.0045

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1741	Ethylenediamine	C2H8N2	0.19542	0.0399	0.0068
2725	O-Aminoaniline	C6H8N2	0.13	0.0149	0.0012
2750	P-Aminoaniline	C6H8N2	0.16772	0.0208	0.0019
2727	M-Aminoaniline	C6H8N2	0.26368	0.0334	0.0028
1750	AEP	C6H15N3	0.14408	0.0235	0.0031
1732	Toluene Diamine	C7H10N2	0.16747	0.0203	0.0017
1731	hexamethyleneDiamine	C6H16N2	0.09433	0.0132	0.0013
3750	P-Benzidine	C12H12N2	0.45141	0.0619	0.0058

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Nitrilies

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1773	Propionitrile	C3H5N	0.097	0.0138	0.0016
1782	Butyronitrile	C4H7N	0.07043	0.0094	0.001
2720	Allyl Cyanide	C4H5N	0.06674	0.0099	0.0012
1783	Valeronitrile	C5H9N	0.06285	0.0077	0.0008
3874	Benzyl Cyanide	C8H7N	0.07794	0.0092	0.0008
1786	Hexanenitrile	C6H11N	0.05902	0.0072	0.0006
1776	Succinonitrile	C4H4N2	0.12348	0.0242	0.0041
1781	Glutaronitrile	C5H6N2	0.11343	0.0179	0.0022
2735	14-2Cyano-2-C4H8	C6H6N2	0.03406	0.0056	0.0008
1777	Adiponitrile	C6H8N2	0.08914	0.0147	0.0019

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Silanes

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
3985	Dimethyl Silane	C2H8Si	0.12509	0.0167	0.0019
3984	Methyl Silane	CH6Si	0.10604	0.0133	0.0012
3986	Trimethyl Silane	C3H10Si	0.10443	0.013	0.0012
1984	TetraMth Silane	C4H12Si	0.07716	0.009	0.0008
2994	TETRAETHYL Si	C8H20Si	0.14999	0.0194	0.0018
1965	HexMthDisiloxane	C6H18OSi2	0.09283	0.0097	0.0007
1966	6C1Cyc3Siloxane	C6H18O3Si3	0.17592	0.0181	0.0012
1988	8C1Cyc4Siloxane	C8H24O4Si4	0.17124	0.0163	0.0011
3991	DecaMethcyclpenS	C10H30O5Si5	0.18974	0.0168	0.0008
3992	DodecaMethCyHexS	C12H36O6Si6	0.23406	0.0207	0.001

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
	Imines				
1767	N-MthPyrrolidine	C5H11N	0.12269	0.0168	0.0018
2797	3-Methylpyridine	C6H7N	0.11301	0.0155	0.0017
1797	2-Methylpyridine	C6H7N	0.07502	0.0094	0.0009
2799	4-Methylpyridine	C6H7N	0.11651	0.0161	0.0018
1753	N,N-DiEthAniline	C10H15N	0.15436	0.0207	0.0021
1754	N-Methylpyrrole	C5H7N	0.13744	0.0261	0.0043
3740	Acridine	C13H9N	0.37208	0.0393	0.0026

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
	Tert-N				
1703	Trimethylamine	C3H9N	0.05354	0.0071	0.0008
2856	DiMth Acetamide	C4H9NO	0.25087	0.0486	0.0077
1706	Triethylamine	C6H15N	0.10565	0.0135	0.0013
2716	Tributylamine	C12H27N	0.0885	0.0114	0.0011
2719	Tripropylamine	C9H21N	0.09093	0.0139	0.0017
3723	Triamylamine	C15H33N	0.05349	0.0061	0.0005

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
	Nitrate				
1761	Nitroethane	C2H5NO2	0.11287	0.0138	0.0013
1763	2-Nitropropane	C3H7NO2	0.0991	0.0123	0.0012
1762	1-Nitropropane	C3H7NO2	0.08776	0.0098	0.0008

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1779	P-Nitrotoluene	C7H7NO2	0.13152	0.0196	0.0027
1886	Nitrobenzene	C6H5NO2	0.11722	0.0183	0.0024
1778	O-Nitrotoluene	C7H7NO2	0.09193	0.0131	0.0015
1780	M-Nitrotoluene	C7H7NO2	0.11465	0.0168	0.0019
1891	O-Nitroanisole	C7H7NO3	0.25781	0.0419	0.0053
2740	M-Dinitrobenzene	C6H4N2O4	0.06016	0.0086	0.0011
2742	P-Dinitrobenzene	C6H4N2O4	0.05633	0.0078	0.0009
2741	O-Dinitrobenzene	C6H4N2O4	0.08499	0.0121	0.0015
2749	3,5-DiNitToluene	C7H6N2O4	0.06084	0.0087	0.0009
2743	DNT	C7H6N2O4	0.06391	0.0082	0.0008
2745	3,4-DiNitToluene	C7H6N2O4	0.09337	0.0131	0.0013
2744	2,6-DiNitToluene	C7H6N2O4	0.03201	0.0036	0.0003
2748	2,5-DiNitToluene	C7H6N2O4	0.06346	0.0082	0.0007
2746	1,3,5-TrinitroBz	C6H3N3O6	0.01932	0.0023	0.0003
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	0.05337	0.0061	0.0005
2747	Trinitrotoluene	C7H5N3O6	0.01531	0.0015	0.0001

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Thiols

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1802	Ethyl Mercaptan	C2H6S	0.11163	0.0167	0.002
1820	Dimethyl Sulfide	C2H6S	0.10251	0.0136	0.0015
1843	Thiacyclopentane	C4H8S	0.20286	0.0286	0.0032
1803	1-Propanethiol	C3H8S	0.10687	0.0153	0.0018
1805	Isobut Mercaptan	C4H10S	0.10612	0.0153	0.0018
6860	Ethylenedithiol	C2H6S2	0.15379	0.027	0.0039
1811	Cyclohexanethiol	C6H12S	0.09278	0.0113	0.0011
1828	DiMth Disulfide	C2H6S2	0.05945	0.008	0.0009
1841	Butanethiol	C4H10S	0.10626	0.0145	0.0016
1814	Methylproylsulf	C4H10S	0.09802	0.0133	0.0014
2816	ETHYLtBUTYL SUL	C6H14S	0.09577	0.011	0.001
1818	Diethyl Sulfide	C4H10S	0.1156	0.014	0.0012
1812	Benzyl Mercaptan	C7H8S	0.12151	0.0148	0.0014
1838	T-OctylMercaptan	C8H18S	0.05035	0.0049	0.0003
1827	1-Pentanethiol	C5H12S	0.10684	0.0144	0.0015
2815	METHnBUTYL SULFD	C5H12S	0.09545	0.0116	0.0011
1824	DiethylDisulfide	C4H10S2	0.10245	0.0111	0.0009
1807	N-Hexylmercaptan	C6H14S	0.10779	0.0141	0.0014
6857	Dimercaptoethyl	C4H10OS2	0.10828	0.0179	0.0024

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1839	1-Heptanethiol	C7H16S	0.10968	0.0143	0.0015
1829	DiProp Disulfide	C6H14S2	0.09917	0.0105	0.0007
1809	1-Octanethiol	C8H18S	0.11014	0.014	0.0014
1808	N-Nonanethiol	C9H20S	0.11079	0.0141	0.0014
1826	1-Decanethiol	C10H22S	0.1126	0.0143	0.0014
2838	tertDodecanThiol	C12H26S	0.06755	0.0078	0.0007
1825	1-Undecanethiol	C11H24S	0.11271	0.0142	0.0014
1837	Dodecylthiol	C12H26S	0.11449	0.0132	0.0012

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Aldehydes

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1037	Methacrolein	C4H6O	0.10656	0.0153	0.0017
1002	Acetaldehyde	C2H4O	0.1803	0.0273	0.0035
1003	Propionaldehyde	C3H6O	0.1296	0.019	0.0022
1041	Benzaldehyde	C7H6O	0.12159	0.0142	0.0012
1034	Acrolein	C3H4O	0.18025	0.0293	0.0039
1005	N-Butyraldehyde	C4H8O	0.10759	0.0146	0.0016
1036	Trans-2-Butenal	C4H6O	0.21516	0.041	0.0065
1007	Valeraldehyde	C5H10O	0.10263	0.0137	0.0015
1006	Isobutyraldehyde	C4H8O	0.10822	0.0171	0.0022
1009	1-Hexanal	C6H12O	0.0975	0.0128	0.0013
1040	P-Tolualdehyde	C8H8O	0.12928	0.0164	0.0016
1016	2-Methylhexanal	C7H14O	0.08805	0.0121	0.0013
1017	3-Methylhexanal	C7H14O	0.09292	0.0123	0.0012
1008	1-Heptanal	C7H14O	0.09706	0.0123	0.0012
1013	2-Ethylhexanal	C8H16O	0.07771	0.0103	0.0011
1010	1-Octanal	C8H16O	0.09241	0.0118	0.0012
1011	1-Nonanal	C9H18O	0.09418	0.0114	0.0012
1020	1-Decanal	C10H20O	0.09272	0.0112	0.0011
1021	1-Undecanal	C11H22O	0.09095	0.0107	0.0011
1025	Dodecanal	C12H24O	0.09203	0.0109	0.001
1026	1-Tridecanal	C13H26O	0.09197	0.0109	0.001
1014	1,2-Ethanedione	C2H2O2	0.06804	0.0111	0.0015
1044	1,4BenzDicarboxAldehy	C8H6O2	0.13034	0.0161	0.0015

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Epoxides

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1440	ISOBUTYLENE OXID	C4H8O	0.31099	0.056	0.0082
1479	Tetrahydrofuran	C4H8O	0.07282	0.0096	0.001
1477	2,5-Dihydrofuran	C4H6O	0.21117	0.0399	0.0061
1408	1-Methoxypropane	C4H10O	0.07809	0.0084	0.0007
1411	2-Methoxypropane	C4H10O	0.0879	0.0103	0.0009
1421	1,4-Dioxane	C4H8O2	0.24309	0.0441	0.0064
2422	1,3-DIOXANE	C4H8O2	0.26447	0.0508	0.0081
1426	2-Methoxybutane	C5H12O	0.08626	0.01	0.0009
1413	1-Methoxybutane	C5H12O	0.0888	0.0098	0.0008
1461	Methoxybenzene	C7H8O	0.14413	0.0163	0.0014
1448	1-Ethoxybutane	C6H14O	0.08838	0.0115	0.0012
1429	1-MethoxyPentane	C6H14O	0.10921	0.0148	0.0016
6885	Ethyl-3-Ethoxypr	C7H14O3	0.10188	0.0138	0.0015

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Ether

Dip ID	Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1401	Dimethyl Ether	C2H6O	0.07113	0.0077	0.0006
1407	MethylEthylEther	C3H8O	0.12672	0.0204	0.0027
1470	VinylMethylEther	C3H6O	0.09394	0.0124	0.0013
1405	MTBE	C5H12O	0.10793	0.0131	0.0012
1445	VinylEthyl Ether	C4H8O	0.12267	0.0199	0.0026
1402	Diethyl Ether	C4H10O	0.09658	0.0134	0.0015
1431	Methylal	C3H8O2	0.07638	0.008	0.0006
1428	T-But EthylEther	C6H14O	0.09343	0.013	0.0014
1427	TAME	C6H14O	0.1197	0.0144	0.0013
1410	Mth Isobut Ether	C5H12O	0.08454	0.0097	0.0008
1430	Eth-t-Pent-Ether	C7H16O	0.0937	0.0123	0.0012
1403	DiisopropylEther	C6H14O	0.09179	0.0123	0.0012
1415	Eth Propyl Ether	C5H12O	0.08989	0.0116	0.0013
1455	Dimethyl Acetal	C4H10O2	0.1867	0.0343	0.0052
1446	Dipropyl Ether	C6H14O	0.08328	0.0104	0.001
1447	Butyl VinylEther	C6H12O	0.09854	0.0148	0.0018
1462	EthylPhenylEther	C8H10O	0.11116	0.0137	0.0013
1406	Di-sec-But Ether	C8H18O	0.08642	0.0111	0.0011
1432	Acetal	C6H14O2	0.0756	0.0105	0.0011

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1460	BenzylEthylEther	C9H12O	0.09141	0.0127	0.0013
1050	Paraldehyde	C6H12O3	0.13239	0.0238	0.0036
1404	Di-n-Butyl Ether	C8H18O	0.08508	0.0106	0.001
1420	Anethole	C10H12O	0.196	0.0221	0.0017
1456	DimethylCarbitol	C6H14O3	0.16509	0.0233	0.0025
1463	Dibenzyl Ether	C14H14O	0.07868	0.0111	0.0012
1425	Di-n-PentylEther	C10H22O	0.0908	0.0109	0.0009
1458	Diethyl Carbitol	C8H18O3	0.08109	0.012	0.0013
1412	Dihexyl Ether	C12H26O	0.09342	0.0125	0.0013
1454	Triglyme	C8H18O4	0.12795	0.0198	0.0024
1459	Dibutyl Carbitol	C12H26O3	0.06512	0.0078	0.0006
1424	Di-n-Octyl Ether	C16H34O	0.08933	0.0118	0.0012
1457	Tetraglyme	C10H22O5	0.07525	0.0128	0.0017
1418	Dinonyl Ether	C18H38O	0.09913	0.0132	0.0013
2432	ETHYLAL	C5H12O2	0.08278	0.0113	0.0012
2405	Diisobutyl Ether	C8H18O	0.07776	0.0102	0.001
2456	Ethyl Glyme	C6H14O2	0.09752	0.015	0.0019
2417	Ethylhexyl Ether	C8H18O	0.09209	0.0123	0.0013
2415	Ethylisopropeth	C5H12O	0.10456	0.0146	0.0016

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Formate

Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1301	Methyl Formate	C2H4O2	0.16787	0.0277	0.0037
1311	Vinyl Formate	C3H4O2	0.10844	0.0182	0.0025
1302	Ethyl Formate	C3H6O2	0.11723	0.0167	0.0019
2306	t-Butyl Formate	C5H10O2	0.08653	0.0111	0.0011
1303	Propyl Formate	C4H8O2	0.10509	0.0145	0.0016
2305	sec-ButylFormate	C5H10O2	0.08842	0.0119	0.0012
2311	CYCLOHEXL FORMAT	C7H12O2	0.09338	0.0118	0.0012
1304	N-Butyl Formate	C5H10O2	0.09877	0.0129	0.0013
1305	Isobutyl Formate	C5H10O2	0.10092	0.0141	0.0014
2350	Benzyl Formate	C8H8O2	0.12712	0.0155	0.0014
2307	n-Hexyl Formate	C7H14O2	0.09995	0.0133	0.0014
1306	N-Pentyl Formate	C6H12O2	0.10105	0.0129	0.0013
2308	n-Heptyl Formate	C8H16O2	0.1042	0.0124	0.0011
1308	N-Octyl Formate	C9H18O2	0.10477	0.0116	0.0009
1309	n-Nonyl Formate	C10H20O2	0.09506	0.0117	0.001
1310	n-Decyl Formate	C11H22O2	0.09884	0.0125	0.0011

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Ester					
Dip ID	**Name**	**Formula**	$P_{760\,nnHg}^{calc}$	$P_{100\,nnHg}^{calc}$	$P_{10\,nnHg}^{calc}$
1351	Mth Methacrylate	C5H8O2	0.10012	0.0118	0.0011
1312	Methyl Acetate	C3H6O2	0.11955	0.0148	0.0014
1331	Vinyl Propionate	C5H8O2	0.11113	0.0168	0.002
1321	Vinyl Acetate	C4H6O2	0.08936	0.0109	0.001
1352	Eth MthAcrylate	C6H10O2	0.10155	0.0133	0.0013
1322	MethylPropionate	C4H8O2	0.10013	0.0117	0.001
1341	Methyl Acrylate	C4H6O2	0.17521	0.0284	0.0037
1313	Ethyl Acetate	C4H8O2	0.14716	0.0225	0.0028
1319	IsopropylAcetate	C5H10O2	0.07649	0.0083	0.0006
1332	Methyl Butyrate	C5H10O2	0.13093	0.0187	0.0021
1342	Ethyl Acrylate	C5H8O2	0.12408	0.0188	0.0022
1318	Allyl Acetate	C5H8O2	0.10494	0.0118	0.0009
1314	N-Propyl Acetate	C5H10O2	0.09002	0.0099	0.0008
1323	Ethyl Propionate	C5H10O2	0.11882	0.0167	0.0019
1360	I-But I-Butyrate	C8H16O2	0.07278	0.0075	0.0006
1320	Sec-ButylAcetate	C6H12O2	0.07478	0.008	0.0006
1336	PropylI-Butyrate	C7H14O2	0.09671	0.0133	0.0014
1353	N-C3-Mthacrylate	C7H12O2	0.12126	0.0161	0.0017
1333	Ethyl Butyrate	C6H12O2	0.10426	0.0127	0.0012
1347	EthylIsovalerate	C7H14O2	0.09357	0.0123	0.0012
1315	N-Butyl Acetate	C6H12O2	0.09253	0.0101	0.0008
1390	Methyl Benzoate	C8H8O2	0.14488	0.0151	0.0011
1388	ISOBUTYL MTHACR	C8H14O2	0.09155	0.0115	0.0011
1343	1-PropylAcrylate	C6H10O2	0.09911	0.0144	0.0017
1316	Isobutyl Acetate	C6H12O2	0.08682	0.0098	0.0008
1344	N-Butyl Acrylate	C7H12O2	0.11317	0.0144	0.0013
1357	Pentyl Acetate	C7H14O2	0.09305	0.0096	0.0008
1327	N-PropN-Butyrate	C7H14O2	0.09646	0.0119	0.0011
1324	N-PropPropionate	C6H12O2	0.10741	0.0142	0.0014
1291	Acetic Anhydride	C4H6O3	0.12203	0.0154	0.0015
1389	N-ButMthacrylate	C8H14O2	0.09429	0.0124	0.0012
1359	Benzyl Acetate	C9H10O2	0.12524	0.0157	0.0015
1326	N-But Propionate	C7H14O2	0.10223	0.0135	0.0014
1391	Ethyl Benzoate	C9H10O2	0.13179	0.015	0.0011
1897	CH3OC3H600CH3	C6H12O3	0.10993	0.0128	0.0011
1392	DiethylCarbonate	C5H10O3	0.12414	0.0175	0.0022
1385	N-But N-Butyrate	C8H16O2	0.09592	0.0113	0.001
1317	IsopentylAcetate	C7H14O2	0.09452	0.0098	0.0008
1363	N-Hexyl Acetate	C8H16O2	0.11462	0.015	0.0015
1387	Ethylene Acetate	C6H10O4	0.16849	0.0217	0.0027
1393	Diethyl Oxalate	C6H10O4	0.16894	0.0262	0.0032
1365	Butyl Benzoate	C11H14O2	0.13109	0.0152	0.0012
1361	I-C5 I-Valerate	C10H20O2	0.09391	0.0108	0.0008

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1367	Heptyl Acetate	C9H18O2	0.11585	0.0152	0.0015
1346	N-Butyl Valerate	C9H18O2	0.09705	0.0124	0.0012
1358	2-C2-C6 Acetate	C10H20O2	0.09237	0.0094	0.0007
1394	Diethyl Malonate	C7H12O4	0.13889	0.0207	0.0023
1292	Propionyl Oxide	C6H10O3	0.09237	0.0117	0.0011
1364	Benzyl Benzoate	C14H12O2	0.14127	0.015	0.0014
1381	2Mth p-Phthalate	C10H10O4	0.26518	0.0244	0.0012
1368	n-Octyl Acetate	C10H20O2	0.11175	0.0145	0.0014
1377	DiMthI-Phthalate	C10H10O4	0.20903	0.0195	0.0013
1896	Ethylene DiAcr	C8H10O4	0.14611	0.0236	0.0029
1386	2-Ethylhexyl Acr	C11H20O2	0.08286	0.0104	0.0009
1395	Methyl Decanoate	C11H22O2	0.1148	0.0148	0.0015
1369	n-Nonyl Acetate	C11H22O2	0.09905	0.0128	0.0013
1370	n-Decyl Acetate	C12H24O2	0.10755	0.0133	0.0013
1345	N-ButylNonanoate	C13H26O2	0.07349	0.0059	0.0003
1375	DiProp Phthalate	C14H18O4	0.13329	0.0138	0.001
1376	Diisobutyl Phtha	C16H22O4	0.08732	0.0093	0.0007
1396	IsopropMyristate	C17H34O2	0.1102	0.0133	0.0012
1383	Butyl Stearate	C22H44O2	0.06009	0.0057	0.0004
1362	Methyl Oleate	C19H36O2	0.08549	0.0109	0.001
1355	Diisooctyl Phtha	C24H38O4	0.14115	0.0155	0.0011
1382	DioctylTerephtha	C24H38O4	0.14798	0.0158	0.0011
1384	DIBUTYL SEBACATE	C18H34O4	0.08981	0.0118	0.0011
1371	Diisodecyl Phtha	C28H46O4	0.18642	0.017	0.0008
1354	DioctylPhthalate	C24H38O4	0.06162	0.0059	0.0004
2375	DiethylPhthalate	C12H14O4	0.13399	0.0152	0.0012
2388	Dipropyl Maleate	C10H16O4	0.09252	0.0134	0.0015
2381	Diallyl Maleate	C10H12O4	0.06019	0.0094	0.0012
2370	Glyceryl Triacet	C9H14O6	0.12811	0.015	0.0013
2382	Dibutyl Maleate	C12H20O4	0.09194	0.0134	0.0015
2376	DibutylPhthalate	C16H22O4	0.12873	0.0139	0.001
2353	CetylMthacrylate	C20H38O2	0.13435	0.0162	0.0012
2379	Dihexyl Adipate	C18H34O4	0.08667	0.0108	0.001
2321	T-Butyl Acetate	C6H12O2	0.08318	0.0113	0.0013
2332	Methl.I-butyrate	C5H10O2	0.12799	0.0188	0.0022
2354	AllylMthacrylate	C7H10O2	0.09051	0.013	0.0016
2364	CYCLOHEXL ACETAT	C8H14O2	0.09842	0.0129	0.0013
2337	EthylIsobutyrate	C6H12O2	0.0953	0.0123	0.0012
2384	IsobutylAcrylate	C7H12O2	0.09914	0.0141	0.0016
2380	1,1-Diacetoxy C2	C6H10O4	0.13514	0.0205	0.0025
2392	n-PropylBenzoate	C10H12O2	0.1266	0.0137	0.0011
2377	DiMth Phthalate	C10H10O4	0.24252	0.0258	0.0017
2386	Diethyl Maleate	C8H12O4	0.13091	0.0191	0.002
2385	Mth Dodecanoate	C13H26O2	0.1221	0.0153	0.0014
3379	Dioctyl Adipate	C22H42O4	0.1726	0.0164	0.0007

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

5886	Mth Acetoacetate	C5H8O3	0.17094	0.0274	0.0035
5884	Ethoxy Acetate	C6H12O3	0.12053	0.0159	0.0016
5887	EthAcetoAcetate	C6H10O3	0.11957	0.0168	0.0017
5885	Carbitol Acetate	C8H16O4	0.1122	0.0142	0.0012

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Dip ID	Ketone Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1096	Methyl Isopropen	C5H8O	0.09452	0.0124	0.0013
1079	Cyclopentanone	C5H8O	0.18004	0.0248	0.0026
1051	Acetone	C3H6O	0.14446	0.0208	0.0023
1052	MEK	C4H8O	0.11038	0.0145	0.0015
1065	Mesityl Oxide	C6H10O	0.09918	0.013	0.0013
1066	T-But Mth Ketone	C6H12O	0.08128	0.0098	0.0009
1060	2-Pentanone	C5H10O	0.09269	0.0115	0.0011
1061	Mth iC3 Ketone	C5H10O	0.09557	0.0123	0.0012
1053	Diethyl Ketone	C5H10O	0.10134	0.0122	0.001
1059	3-Hexanone	C6H12O	0.09104	0.0105	0.0009
1099	Diketene	C4H4O2	0.54008	0.1222	0.0224
1055	Sec-ButMthKetone	C6H12O	0.08653	0.0107	0.001
1054	MIBK	C6H12O	0.0828	0.01	0.001
1095	EthIsopropKetone	C6H12O	0.08609	0.0107	0.001
1063	2-Heptanone	C7H14O	0.09159	0.0109	0.001
1064	5-Mth-2-Hexanone	C7H14O	0.09308	0.0116	0.0011
1058	4-Heptanone	C7H14O	0.08402	0.0091	0.0007
1057	3-Heptanone	C7H14O	0.09146	0.0109	0.001
1076	2,4-Pentanedione	C5H8O2	0.05356	0.0038	0.0002
1068	DiisobutylKetone	C9H18O	0.07011	0.0077	0.0007
1097	2-CycC6 CycC6one	C12H20O	0.08986	0.0105	0.0011
1083	2-Octanone	C8H16O	0.09164	0.0109	0.001
1073	Dibutyl Ketone	C9H18O	0.09057	0.01	0.0008
1062	2-Hexanone	C6H12O	0.09205	0.0111	0.001
1077	Isophorone	C9H14O	0.1811	0.0234	0.0021
1090	Acetophenone	C8H8O	0.12836	0.0147	0.0012
1080	Cyclohexanone	C6H10O	0.16406	0.021	0.002
1074	2-Nonanone	C9H18O	0.09312	0.0111	0.001

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Dip ID	Alcohol-Ethers Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
2862	2-Butoxyethanol	C6H14O2	0.09727	0.0112	0.0009
4857	butyl carbitol	C8H18O3	0.09089	0.0107	0.001
2898	2-Chloroethanol	C2H5ClO	0.16503	0.0222	0.0019
2864	Carbitol	C6H14O3	0.11758	0.0158	0.0016
3854	Methyl propasol	C4H10O2	0.10275	0.0102	0.0006
2860	2-Methoxyethanol	C3H8O2	0.20363	0.0233	0.0019
2854	DiacetoneAlcohol	C6H12O2	0.06833	0.0066	0.0004
2861	2-Ethoxyethanol	C4H10O2	0.1292	0.0151	0.0013
2889	HydroxyAcetone	C3H6O2	0.17396	0.0206	0.0016
3856	1tButoxy2Propnol	C7H16O2	0.03972	0.0047	0.0004
3858	PROPGLYC2tBUTYL	C7H16O2	0.06152	0.008	0.0008
4855	2-Propoxyethanol	C5H12O2	0.10364	0.0111	0.0009
4849	Acetovanillone	C9H10O3	0.24018	0.028	0.0021
5883	Ethyl Lactate	C5H10O3	0.07822	0.0075	0.0004
6883	2-HydroxyEth Acr	C5H8O3	0.28586	0.055	0.0078
2863	Methyl Carbitol	C5H12O3	0.16543	0.0248	0.0027
3855	Dowanol DPM	C7H16O3	0.05459	0.005	0.0003
3857	TriPropGlymEthlE	C10H22O4	0.03677	0.0045	0.0004

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

Dip ID	Hydrocarbons Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
404	DiMth-Acetylene	C4H6	0.15406	0.0203	0.002
202	Propylene	C3H6	0.06192	0.0076	0.0007
412	2-Pentyne	C5H8	0.0209	0.0014	0.0001
207	2-Methylpropene	C4H8	0.08462	0.0109	0.0011
204	1-Butene	C4H8	0.07571	0.0095	0.0009
205	Cis-2-Butene	C4H8	0.09782	0.0139	0.0016
402	Propyne	C3H4	0.11493	0.0189	0.0025
406	3-Hexyne	C6H10	0.1336	0.0157	0.0013
206	Trans-2-Butene	C4H8	0.08806	0.0119	0.0013
407	2-Hexyne	C6H10	0.14723	0.0178	0.0017
231	33-2Mth-1-Butene	C6H12	0.04002	0.0038	0.0003
230	23-2Mth-1-Butene	C6H12	0.06811	0.0076	0.0006
229	2-Ethyl-1-Butene	C6H12	0.10205	0.0136	0.0014
8	I-Pentane	C5H12	0.0946	0.0114	0.0011

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

14	2,2-DiMth-Butane	C6H14	0.10263	0.0124	0.0012
232	23-2Mth-2-Butene	C6H12	0.08306	0.0109	0.0011
213	3-Mth-1-Butene	C5H10	0.09181	0.0122	0.0013
212	2-Mth-1-Butene	C5H10	0.09688	0.0128	0.0013
211	Trans-2-Pentene	C5H10	0.0902	0.0121	0.0013
210	Cis-2-Pentene	C5H10	0.09166	0.0124	0.0014
223	4-Mth-1-Pentene	C6H12	0.09445	0.0123	0.0013
221	2-Mth-1-Pentene	C6H12	0.09437	0.012	0.0012
248	2-t-Butylpropene	C7H14	0.12004	0.0165	0.0018
227	Cs-4-Mth-2-C5H10	C6H12	0.08855	0.012	0.0013
224	2-Mth-2-Pentene	C6H12	0.1005	0.013	0.0013
403	1-Butyne	C4H6	0.09069	0.0135	0.0016
15	2,3-DiMth-Butane	C6H14	0.13397	0.0182	0.0019
214	2-Mth-2-Butene	C5H10	0.10902	0.0144	0.0015
228	Ts-4-Mth-2-C5H10	C6H12	0.09519	0.0132	0.0015
225	Cs-3-Mth-2-C5H10	C6H12	0.10187	0.013	0.0013
218	Trans-2-Hexene	C6H12	0.08964	0.0117	0.0012
2226	3-METH-Tr-2Pente	C6H12	0.11093	0.0148	0.0015
222	3-Mth-1-Pentene	C6H12	0.09489	0.0122	0.0013
257	2-Diisobutylene	C8H16	0.10484	0.0138	0.0014
256	1-Diisobutylene	C8H16	0.10303	0.013	0.0013
217	Cis-2-Hexene	C6H12	0.09213	0.0121	0.0012
2414	1-Heptyne	C7H12	0.08868	0.0114	0.0011
13	3-Methylpentane	C6H14	0.10988	0.0138	0.0013
219	Cis-3-Hexene	C6H12	0.09784	0.0124	0.0012
12	2-Methylpentane	C6H14	0.09954	0.0123	0.0011
220	Trans-3-Hexene	C6H12	0.10026	0.0129	0.0013
405	1-Pentyne	C5H8	0.08561	0.0115	0.0012
209	1-Pentene	C5H10	0.08218	0.0102	0.001
11	N-Hexane	C6H14	0.09289	0.0108	0.001
235	Cis-2-Heptene	C7H14	0.09368	0.0117	0.0011
249	Cis-3-Heptene	C7H14	0.088	0.0108	0.0011
216	1-Hexene	C6H12	0.08856	0.0112	0.0011
239	3-Eth-1-Pentene	C7H14	0.09369	0.0125	0.0013
226	4-Mth-1-Hexene	C7H14	0.1016	0.0138	0.0015
240	3-Mth-1-Hexene	C7H14	0.09312	0.0124	0.0013
419	3-Mth-1-Butyne	C5H8	0.09059	0.0129	0.0015
233	2-Eth-1-Pentene	C7H14	0.10348	0.013	0.0013
238	2-Mth-1-Hexene	C7H14	0.09743	0.0122	0.0012
416	1-Octyne	C8H14	0.08983	0.0116	0.0011
289	2,3Dimeth Hexene	C8H16	0.09873	0.013	0.0013
234	1-Heptene	C7H14	0.09304	0.0116	0.0011
413	1-Hexyne	C6H10	0.08618	0.0113	0.0012
237	Trans-3-Heptene	C7H14	0.08594	0.0108	0.0011
236	Trans-2-Heptene	C7H14	0.09251	0.0116	0.0011

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

251	Trans-2-Octene	C8H16	0.09347	0.0114	0.0011
279	Trans-4-Octene	C8H16	0.08691	0.0104	0.001
277	Trans-3-Octene	C8H16	0.08946	0.0108	0.001
2252	2Methl-1-Heptene	C8H16	0.09883	0.012	0.0011
250	1-Octene	C8H16	0.09612	0.012	0.0012
258	2-Ethyl-1-Hexene	C8H16	0.10131	0.0126	0.0011
280	3-Octene	C8H16	0.08818	0.0106	0.001
278	4-Octene	C8H16	0.08794	0.0106	0.0009
276	2-Octene	C8H16	0.09501	0.0116	0.0011
259	1-Nonene	C9H18	0.09934	0.0124	0.0012
262	1-Dodecene	C12H24	0.10777	0.0133	0.0012
263	1-Tridecene	C13H26	0.11001	0.0136	0.0013
264	1-Tetradecene	C14H28	0.11294	0.0138	0.0013
265	1-Pentadecene	C15H30	0.11554	0.0141	0.0013
266	1-Hexadecene	C16H32	0.1182	0.0144	0.0013
267	1-Octadecene	C18H36	0.12129	0.0146	0.0014
281	1-Heptadecene	C17H34	0.11952	0.0143	0.0013
284	1-Eicosene	C20H40	0.12721	0.0156	0.0014
283	1-Nonadecene	C19H38	0.12397	0.015	0.0014
3	Propane	C3H8	0.04518	0.0044	0.0003
4	I-Butane	C4H10	0.07366	0.0085	0.0008
9	Neopentane	C5H12	0.07528	0.0084	0.0007
5	N-Butane	C4H10	0.06663	0.0072	0.0006
7	pentane	C5H12	0.08196	0.0093	0.0008
44	Hexamethylethane	C8H18	0.18135	0.0263	0.003
25	223-TriMthButane	C7H16	0.14988	0.0203	0.0022
24	3,3-DiMthPentane	C7H16	0.12747	0.016	0.0015
51	2,2,3,3-4Mth-C5	C9H20	0.21057	0.0308	0.0035
21	2,2-DiMthPentane	C7H16	0.10339	0.0125	0.0012
42	2,3,3-TriMth-C5	C8H18	0.17034	0.0236	0.0025
22	2,3-DiMthPentane	C7H16	0.14001	0.0191	0.002
40	2,2,3-TriMth-C5	C8H18	0.14937	0.0202	0.0021
23	2,4-DiMthPentane	C7H16	0.10589	0.0135	0.0013
41	2,2,4-TriMth-C5	C8H18	0.11033	0.0137	0.0013
39	3-Mth-3-Eth-C5	C8H18	0.14562	0.0186	0.0018
20	3-Ethylpentane	C7H16	0.11551	0.0145	0.0014
52	2,2,3,4-4Mth-C5	C9H20	0.16979	0.0241	0.0027
54	2334TetrMethPent	C9H20	0.21116	0.0317	0.0037
53	2,2,4,4-4Mth-C5	C9H20	0.13282	0.017	0.0017
43	2,3,4-TriMth-C5	C8H18	0.16023	0.023	0.0026
36	3,3-DiMth-Hexane	C8H18	0.12202	0.0151	0.0014
19	3-Methylhexane	C7H16	0.11004	0.0138	0.0013
18	2-Methylhexane	C7H16	0.104	0.0129	0.0012
38	2-Mth-3-Eth-C5	C8H18	0.1317	0.0174	0.0018
190	2,2-2C1-3-C2-C5	C9H20	0.13898	0.0186	0.0019

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

32	2,2-DiMth-Hexane	C8H18	0.1051	0.0128	0.0012
37	3,4-DiMth-Hexane	C8H18	0.13934	0.0188	0.002
50	3,3-DiEthPentane	C9H20	0.15504	0.0196	0.0019
34	2,4-DiMth-Hexane	C8H18	0.10832	0.0138	0.0014
33	2,3-DiMth-Hexane	C8H18	0.13136	0.0175	0.0018
17	N-Heptane	C7H16	0.10121	0.0121	0.0011
49	244TriMethHexane	C9H20	0.12769	0.0162	0.0016
192	2,4-2C1-3-C2-C5	C9H20	0.14465	0.0199	0.0021
47	2,2,5-TriMth-C6	C9H20	0.10647	0.0131	0.0013
35	2,5-DiMth-Hexane	C8H18	0.10954	0.014	0.0014
31	3-Ethylhexane	C8H18	0.1115	0.0138	0.0013
30	4-Methylheptane	C8H18	0.10883	0.0135	0.0013
29	3-Methylheptane	C8H18	0.11304	0.0141	0.0013
28	2-Methylheptane	C8H18	0.10865	0.0135	0.0013
96	2,2-DiMthHeptane	C9H20	0.10834	0.0129	0.0012
176	2,6-DiMthHeptane	C9H20	0.11021	0.0143	0.0014
27	N-Octane	C8H18	0.10818	0.013	0.0012
94	3-Ethylheptane	C9H20	0.11177	0.0137	0.0013
92	3-Methyloctane	C9H20	0.11555	0.0143	0.0014
93	4-Methyloctane	C9H20	0.11043	0.0135	0.0013
91	2-Methyloctane	C9H20	0.1128	0.0141	0.0014
72	2,2-DiMthOctane	C10H22	0.11063	0.0136	0.0012
2095	2,3Dimethloctane	C10H22	0.12935	0.0167	0.0017
2096	2,4Dimethloctane	C10H22	0.10361	0.013	0.0012
2098	2,6DimethlOctane	C10H22	0.11669	0.015	0.0015
2097	2,5Dimethloctane	C10H22	0.11117	0.0139	0.0013
2099	2,7DimethlOctane	C10H22	0.11563	0.0147	0.0014
46	N-Nonane	C9H20	0.11325	0.0138	0.0013
88	5-Methylnonane	C10H22	0.11046	0.0133	0.0013
85	3-Methylnonane	C10H22	0.12083	0.0151	0.0014
87	4-Methylnonane	C10H22	0.11213	0.0137	0.0013
86	2-Methylnonane	C10H22	0.11747	0.0146	0.0014
56	N-Decane	C10H22	0.11882	0.0145	0.0013
63	N-Undecane	C11H24	0.12259	0.015	0.0014
64	N-Dodecane	C12H26	0.12666	0.0155	0.0014
65	N-Tridecane	C13H28	0.12937	0.016	0.0015
66	N-Tetradecane	C14H30	0.13306	0.0165	0.0015
67	N-Pentadecane	C15H32	0.13632	0.017	0.0016
68	N-Hexadecane	C16H34	0.13933	0.0172	0.0016
69	N-Heptadecane	C17H36	0.14337	0.018	0.0017
70	N-Octadecane	C18H38	0.14361	0.018	0.0017
71	N-Nonadecane	C19H40	0.14621	0.0182	0.0017
73	N-Eicosane	C20H42	0.15089	0.0189	0.0017
74	n-HENEICOSANE	C21H44	0.15316	0.019	0.0017
75	n-DOCOSANE	C22H46	0.1548	0.0188	0.0017

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

76	n-TRICOSANE	C23H48	0.15562	0.0197	0.0018
77	n-Tetracosane	C24H50	0.15766	0.0201	0.0018
78	n-PENTACOSANE	C25H52	0.1602	0.0201	0.0018
79	n-HEXACOSANE	C26H54	0.16197	0.0207	0.0019
81	n-Octacosane	C28H58	0.16171	0.0208	0.0019
2081	n-TRICONTANE	C30H62	0.17325	0.0217	0.0018
2082	n-Dotriacontane	C32H66	0.17382	0.0218	0.0018
2086	Hexatriacontane	C36H74	0.18335	0.023	0.0018

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

	Cyclic Hydrocarbons				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
269	Cyclopentene	C5H8	0.08423	0.0112	0.0012
270	Cyclohexene	C6H10	0.0977	0.0131	0.0014
287	3MthCyclopentene	C6H10	0.08036	0.0112	0.0012
286	1-MthCyclPentene	C6H10	0.09472	0.0122	0.0012
288	4MthCyclopenten	C6H10	0.08367	0.0118	0.0013
273	Cycloheptene	C7H12	0.10014	0.0134	0.0014
274	Cyclooctene	C8H14	0.09947	0.0131	0.0013
101	Cyclopropane	C3H6	0.05308	0.0057	0.0005
810	ADAMANTANE	C10H16	0.11751	0.0138	0.0012
102	Cyclobutane	C4H8	0.08124	0.0095	0.0008
104	Cyclopentane	C5H10	0.08991	0.0108	0.001
137	Cyclohexane	C6H12	0.09109	0.0107	0.0009
105	MthCyclopentane	C6H12	0.09789	0.0123	0.0012
146	Cs-1,4-2C1-CycC6	C8H16	0.10751	0.0136	0.0013
142	Cs-1,2-2C1-CycC6	C8H16	0.12445	0.0163	0.0017
141	1,1-2C1-CycC6	C8H16	0.09876	0.0116	0.001
145	Ts-1,3-2C1-CycC6	C8H16	0.108	0.0137	0.0014
144	Cs-1,3-2C1-CycC6	C8H16	0.09601	0.0117	0.0011
147	Ts-1,4-2C1-CycC6	C8H16	0.09367	0.0112	0.001
143	Ts-1,2-2C1-CycC6	C8H16	0.1053	0.0129	0.0012
138	MthCyclohexane	C7H14	0.09369	0.0111	0.001
159	Cycloheptane	C7H14	0.11913	0.0147	0.0014
140	Ethylcyclohexane	C8H16	0.10201	0.0123	0.0011
154	Trans-Decalin	C10H18	0.10609	0.0127	0.0012
149	N-PropylCyc-C6	C9H18	0.0992	0.0119	0.0011
109	Cs-1,2-2C1-CycC5	C7H14	0.12305	0.0168	0.0018
110	Ts-1,2-2C1-CycC5	C7H14	0.09861	0.0127	0.0013

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

112	Ts-1,3-2C1-CycC5	C7H14	0.09973	0.0128	0.0013
107	Eth-Cyclopentane	C7H14	0.10127	0.0127	0.0012
114	N-PropCycPentane	C8H16	0.09977	0.0124	0.0012
108	1,1-DiMthCycC5	C7H14	0.08933	0.0108	0.001
111	Cs-1,3-2C1-CycC5	C7H14	0.09754	0.0125	0.0012
152	N-ButylCycHexane	C10H20	0.09899	0.0118	0.0011
160	Cyclooctane	C8H16	0.13523	0.0169	0.0016
153	Cis-Decalin	C10H18	0.13129	0.0167	0.0017
115	ISOPROPYLCYCLOPENTANE	C8H16	0.11417	0.0149	0.0015
150	Isopropyl-CycC6	C9H18	0.1161	0.0149	0.0015
116	1-C1-1-C2-CycC5	C8H16	0.09977	0.0125	0.0012
122	Butylcyclpentane	C9H18	0.09817	0.0122	0.0012
155	1,1-Bicyclohexyl	C12H22	0.1207	0.0146	0.0013
158	N-Decylcyclo-C6	C16H32	0.09761	0.0113	0.001

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

	Aromatic Hydrocarbons				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
307	1,4-Pentadiene	C5H8	0.08864	0.0128	0.0015
306	1-ts3-Pentadiene	C5H8	0.1293	0.0212	0.0029
414	2-Methyl-1-Butenyne	C5H6	0.09021	0.0121	0.0013
305	Cs1,3-Pentadiene	C5H8	0.1374	0.0231	0.0033
309	Isoprene	C5H8	0.13129	0.0206	0.0027
421	1-Pentene-4-yne	C5H6	0.10851	0.0156	0.0018
303	1,3-Butadiene	C4H6	0.11545	0.0182	0.0024
332	1,4-CyclHexadien	C6H8	0.1066	0.0183	0.0025
501	Benzene	C6H6	0.11495	0.0171	0.0021
315	Cyclopentadiene	C5H6	0.08122	0.0106	0.001
319	Diisopropenyl	C6H10	0.14517	0.0227	0.0029
615	Ethynylbezene	C8H6	0.07973	0.0081	0.0006
601	Styrene	C8H8	0.10551	0.012	0.0011
331	1,3-CycHexadiene	C6H8	0.08769	0.013	0.0016
310	1,5-Hexadiene	C6H10	0.08712	0.0116	0.0012
312	MthCycPentadiene	C6H8	0.09347	0.0136	0.0016
420	1-Pentene-3-yne	C5H6	0.19377	0.0256	0.0027
502	Toluene	C7H8	0.10725	0.0144	0.0015
521	T-Butylbenzene	C10H14	0.09199	0.0094	0.0007
320	Dipropylene	C6H10	0.13289	0.0219	0.003
520	Sec-Butylbenzene	C10H14	0.10314	0.0124	0.0012

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

313	1,4-Hexadiene	C6H10	0.09075	0.0129	0.0015
314	Dipropylene	C6H10	0.12756	0.0209	0.0029
316	DiCycPentadiene	C10H12	0.04571	0.0063	0.0007
333	1,5-CycOctadiene	C8H12	0.10314	0.0156	0.0019
701	Naphthalene	C10H8	0.16945	0.0168	0.0011
504	Ethylbenzene	C8H10	0.0983	0.0127	0.0013
820	Indan	C9H10	0.11438	0.0145	0.0014
505	O-Xylene	C8H10	0.12171	0.0161	0.0017
612	P-Methylstyrene	C9H10	0.11197	0.0125	0.001
330	DIISOCROTYL	C8H14	0.14782	0.0226	0.0028
507	P-Xylene	C8H10	0.1035	0.013	0.0013
329	DIISOBUTENYL	C8H14	0.0956	0.0127	0.0013
506	M-Xylene	C8H10	0.10578	0.0135	0.0013
603	Methylstyrene	C9H10	0.1107	0.0125	0.001
613	Alpha-MthStyrene	C9H10	0.10568	0.0118	0.001
510	Isopropylbenzene	C9H12	0.11197	0.0145	0.0015
724	2-Methylindene	C10H10	0.1293	0.0141	0.0011
285	Vinylcyclohexene	C8H12	0.08383	0.0112	0.0012
803	Indene	C9H8	0.11687	0.0098	0.0006
706	Tetralin	C10H12	0.12925	0.0167	0.0017
511	O-Ethyltoluene	C9H12	0.10607	0.0134	0.0013
723	1-Methylindene	C10H10	0.08478	0.0132	0.0017
738	Fluorene	C13H10	0.27847	0.0277	0.0018
619	Tr-1PropenylBz	C9H10	0.12031	0.0145	0.0013
525	O-Diethylbenzene	C10H14	0.09111	0.011	0.001
618	Propenyl Bz(cis)	C9H10	0.12208	0.0143	0.0012
602	O-Methylstyrene	C9H10	0.10642	0.0121	0.001
702	1-MthNaphthalene	C11H10	0.20251	0.0213	0.0015
509	N-Propylbenzene	C9H12	0.0933	0.0116	0.0011
526	M-Diethylbenzene	C10H14	0.08656	0.0102	0.0009
583	Cs-2-PhnButene-2	C10H12	0.12394	0.014	0.0012
543	M-DiisopropylBz	C12H18	0.09877	0.0116	0.001
584	Ts-2-PhnButene-2	C10H12	0.07079	0.0069	0.0005
580	1,2-DiC1-3C2-Bz	C10H14	0.12133	0.0154	0.0015
704	1-EthNaphthalene	C12H12	0.17973	0.0186	0.0013
512	M-Ethyltoluene	C9H12	0.09576	0.0119	0.0011
522	1-Mth-2-iC3-Benz	C10H14	0.11523	0.0143	0.0013
513	P-Ethyltoluene	C9H12	0.0981	0.0119	0.0011
514	1,2,3-Mesitylene	C9H12	0.14195	0.0187	0.0019
614	M-Divinylbenzene	C10H10	0.12014	0.0118	0.0008
524	1-Mth-4-iC3-Benz	C10H14	0.11101	0.0135	0.0013
822	Gamma-Terpinene	C10H16	0.12215	0.0173	0.0019
821	Alpha-Terpinene	C10H16	0.09872	0.0129	0.0013
523	1-Mth-3-iC3-Benz	C10H14	0.1065	0.0129	0.0012
703	2-MthNaphthalene	C11H10	0.18956	0.0187	0.0013

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

557	CycHexylBenzene	C12H16	0.12722	0.0174	0.0019
515	1,2,4-Mesitylene	C9H12	0.12014	0.0151	0.0014
519	Isobutylbenzene	C10H14	0.08505	0.0106	0.001
424	DiPhnAcetylene	C14H10	0.25184	0.0259	0.0017
544	P-DiisopropylBz	C12H18	0.11614	0.0146	0.0014
518	N-Butylbenzene	C10H14	0.09605	0.0118	0.0011
516	1,3,5-Mesitylene	C9H12	0.10561	0.0131	0.0012
809	Acenaphthalene	C12H8	0.25107	0.0229	0.0013
725	123-TriMthIndene	C12H14	0.13793	0.0144	0.001
527	1,4-DiEthBenzene	C10H14	0.09197	0.011	0.001
558	Diphenyl	C12H10	0.15791	0.0169	0.0013
576	2-Ethyl-m-Xylene	C10H14	0.11078	0.0136	0.0013
620	p-ISOPROPENYLSTY	C11H12	0.22676	0.0206	0.0014
585	o-PropylToluene	C10H14	0.09858	0.0117	0.0011
577	2-Ethyl-p-Xylene	C10H14	0.10211	0.0125	0.0011
579	4-Ethyl-o-Xylene	C10H14	0.10846	0.0133	0.0012
586	m-Propyltoluene	C10H14	0.09094	0.0108	0.001
587	p-Propyltoluene	C10H14	0.09398	0.0112	0.001
578	4-Ethyl-m-Xylene	C10H14	0.10665	0.013	0.0012
575	5-Ethyl-m-Xylene	C10H14	0.09176	0.0107	0.0009
530	Prehnitene	C10H14	0.16244	0.0216	0.0022
709	2,6-2Mth-Naphtha	C12H12	0.20508	0.0215	0.0015
715	2,7-2Mth-Naphtha	C12H12	0.2102	0.0224	0.0015
719	2-ETHYLNAPHTHALENE	C12H12	0.19559	0.0166	0.0009
621	p-tert-BUTYLSTY	C12H16	0.13306	0.0122	0.0008
532	1,2,4,5-TetMthBz	C10H14	0.13275	0.0168	0.0016
531	1,2,3,5-TetMthBz	C10H14	0.13739	0.0176	0.0017
533	p-tert-BUTYL ET	C12H18	0.09611	0.0081	0.0005
567	N-Pentylbenzene	C11H16	0.09804	0.0118	0.0011
718	1-n-PROPYLNAPHTH	C13H14	0.19178	0.0163	0.0009
562	1,1-DiPhnEthane	C14H14	0.11977	0.0134	0.0011
616	4-ISOBUTYLSTYRE	C12H16	0.20689	0.0235	0.0019
260	1-Decene	C10H20	0.10245	0.0128	0.0012
735	Cis-Stilbene	C14H12	0.10475	0.0102	0.0007
568	Hexylbenzene	C12H18	0.09994	0.012	0.0011
563	Diphenylmethane	C13H12	0.11269	0.0126	0.0011
564	1,2-DiPhnEthane	C14H14	0.08377	0.0102	0.0009
804	Anthracene	C14H10	0.54488	0.0569	0.0036
736	Trans-Stilbene	C14H12	0.18979	0.0243	0.0022
805	Phenanthrene	C14H10	0.49513	0.053	0.0035
713	1-ButNaphthalene	C14H16	0.17584	0.0184	0.0013
807	Pyrene	C16H10	1.00681	0.1079	0.0066
261	1-Undecene	C11H22	0.10515	0.013	0.0013
581	23-2C1-23-2PhnC4	C18H22	0.11218	0.0102	0.0006
549	N-Heptylbenzene	C13H20	0.10396	0.0119	0.0011

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

710	1-PhnNaphthalene	C16H12	0.24426	0.0233	0.0014
566	2,4-Diphenyl-4-M	C18H20	0.15396	0.0157	0.0011
561	O-Terphenyl	C18H14	0.13323	0.0104	0.0005
569	N-Octylbenzene	C14H22	0.10486	0.0123	0.0011
565	Triphenylmethane	C19H16	0.14673	0.014	0.0009
714	N-C6-Naphthalene	C16H20	0.1919	0.0211	0.0016
717	Fluoranthene	C16H10	0.81953	0.0764	0.0036
716	1-Hexyl-Tetralin	C16H24	0.15104	0.0151	0.001
731	TriPhnEthylene	C20H16	0.21831	0.0231	0.0016
806	Chrysene	C18H12	1.35847	0.1957	0.0182
588	1,1,2TriPhenEth	C20H18	0.08878	0.0072	0.0004
711	1-n-NonylNaphtha	C19H26	0.21859	0.0225	0.0015
570	N-Nonylbenzene	C15H24	0.10929	0.0126	0.0012
712	1-Decyl Naphtha	C20H28	0.22548	0.0232	0.0016
559	P-Terphenyl	C18H14	0.36067	0.0447	0.0037
560	M-Terphenyl	C18H14	0.30927	0.0343	0.0024
589	TetraPhenylMetha	C25H20	0.33702	0.0379	0.0028
554	Decylbenzene	C16H26	0.1097	0.0129	0.0012
732	TetraPhnEthylene	C26H20	0.27429	0.0294	0.002
574	N-Dodecylbenzene	C18H30	0.11212	0.0136	0.0012
571	N-Undecylbenzene	C17H28	0.11181	0.013	0.0012
572	Tridecylbenzene	C19H32	0.11461	0.0138	0.0012
573	n-TETRADECYLBENZ	C20H34	0.14796	0.0169	0.0013
2575	n-PENTADECYLBENZ	C21H36	0.15123	0.0175	0.0014
2576	n-HEXADECYLBENZ	C22H38	0.15398	0.0183	0.0015
2577	n-HEPTADECYLBENZ	C23H40	0.15523	0.0178	0.0014
2578	n-OCTADECYLBENZE	C24H42	0.15731	0.0179	0.0014

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

	Halocarbons				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1544	Allyl Chloride	C3H5Cl	0.1045	0.0149	0.0017
1595	2-Chloropropene	C3H5Cl	0.13289	0.0177	0.0018
1531	3-Chloropropyne	C3H3Cl	0.11306	0.0162	0.0018
1561	6Cl-1,3Butadiene	C4Cl6	0.15126	0.0166	0.0014
1535	T-Butyl Chloride	C4H9Cl	0.12388	0.0156	0.0015
1583	Chloroprene	C4H5Cl	0.04499	0.0046	0.0004
1530	Isopropyl Cl	C3H7Cl	0.12358	0.0168	0.0017

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1572	O-DiCl-Benzene	C6H4Cl2	0.11404	0.0154	0.0016
1585	Propyl Chloride	C3H7Cl	0.09268	0.012	0.0012
1684	Isopropyl Iodide	C3H7I	0.09625	0.0135	0.0015
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	0.12918	0.0183	0.0022
1651	2-Bromopropane	C3H7Br	0.13459	0.0188	0.0021
1691	Iodobenzene	C6H5I	0.07772	0.0081	0.0006
1860	Fluorobenzene	C6H5F	0.131	0.0195	0.0023
1571	Chlorobenzene	C6H5Cl	0.1111	0.0154	0.0017
1680	Bromobenzene	C6H5Br	0.08536	0.0083	0.0006
1526	1,2-DiCl-Propane	C3H6Cl2	0.08873	0.0109	0.001
1683	Propyl Iodide	C3H7I	0.10391	0.0142	0.0015
1576	Benzotrichloride	C7H5Cl3	0.15016	0.0105	0.0004
1536	2,3-DICHLOROBUT	C4H8Cl2	0.08933	0.0108	0.001
2638	2-Bromobutane	C4H9Br	0.136	0.0202	0.0023
1586	1-Chlorobutane	C4H9Cl	0.09603	0.0122	0.0012
1573	M-DiCl-Benzene	C6H4Cl2	0.09451	0.012	0.0011
2634	Benzotrifluoride	C7H5F3	0.09527	0.0074	0.0004
1574	P-DiCl-Benzene	C6H4Cl2	0.09768	0.0127	0.0013
1650	1-Bromopropane	C3H7Br	0.13556	0.0182	0.0019
1587	2-Chlorobutane	C4H9Cl	0.1258	0.0161	0.0016
2653	8F-2-Butene	C4F8	0.00574	0.0001	0
1678	M-Dibromobenzene	C6H4Br2	0.09104	0.0069	0.0003
1537	1,2-DiCl-Butane	C4H8Cl2	0.1322	0.0171	0.0017
1597	34-DiCl-1-Butene	C4H6Cl2	0.06786	0.0095	0.0011
1577	O-Chlorotoluene	C7H7Cl	0.10875	0.0143	0.0015
1532	123-3Cl-Propane	C3H5Cl3	0.07765	0.0095	0.0009
1578	P-Chlorotoluene	C7H7Cl	0.11654	0.0158	0.0017
1562	Benzyl Chloride	C7H7Cl	0.11231	0.0128	0.001
2661	P-Bromotoluene	C7H7Br	0.10139	0.0102	0.0007
1508	1,4-DiCl-Butane	C4H8Cl2	0.12401	0.0174	0.0019
1655	1-Bromobutane	C4H9Br	0.13998	0.018	0.0019
1599	BenzylDichloride	C7H6Cl2	0.15197	0.0158	0.0011
2652	Perfluoropropane	C3F8	0.0174	0.0005	0
1505	2-Butylene DiCl	C4H6Cl2	0.15601	0.0255	0.0034
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	0.09176	0.0135	0.0016
1588	1-Chloropentane	C5H11Cl	0.10083	0.012	0.0011
1592	1,2,4-TriCl-Bz	C6H3Cl3	0.08949	0.0108	0.0009
1579	2,4-2Cl-Toluene	C7H6Cl2	0.10636	0.0139	0.0014
2593	1,3,5-TriCl-BZ	C6H3Cl3	0.0802	0.0094	0.0008
1697	1-Br-Naphthalene	C10H7Br	0.23843	0.0232	0.0014
1622	Perfluorobutane	C4F10	0.10718	0.0057	0.0002
1857	P-Cl-Benzo-TriF	C7H4ClF3	0.10627	0.0087	0.0005
1509	1,5-DiCl-Pentane	C5H10Cl2	0.134	0.019	0.0021
1589	1-Cl-Naphthalene	C10H7Cl	0.21451	0.0219	0.0016
1582	6ClCycPentadiene	C5Cl6	0.13031	0.0146	0.0012

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1864	Perfluorobenzene	C6F6	0.09589	0.0124	0.0012
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	0.13452	0.0122	0.0007
1667	1-Bromoheptane	C7H15Br	0.14056	0.0182	0.0018
1575	HexaCl-Benzene	C6Cl6	0.07187	0.0108	0.0014
2640	Freon 123B1	C2HBrClF3	0.07579	0.0061	0.0004
1504	Vinyl Chloride	C2H3Cl	0.05556	0.0066	0.0007
1672	1,1-DiBr-Ethane	C2H4Br2	0.11526	0.0176	0.0022
1580	Acetylene DiCl	C2H2Cl2	0.11729	0.0158	0.0017
1692	Diiodomethane	CH2I2	0.11097	0.0184	0.0027
1698	Bromoform	CHBr3	0.08832	0.0111	0.0011
2687	Freon 13B1	CBrF3	0.00215	0.0001	0
2690	Br-3F-Ethylene	C2BrF3	0.0448	0.003	0.0001
1649	Tetrabromoethane	C2H2Br4	0.10249	0.0141	0.0015
2686	Freon 12B1	CBrClF2	0.04657	0.0036	0.0002
1503	Ethyl Chloride	C2H5Cl	0.09187	0.0122	0.0013
2641	Br-TriCl-Methane	CBrCl3	0.04865	0.0029	0.0001
1641	Methyl Bromide	CH3Br	0.14693	0.0214	0.0025
2688	Freon 12B2	CBr2F2	0.04159	0.0032	0.0002
2545	2,3-DiCl-Propene	C3H4Cl2	0.11138	0.0161	0.002
1673	1,2-DiBr-Ethane	C2H4Br2	0.17125	0.0237	0.0024
2637	Dibromomethane	CH2Br2	0.15478	0.0232	0.0028
1542	TetraCl-Ethylene	C2Cl4	0.07769	0.0081	0.0006
1541	TriCl-Ethylene	C2HCl3	0.12905	0.0156	0.0014
1527	111-TriCl-Ethane	C2H3Cl3	0.05718	0.0037	0.0002
1612	Cl-2F-Ethylene	C2HClF2	0.14817	0.0182	0.0016
2639	Br-Cl-Methane	CH2BrCl	0.09337	0.013	0.0014
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	0.07609	0.009	0.0009
1682	Ethyl Iodide	C2H5I	0.10848	0.0159	0.0018
1522	1,1-DiCl-Ethane	C2H4Cl2	0.1224	0.017	0.0018
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	0.18794	0.0301	0.0039
1525	Hexachloroethane	C2Cl6	0.15248	0.0102	0.0004
1528	1112-4Cl-Ethane	C2H2Cl4	0.07697	0.0058	0.0003
1590	Penta-Cl-Ethane	C2HCl5	0.10468	0.0076	0.0004
1529	1122-4Cl-Ethane	C2H2Cl4	0.09395	0.0119	0.0011
2693	Perfluoroethane	C2F6	0.00079	0	0
2692	Cl-PentaF-Ethane	C2ClF5	0.01956	0.0011	0
2655	122-3Cl-112-3FC2	C2Cl3F3	0.09043	0.0123	0.0013
1609	12-2Cl-1122-4FC2	C2Cl2F4	0.07783	0.01	0.001
2526	1,1-DiCl-Propane	C3H6Cl2	0.12306	0.0163	0.0017
1645	Ethyl Bromide	C2H5Br	0.1365	0.019	0.0022
2658	1112-4Cl-22-2FC2	C2Cl4F2	0.04708	0.0032	0.0001
1619	111-3F-Ethane	C2H3F3	0.05238	0.0038	0.0002
1524	1,1,2-3Cl-Ethane	C2H3Cl3	0.0833	0.0104	0.001
2691	Genetron 1113	C2ClF3	0.04216	0.0028	0.0001
1591	Vinylidene DiCl	C2H2Cl2	0.10648	0.0121	0.0011

Table B.8 Detailed Vapor Pressures for Different Organic Compounds Calculated by GC-ESD Equation of State (Continued)

1614	Difluoromethane	CH2F2	0.06797	0.0014	0.0009
2694	Vinyl Bromide	C2H3Br	0.07812	0.0099	0.0009
1694	Refrigerant 123	C2HCl2F3	0.04484	0.0032	0.0002
1523	1,2-DiCl-Ethane	C2H4Cl2	0.08256	0.0109	0.0012
2656	1122-4Cl-12-2FC2	C2Cl4F2	0.10426	0.0148	0.0017
2527	1,3-DiCl-Propane	C3H6Cl2	0.10172	0.0134	0.0014

TableB. 9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG.

Dip ID	Nitrates Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1761	Nitroethane	C2H5NO2	0.12339	0.0168	0.0018
1763	2-Nitropropane	C3H7NO2	0.06112	0.0065	0.0005
1762	1-Nitropropane	C3H7NO2	0.08659	0.0106	0.001
1779	P-Nitrotoluene	C7H7NO2	0.11794	0.0136	0.0013
1886	Nitrobenzene	C6H5NO2	0.11672	0.0138	0.0013
1778	O-Nitrotoluene	C7H7NO2	0.07857	0.0086	0.0007
1780	M-Nitrotoluene	C7H7NO2	0.10082	0.0114	0.0009
1891	O-Nitroanisole	C7H7NO3	0.13644	0.0193	0.0021
2740	M-Dinitrobenzene	C6H4N2O4	0.09363	0.0093	0.0007
2742	P-Dinitrobenzene	C6H4N2O4	0.08495	0.0081	0.0006
2741	O-Dinitrobenzene	C6H4N2O4	0.13681	0.0139	0.0011
2749	3,5-DiNitToluene	C7H6N2O4	0.07738	0.0079	0.0005
2743	DNT	C7H6N2O4	0.08158	0.0073	0.0004
2745	3,4-DiNitToluene	C7H6N2O4	0.1267	0.0128	0.0008
2744	2,6-DiNitToluene	C7H6N2O4	0.08158	0.0073	0.0004
2748	2,5-DiNitToluene	C7H6N2O4	0.08116	0.0073	0.0004
2746	1,3,5-TrinitroBz	C6H3N3O6	0.05561	0.0044	0.0003
2747	Trinitrotoluene	C7H5N3O6	0.03238	0.0021	0.0001

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	Thiols Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1802	Ethyl Mercaptan	C2H6S	0.29672	0.0562	0.0087
1820	Dimethyl Sulfide	C2H6S	0.1493	0.0228	0.0028
1843	Thiacyclopentane	C4H8S	0.35892	0.0701	0.0112
1803	1-Propanethiol	C3H8S	0.23809	0.0424	0.0062
1805	Isobut Mercaptan	C4H10S	0.15259	0.0237	0.0029
6860	Ethylenedithiol	C2H6S2	0.37218	0.0746	0.0121
1811	Cyclohexanethiol	C6H12S	0.18811	0.0289	0.0034
1828	DiMth Disulfide	C2H6S2	0.15486	0.0241	0.003
1841	Butanethiol	C4H10S	0.20474	0.0342	0.0046
1814	Methylproylsulf	C4H10S	0.19062	0.0317	0.0042
2816	ETHYLtBUTYL SUL	C6H14S	0.08643	0.0111	0.0011
1818	Diethyl Sulfide	C4H10S	0.17001	0.0266	0.0031
1812	Benzyl Mercaptan	C7H8S	0.14585	0.0224	0.0028
1838	T-OctylMercaptan	C8H18S	0.05399	0.0056	0.0004
1827	1-Pentanethiol	C5H12S	0.18247	0.0296	0.0038

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

2815	METHnBUTYL SULFD	C5H12S	0.0968	0.0121	0.0012
1824	DiethylDisulfide	C4H10S2	0.10677	0.0142	0.0014
1807	N-Hexylmercaptan	C6H14S	0.16535	0.0257	0.0031
6857	Dimercaptoethyl	C4H10OS2	0.24164	0.0411	0.0055
1839	1-Heptanethiol	C7H16S	0.15387	0.0234	0.0028
1829	DiProp Disulfide	C6H14S2	0.08712	0.0108	0.0009
1809	1-Octanethiol	C8H18S	0.14225	0.021	0.0024
1808	N-Nonanethiol	C9H20S	0.13268	0.0192	0.0023
1826	1-Decanethiol	C10H22S	0.12567	0.018	0.002
2838	tertDodecanThiol	C12H26S	0.05834	0.0071	0.0006
1825	1-Undecanethiol	C11H24S	0.11841	0.0167	0.0019
1837	Dodecylthiol	C12H26S	0.11342	0.0146	0.0015

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	Epoxides Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1440	ISOBUTYLENE OXID	C4H8O	0.35806	0.0651	0.0093
1479	Tetrahydrofuran	C4H8O	0.38287	0.0731	0.0112
1477	2,5-Dihydrofuran	C4H6O	0.24369	0.0405	0.0051
1408	1-Methoxypropane	C4H10O	0.10127	0.0132	0.0013
1411	2-Methoxypropane	C4H10O	0.07512	0.0091	0.0008
1421	1,4-Dioxane	C4H8O2	0.32595	0.0548	0.0069
2422	1,3-DIOXANE	C4H8O2	0.35673	0.0638	0.0089
1426	2-Methoxybutane	C5H12O	0.06819	0.0081	0.0007
1413	1-Methoxybutane	C5H12O	0.09922	0.0128	0.0012
1461	Methoxybenzene	C7H8O	0.13078	0.0185	0.002
1448	1-Ethoxybutane	C6H14O	0.10345	0.0137	0.0013
1429	1-MethoxyPentane	C6H14O	0.12632	0.0174	0.0018
6885	Ethyl-3-Ethoxypr	C7H14O3	0.11031	0.0144	0.0014

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	Ether Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1401	Dimethyl Ether	C2H6O	0.15098	0.022	0.0024
1407	MethylEthylEther	C3H8O	0.16663	0.0269	0.0034

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

1470	VinylMethylEther	C3H6O	0.09826	0.0131	0.0013
1405	MTBE	C5H12O	0.08324	0.0103	0.001
1445	VinylEthyl Ether	C4H8O	0.11627	0.0157	0.0016
1402	Diethyl Ether	C4H10O	0.12089	0.0168	0.0018
1431	Methylal	C3H8O2	0.06511	0.0071	0.0006
1428	T-But EthylEther	C6H14O	0.07431	0.0091	0.0008
1427	TAME	C6H14O	0.08626	0.0105	0.001
1410	Mth Isobut Ether	C5H12O	0.06681	0.0078	0.0007
1430	Eth-t-Pent-Ether	C7H16O	0.0758	0.0089	0.0007
1403	DiisopropylEther	C6H14O	0.04067	0.0037	0.0002
1415	Eth Propyl Ether	C5H12O	0.10823	0.0141	0.0015
1455	Dimethyl Acetal	C4H10O2	0.17377	0.026	0.0029
1446	Dipropyl Ether	C6H14O	0.09686	0.0122	0.0012
1447	Butyl VinylEther	C6H12O	0.10183	0.0137	0.0014
1462	EthylPhenylEther	C8H10O	0.1225	0.0174	0.0019
1406	Di-sec-But Ether	C8H18O	0.04695	0.0045	0.0003
1432	Acetal	C6H14O2	0.05368	0.0054	0.0004
1460	BenzylEthylEther	C9H12O	0.11477	0.0155	0.0015
1050	Paraldehyde	C6H12O3	0.03992	0.0032	0.0002
1404	Di-n-Butyl Ether	C8H18O	0.09125	0.0116	0.0011
1420	Anethole	C10H12O	0.10125	0.0133	0.0013
1456	DimethylCarbitol	C6H14O3	0.09616	0.0118	0.0011
1463	Dibenzyl Ether	C14H14O	0.06836	0.0102	0.0011
1425	Di-n-PentylEther	C10H22O	0.0901	0.0111	0.001
1458	Diethyl Carbitol	C8H18O3	0.08593	0.0103	0.0008
1412	Dihexyl Ether	C12H26O	0.08634	0.0118	0.0012
1454	Triglyme	C8H18O4	0.0744	0.0094	0.0009
1459	Dibutyl Carbitol	C12H26O3	0.07258	0.0076	0.0005
1424	Di-n-Octyl Ether	C16H34O	0.07163	0.0096	0.001
1457	Tetraglyme	C10H22O5	0.11967	0.0162	0.0015
1418	Dinonyl Ether	C18H38O	0.07435	0.0099	0.001
2432	ETHYLAL	C5H12O2	0.07623	0.0084	0.0006
2405	DIISOBUTYL ETHER	C8H18O	0.05057	0.0054	0.0004
2456	Ethyl Glyme	C6H14O2	0.09574	0.0126	0.0013
2417	ETHYLHEXYL ETHER	C8H18O	0.09873	0.0135	0.0014
2415	ETHYLISOPROPETH	C5H12O	0.06359	0.0067	0.0005

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	Formate Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1301	Methyl Formate	C2H4O2	0.28781	0.0522	0.0076
1311	Vinyl Formate	C3H4O2	0.12913	0.02	0.0024

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

1302	Ethyl Formate	C3H6O2	0.17493	0.0272	0.0033
2306	t-Butyl Formate	C5H10O2	0.07486	0.009	0.0008
1303	Propyl Formate	C4H8O2	0.14018	0.0208	0.0024
2305	sec-ButylFormate	C5H10O2	0.08032	0.0103	0.001
2311	CYCLOHEXL FORMAT	C7H12O2	0.12256	0.0165	0.0017
1304	N-Butyl Formate	C5H10O2	0.11987	0.0168	0.0018
1305	Isobutyl Formate	C5H10O2	0.09179	0.0122	0.0011
2350	Benzyl Formate	C8H8O2	0.11884	0.0166	0.0018
2307	n-Hexyl Formate	C7H14O2	0.10523	0.0148	0.0016
1306	N-Pentyl Formate	C6H12O2	0.11363	0.0154	0.0016
2308	n-Heptyl Formate	C8H16O2	0.10247	0.0129	0.0012
1308	N-Octyl Formate	C9H18O2	0.09794	0.0114	0.0009
1309	n-Nonyl Formate	C10H20O2	0.08448	0.0109	0.001
1310	n-Decyl Formate	C11H22O2	0.08353	0.0109	0.001

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	Ester Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1351	Mth Methacrylate	C5H8O2	0.11073	0.0145	0.0015
1312	Methyl Acetate	C3H6O2	0.23683	0.0401	0.0053
1331	Vinyl Propionate	C5H8O2	0.14745	0.0221	0.0025
1321	Vinyl Acetate	C4H6O2	0.12637	0.0178	0.0019
1352	Eth MthAcrylate	C6H10O2	0.11502	0.0145	0.0013
1322	MethylPropionate	C4H8O2	0.1656	0.0255	0.0031
1341	Methyl Acrylate	C4H6O2	0.22731	0.0369	0.0046
1313	Ethyl Acetate	C4H8O2	0.2351	0.0406	0.0056
1319	IsopropylAcetate	C5H10O2	0.08445	0.0106	0.001
1332	Methyl Butyrate	C5H10O2	0.19284	0.0309	0.0039
1342	Ethyl Acrylate	C5H8O2	0.15475	0.0236	0.0027
1318	Allyl Acetate	C5H8O2	0.13175	0.017	0.0015
1314	N-Propyl Acetate	C5H10O2	0.12814	0.0182	0.002
1323	Ethyl Propionate	C5H10O2	0.17566	0.0276	0.0034
1360	I-But I-Butyrate	C8H16O2	0.06352	0.0073	0.0006
1320	Sec-ButylAcetate	C6H12O2	0.07478	0.0091	0.0008
1336	PropylI-Butyrate	C7H14O2	0.09178	0.0127	0.0013
1353	N-C3-Mthacrylate	C7H12O2	0.14467	0.0212	0.0025
1333	Ethyl Butyrate	C6H12O2	0.14359	0.0196	0.002
1347	EthylIsovalerate	C7H14O2	0.09657	0.0128	0.0012
1315	N-Butyl Acetate	C6H12O2	0.11658	0.0159	0.0017

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

1390	Methyl Benzoate	C8H8O2	0.13454	0.0181	0.0019
1388	ISOBUTYL MTHACR	C8H14O2	0.07324	0.0083	0.0007
1343	1-PropylAcrylate	C6H10O2	0.12803	0.0187	0.0021
1316	Isobutyl Acetate	C6H12O2	0.0862	0.011	0.001
1344	N-Butyl Acrylate	C7H12O2	0.14032	0.0197	0.002
1357	Pentyl Acetate	C7H14O2	0.10424	0.0133	0.0013
1327	N-PropN-Butyrate	C7H14O2	0.12409	0.0171	0.0017
1324	N-PropPropionate	C6H12O2	0.14772	0.0218	0.0024
1291	Acetic Anhydride	C4H6O3	0.12242	0.017	0.0018
1389	N-ButMthacrylate	C8H14O2	0.09284	0.012	0.0012
1359	Benzyl Acetate	C9H10O2	0.12716	0.0177	0.0019
1326	N-But Propionate	C7H14O2	0.13136	0.0192	0.0021
1391	Ethyl Benzoate	C9H10O2	0.12624	0.0171	0.0016
1897	CH3OC3H600CH3	C6H12O3	0.07292	0.0086	0.0007
1392	DiethylCarbonate	C5H10O3	0.15129	0.0199	0.0022
1385	N-But N-Butyrate	C8H16O2	0.11625	0.0152	0.0015
1317	IsopentylAcetate	C7H14O2	0.08595	0.01	0.0009
1363	N-Hexyl Acetate	C8H16O2	0.12687	0.0183	0.002
1387	Ethylene Acetate	C6H10O4	0.15891	0.024	0.0035
1393	Diethyl Oxalate	C6H10O4	0.23396	0.0373	0.0047
1365	Butyl Benzoate	C11H14O2	0.10729	0.0143	0.0014
1361	I-C5 I-Valerate	C10H20O2	0.07368	0.0079	0.0005
1367	Heptyl Acetate	C9H18O2	0.12015	0.0173	0.0019
1346	N-Butyl Valerate	C9H18O2	0.11107	0.0156	0.0016
1358	2-C2-C6 Acetate	C10H20O2	0.06924	0.0076	0.0006
1394	Diethyl Malonate	C7H12O4	0.16837	0.0259	0.0029
1292	Propionyl Oxide	C6H10O3	0.11242	0.0153	0.0015
1364	Benzyl Benzoate	C14H12O2	0.10759	0.0124	0.0013
1381	2Mth p-Phthalate	C10H10O4	0.1275	0.0148	0.0011
1368	n-Octyl Acetate	C10H20O2	0.11179	0.0157	0.0016
1377	DiMthI-Phthalate	C10H10O4	0.13835	0.0156	0.0013
1896	Ethylene DiAcr	C8H10O4	0.17957	0.027	0.0029
1386	2-Ethylhexyl Acr	C11H20O2	0.07126	0.0085	0.0007
1395	Methyl Decanoate	C11H22O2	0.12037	0.0167	0.0018
1369	n-Nonyl Acetate	C11H22O2	0.09265	0.0129	0.0014
1370	n-Decyl Acetate	C12H24O2	0.09553	0.0126	0.0013
1345	N-ButylNonanoate	C13H26O2	0.07025	0.0061	0.0004
1375	DiProp Phthalate	C14H18O4	0.06727	0.0078	0.0007
1376	Diisobutyl Phtha	C16H22O4	0.03382	0.0036	0.0003
1396	IsopropMyristate	C17H34O2	0.07223	0.0086	0.0008
1383	Butyl Stearate	C22H44O2	0.03971	0.0039	0.0003
1362	Methyl Oleate	C19H36O2	0.06927	0.0087	0.0008
1355	Diisooctyl Phtha	C24H38O4	0.04204	0.0042	0.0003
1382	DioctylTerephtha	C24H38O4	0.04938	0.0051	0.0004
1384	DIBUTYL SEBACATE	C18H34O4	0.07896	0.0105	0.001

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

1371	Diisodecyl Phtha	C28H46O4	0.05111	0.004	0.0002
1354	DioctylPhthalate	C24H38O4	0.01752	0.0016	0.0001
2375	DiethylPhthalate	C12H14O4	0.09384	0.0125	0.0013
2388	Dipropyl Maleate	C10H16O4	0.09205	0.0126	0.0013
2381	Diallyl Maleate	C10H12O4	0.09638	0.0132	0.0014
2370	Glyceryl Triacet	C9H14O6	0.0726	0.0089	0.0008
2382	Dibutyl Maleate	C12H20O4	0.08702	0.0121	0.0013
2376	DibutylPhthalate	C16H22O4	0.05815	0.0068	0.0006
2353	CetylMthacrylate	C20H38O2	0.09101	0.0106	0.0008
2379	Dihexyl Adipate	C18H34O4	0.07896	0.0105	0.001
2321	T-Butyl Acetate	C6H12O2	0.08091	0.011	0.0012
2332	Methl.I-butyrate	C5H10O2	0.13237	0.0196	0.0023
2354	AllylMthacrylate	C7H10O2	0.09046	0.0116	0.0012
2364	CYCLOHEXL ACETAT	C8H14O2	0.13226	0.0194	0.0021
2337	EthylIsobutyrate	C6H12O2	0.09485	0.0124	0.0012
2384	IsobutylAcrylate	C7H12O2	0.09101	0.0119	0.0011
2380	1,1-Diacetoxy C2	C6H10O4	0.13058	0.0189	0.0021
2392	n-PropylBenzoate	C10H12O2	0.1122	0.0143	0.0014
2377	DiMth Phthalate	C10H10O4	0.11754	0.0155	0.0014
2386	Diethyl Maleate	C8H12O4	0.13742	0.0186	0.0017
2385	Mth Dodecanoate	C13H26O2	0.11381	0.0151	0.0015
3379	Dioctyl Adipate	C22H42O4	0.09928	0.0081	0.0003
5886	Mth Acetoacetate	C5H8O3	0.18993	0.0306	0.0039
5884	Ethoxy Acetate	C6H12O3	0.1241	0.0171	0.0018
5887	EthAcetoAcetate	C6H10O3	0.12781	0.0181	0.0018
5885	Carbitol Acetate	C8H16O4	0.1055	0.0125	0.001

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	**Ketone Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1096	Methyl Isopropen	C5H8O	0.08128	0.0098	0.0009
1079	Cyclopentanone	C5H8O	0.31153	0.0566	0.0081
1051	Acetone	C3H6O	0.18542	0.0296	0.0036
1052	MEK	C4H8O	0.13064	0.0189	0.0021
1065	Mesityl Oxide	C6H10O	0.07518	0.0091	0.0008
1066	T-But Mth Ketone	C6H12O	0.06141	0.0072	0.0006
1060	2-Pentanone	C5H10O	0.10201	0.0138	0.0014
1061	Mth iC3 Ketone	C5H10O	0.07811	0.0097	0.0009
1053	Diethyl Ketone	C5H10O	0.13969	0.0204	0.0021

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

1059	3-Hexanone	C6H12O	0.11339	0.0156	0.0017
1099	Diketene	C4H4O2	0.83571	0.2019	0.0393
1055	Sec-ButMthKetone	C6H12O	0.0689	0.0083	0.0007
1054	MIBK	C6H12O	0.06578	0.0077	0.0007
1095	EthIsopropKetone	C6H12O	0.08351	0.0111	0.0011
1063	2-Heptanone	C7H14O	0.08814	0.0113	0.0011
1064	5-Mth-2-Hexanone	C7H14O	0.07196	0.0088	0.0008
1058	4-Heptanone	C7H14O	0.09609	0.0123	0.0012
1057	3-Heptanone	C7H14O	0.104	0.0145	0.0016
1076	2,4-Pentanedione	C5H8O2	0.04409	0.003	0.0001
1068	DiisobutylKetone	C9H18O	0.04768	0.0051	0.0004
1097	2-CycC6 CycC6one	C12H20O	0.09608	0.0125	0.0015
1083	2-Octanone	C8H16O	0.08343	0.0106	0.001
1073	Dibutyl Ketone	C9H18O	0.08808	0.0111	0.0011
1062	2-Hexanone	C6H12O	0.09443	0.0124	0.0012
1077	Isophorone	C9H14O	0.14058	0.0183	0.0016
1090	Acetophenone	C8H8O	0.10453	0.014	0.0014
1080	Cyclohexanone	C6H10O	0.25985	0.0431	0.0056
1074	2-Nonanone	C9H18O	0.08056	0.0102	0.0009

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	**Hydrocarbons Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
404	DiMth-Acetylene	C4H6	0.1362	0.0215	0.0027
202	Propylene	C3H6	0.13348	0.02	0.0023
412	2-Pentyne	C5H8	0.01325	0.001	0.0001
207	2-Methylpropene	C4H8	0.11951	0.0171	0.0019
204	1-Butene	C4H8	0.13179	0.0193	0.0022
205	Cis-2-Butene	C4H8	0.10881	0.0151	0.0016
402	Propyne	C3H4	0.19193	0.0337	0.0047
406	3-Hexyne	C6H10	0.08831	0.0115	0.0011
206	Trans-2-Butene	C4H8	0.09794	0.0129	0.0013
407	2-Hexyne	C6H10	0.09702	0.013	0.0014
231	33-2Mth-1-Butene	C6H12	0.08387	0.0107	0.0011
230	23-2Mth-1-Butene	C6H12	0.08912	0.0114	0.0011
229	2-Ethyl-1-Butene	C6H12	0.12008	0.0173	0.0019
8	I-Pentane	C5H12	0.12707	0.0182	0.002
14	2,2-DiMth-Butane	C6H14	0.12071	0.017	0.0019
232	23-2Mth-2-Butene	C6H12	0.10089	0.0135	0.0014

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

213	3-Mth-1-Butene	C5H10	0.08802	0.0112	0.0011
212	2-Mth-1-Butene	C5H10	0.12301	0.0178	0.002
211	Trans-2-Pentene	C5H10	0.09772	0.0129	0.0013
210	Cis-2-Pentene	C5H10	0.09968	0.0133	0.0014
223	4-Mth-1-Pentene	C6H12	0.08898	0.0112	0.0011
221	2-Mth-1-Pentene	C6H12	0.11141	0.0154	0.0016
248	2-t-Butylpropene	C7H14	0.09152	0.0118	0.0012
227	Cs-4-Mth-2-C5H10	C6H12	0.06357	0.0073	0.0006
224	2-Mth-2-Pentene	C6H12	0.10431	0.0143	0.0015
403	1-Butyne	C4H6	0.13319	0.0207	0.0025
15	2,3-DiMth-Butane	C6H14	0.10868	0.0147	0.0015
214	2-Mth-2-Butene	C5H10	0.12087	0.0171	0.0019
228	Ts-4-Mth-2-C5H10	C6H12	0.06873	0.0081	0.0007
225	Cs-3-Mth-2-C5H10	C6H12	0.10549	0.0143	0.0015
218	Trans-2-Hexene	C6H12	0.09468	0.0123	0.0012
2226	3-METH-Tr-2Pente	C6H12	0.11489	0.0162	0.0018
222	3-Mth-1-Pentene	C6H12	0.09024	0.0113	0.0011
257	2-Diisobutylene	C8H16	0.07039	0.0086	0.0008
256	1-Diisobutylene	C8H16	0.07766	0.0093	0.0008
217	Cis-2-Hexene	C6H12	0.09771	0.0128	0.0012
2414	1-Heptyne	C7H12	0.10327	0.0138	0.0014
13	3-Methylpentane	C6H14	0.12994	0.0188	0.0021
219	Cis-3-Hexene	C6H12	0.0905	0.0115	0.0011
12	2-Methylpentane	C6H14	0.11865	0.0168	0.0018
220	Trans-3-Hexene	C6H12	0.09233	0.012	0.0012
405	1-Pentyne	C5H8	0.11494	0.016	0.0017
209	1-Pentene	C5H10	0.12552	0.0179	0.002
11	N-Hexane	C6H14	0.15569	0.0238	0.0029
235	Cis-2-Heptene	C7H14	0.09657	0.0121	0.0011
249	Cis-3-Heptene	C7H14	0.08927	0.011	0.001
216	1-Hexene	C6H12	0.12241	0.0174	0.0018
239	3-Eth-1-Pentene	C7H14	0.08769	0.0115	0.0011
226	4-Mth-1-Hexene	C7H14	0.09501	0.0127	0.0013
240	3-Mth-1-Hexene	C7H14	0.08721	0.0114	0.0011
419	3-Mth-1-Butyne	C5H8	0.07672	0.0096	0.0009
233	2-Eth-1-Pentene	C7H14	0.11374	0.0153	0.0016
238	2-Mth-1-Hexene	C7H14	0.1074	0.0145	0.0015
416	1-Octyne	C8H14	0.09864	0.0132	0.0013
289	2,3Dimeth Hexene	C8H16	0.0785	0.0098	0.0009
234	1-Heptene	C7H14	0.11896	0.0166	0.0018
413	1-Hexyne	C6H10	0.10833	0.0148	0.0015
237	Trans-3-Heptene	C7H14	0.08869	0.0111	0.001
236	Trans-2-Heptene	C7H14	0.09494	0.0119	0.0011
251	Trans-2-Octene	C8H16	0.09346	0.0114	0.001
279	Trans-4-Octene	C8H16	0.08656	0.0104	0.0009

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

277	Trans-3-Octene	C8H16	0.0893	0.0108	0.001
2252	2Methl-1-Heptene	C8H16	0.10325	0.0134	0.0013
250	1-Octene	C8H16	0.11465	0.0158	0.0017
258	2-Ethyl-1-Hexene	C8H16	0.10525	0.014	0.0013
280	3-Octene	C8H16	0.08805	0.0106	0.0009
278	4-Octene	C8H16	0.08748	0.0106	0.0009
276	2-Octene	C8H16	0.09541	0.0117	0.001
259	1-Nonene	C9H18	0.11126	0.0152	0.0016
262	1-Dodecene	C12H24	0.10283	0.0136	0.0014
263	1-Tridecene	C13H26	0.10009	0.0132	0.0013
264	1-Tetradecene	C14H28	0.09829	0.0128	0.0013
265	1-Pentadecene	C15H30	0.09636	0.0124	0.0012
266	1-Hexadecene	C16H32	0.09468	0.0121	0.0012
267	1-Octadecene	C18H36	0.09003	0.0112	0.0011
281	1-Heptadecene	C17H34	0.0921	0.0114	0.0011
284	1-Eicosene	C20H40	0.08814	0.0109	0.001
283	1-Nonadecene	C19H38	0.08876	0.0109	0.0011
3	Propane	C3H8	0.19109	0.0317	0.0042
4	I-Butane	C4H10	0.1188	0.0171	0.002
9	Neopentane	C5H12	0.10395	0.0141	0.0014
5	N-Butane	C4H10	0.17975	0.0288	0.0036
7	pentane	C5H12	0.16732	0.0263	0.0032
44	Hexamethylethane	C8H18	0.12635	0.0182	0.002
25	223-TriMthButane	C7H16	0.11253	0.0152	0.0016
24	3,3-DiMthPentane	C7H16	0.13348	0.019	0.0021
51	2,2,3,3-4Mth-C5	C9H20	0.14267	0.0206	0.0023
21	2,2-DiMthPentane	C7H16	0.10965	0.0151	0.0016
42	2,3,3-TriMth-C5	C8H18	0.12425	0.0171	0.0018
22	2,3-DiMthPentane	C7H16	0.10972	0.0149	0.0015
40	2,2,3-TriMth-C5	C8H18	0.10878	0.0146	0.0015
23	2,4-DiMthPentane	C7H16	0.08309	0.0105	0.001
41	2,2,4-TriMth-C5	C8H18	0.08034	0.0099	0.0009
39	3-Mth-3-Eth-C5	C8H18	0.13973	0.0199	0.0022
20	3-Ethylpentane	C7H16	0.12416	0.0176	0.0019
52	2,2,3,4-4Mth-C5	C9H20	0.09371	0.0118	0.0011
54	2334TetrMethPent	C9H20	0.11701	0.0157	0.0016
53	2,2,4,4-4Mth-C5	C9H20	0.08964	0.0113	0.0011
43	2,3,4-TriMth-C5	C8H18	0.09225	0.0117	0.0011
36	3,3-DiMth-Hexane	C8H18	0.11816	0.0163	0.0017
19	3-Methylhexane	C7H16	0.11837	0.0168	0.0018
18	2-Methylhexane	C7H16	0.11237	0.0157	0.0017
38	2-Mth-3-Eth-C5	C8H18	0.10043	0.0131	0.0013
190	2,2-2C1-3-C2-C5	C9H20	0.09822	0.013	0.0013
32	2,2-DiMth-Hexane	C8H18	0.10249	0.0139	0.0015
37	3,4-DiMth-Hexane	C8H18	0.1063	0.0142	0.0015

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

50	3,3-DiEthPentane	C9H20	0.13852	0.0192	0.002
34	2,4-DiMth-Hexane	C8H18	0.0842	0.0106	0.001
33	2,3-DiMth-Hexane	C8H18	0.1001	0.0133	0.0013
17	N-Heptane	C7H16	0.14578	0.0221	0.0026
49	244TriMethHexane	C9H20	0.0903	0.0113	0.0011
192	2,4-2C1-3-C2-C5	C9H20	0.08375	0.0103	0.0009
47	2,2,5-TriMth-C6	C9H20	0.0757	0.0092	0.0009
35	2,5-DiMth-Hexane	C8H18	0.08356	0.0106	0.001
31	3-Ethylhexane	C8H18	0.11117	0.0153	0.0016
30	4-Methylheptane	C8H18	0.10876	0.015	0.0016
29	3-Methylheptane	C8H18	0.11274	0.0156	0.0017
28	2-Methylheptane	C8H18	0.1085	0.0149	0.0016
96	2,2-DiMthHeptane	C9H20	0.09802	0.0129	0.0013
176	2,6-DiMthHeptane	C9H20	0.08268	0.0106	0.001
27	N-Octane	C8H18	0.13788	0.0205	0.0024
94	3-Ethylheptane	C9H20	0.10415	0.014	0.0014
92	3-Methyloctane	C9H20	0.10772	0.0147	0.0015
93	4-Methyloctane	C9H20	0.10296	0.0138	0.0014
91	2-Methyloctane	C9H20	0.10525	0.0144	0.0015
72	2,2-DiMthOctane	C10H22	0.09443	0.0126	0.0013
2095	2,3Dimethloctane	C10H22	0.09277	0.0119	0.0011
2096	2,4Dimethloctane	C10H22	0.07407	0.0092	0.0009
2098	2,6DimethlOctane	C10H22	0.08382	0.0107	0.001
2097	2,5Dimethloctane	C10H22	0.07974	0.0099	0.0009
2099	2,7DimethlOctane	C10H22	0.08293	0.0104	0.001
46	N-Nonane	C9H20	0.13046	0.0191	0.0022
88	5-Methylnonane	C10H22	0.09718	0.0127	0.0013
85	3-Methylnonane	C10H22	0.10415	0.0141	0.0015
87	4-Methylnonane	C10H22	0.09869	0.0131	0.0013
86	2-Methylnonane	C10H22	0.10214	0.0138	0.0015
56	N-Decane	C10H22	0.12561	0.0181	0.002
63	N-Undecane	C11H24	0.12014	0.017	0.0019
64	N-Dodecane	C12H26	0.11589	0.0162	0.0018
65	N-Tridecane	C13H28	0.11144	0.0155	0.0017
66	N-Tetradecane	C14H30	0.10833	0.0148	0.0016
67	N-Pentadecane	C15H32	0.10519	0.0143	0.0015
68	N-Hexadecane	C16H34	0.10264	0.0137	0.0014
69	N-Heptadecane	C17H36	0.10098	0.0134	0.0014
70	N-Octadecane	C18H38	0.09691	0.0128	0.0013
71	N-Nonadecane	C19H40	0.09465	0.0123	0.0012
73	N-Eicosane	C20H42	0.09411	0.0121	0.0012
74	n-HENEICOSANE	C21H44	0.09207	0.0116	0.0011
75	n-DOCOSANE	C22H46	0.08986	0.011	0.0011
76	n-TRICOSANE	C23H48	0.08735	0.011	0.0011
77	n-Tetracosane	C24H50	0.08574	0.0108	0.001

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

78	n-PENTACOSANE	C25H52	0.08438	0.0103	0.001
79	n-HEXACOSANE	C26H54	0.08281	0.0102	0.001
81	n-Octacosane	C28H58	0.08004	0.0097	0.0009
2081	n-TRICONTANE	C30H62	0.07846	0.0091	0.0008
2082	n-Dotriacontane	C32H66	0.07432	0.0085	0.0007
2086	Hexatriacontane	C36H74	0.07204	0.0079	0.0006

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

	Cyclic Hydrocarbons				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
269	Cyclopentene	C5H8	0.14617	0.0221	0.0026
270	Cyclohexene	C6H10	0.16044	0.0243	0.0029
287	3MthCyclopentene	C6H10	0.09117	0.0124	0.0013
286	1-MthCyclPentene	C6H10	0.14293	0.0221	0.0026
288	4MthCyclopenten	C6H10	0.09455	0.013	0.0013
273	Cycloheptene	C7H12	0.15753	0.0237	0.0027
274	Cyclooctene	C8H14	0.15228	0.0226	0.0025
101	Cyclopropane	C3H6	0.36203	0.0741	0.0125
810	ADAMANTANE	C10H16	0.11853	0.015	0.0014
102	Cyclobutane	C4H8	0.33736	0.0664	0.0107
104	Cyclopentane	C5H10	0.2835	0.0528	0.0079
137	Cyclohexane	C6H12	0.23625	0.041	0.0056
105	MthCyclopentane	C6H12	0.18084	0.0296	0.0037
146	Cs-1,4-2C1-CycC6	C8H16	0.12727	0.0179	0.0019
142	Cs-1,2-2C1-CycC6	C8H16	0.14614	0.0213	0.0024
141	1,1-2C1-CycC6	C8H16	0.14487	0.0213	0.0024
145	Ts-1,3-2C1-CycC6	C8H16	0.12778	0.0181	0.002
144	Cs-1,3-2C1-CycC6	C8H16	0.11397	0.0155	0.0016
147	Ts-1,4-2C1-CycC6	C8H16	0.11179	0.0149	0.0015
143	Ts-1,2-2C1-CycC6	C8H16	0.12444	0.0171	0.0018
138	MthCyclohexane	C7H14	0.15817	0.0239	0.0029
159	Cycloheptane	C7H14	0.25592	0.0443	0.0061
140	Ethylcyclohexane	C8H16	0.1584	0.0238	0.0028
154	Trans-Decalin	C10H18	0.1429	0.0205	0.0023
149	N-PropylCyc-C6	C9H18	0.14504	0.0212	0.0024
109	Cs-1,2-2C1-CycC5	C7H14	0.14885	0.0228	0.0028
110	Ts-1,2-2C1-CycC5	C7H14	0.12083	0.0174	0.002
112	Ts-1,3-2C1-CycC5	C7H14	0.12055	0.0173	0.002
107	Eth-Cyclopentane	C7H14	0.16943	0.0268	0.0034

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

114	N-PropCycPentane	C8H16	0.15509	0.0239	0.0029
108	1,1-DiMthCycC5	C7H14	0.14541	0.0224	0.0028
111	Cs-1,3-2C1-CycC5	C7H14	0.11823	0.017	0.0018
152	N-ButylCycHexane	C10H20	0.138	0.0199	0.0022
160	Cyclooctane	C8H16	0.25707	0.0436	0.0059
153	Cis-Decalin	C10H18	0.17361	0.0263	0.0032
115	ISOPROPYLCYCLOPENTANE	C8H16	0.13409	0.0195	0.0022
150	Isopropyl-CycC6	C9H18	0.13343	0.019	0.0021
116	1-C1-1-C2-CycC5	C8H16	0.15203	0.0234	0.0028
122	Butylcyclpentane	C9H18	0.14385	0.0218	0.0026
155	1,1-Bicyclohexyl	C12H22	0.15083	0.0214	0.0023
158	N-Decylcyclo-C6	C16H32	0.11428	0.0153	0.0016

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

	Aromatic Hydrocarbons				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
307	1,4-Pentadiene	C5H8	0.09983	0.0134	0.0014
306	1-ts3-Pentadiene	C5H8	0.10881	0.0146	0.0015
414	2-Methyl-1-Butenyne	C5H6	0.07486	0.0081	0.0006
305	Cs1,3-Pentadiene	C5H8	0.11647	0.0162	0.0017
309	Isoprene	C5H8	0.12389	0.0175	0.0019
421	1-Pentene-4-yne	C5H6	0.11358	0.014	0.0013
303	1,3-Butadiene	C4H6	0.12649	0.0183	0.0021
332	1,4-CyclHexadien	C6H8	0.11771	0.0177	0.002
501	Benzene	C6H6	0.1638	0.026	0.0033
315	Cyclopentadiene	C5H6	0.07815	0.0082	0.0005
319	Diisopropenyl	C6H10	0.11974	0.0167	0.0018
615	Ethynylbezene	C8H6	0.09209	0.0112	0.001
601	Styrene	C8H8	0.12676	0.0182	0.0021
331	1,3-CycHexadiene	C6H8	0.09549	0.0122	0.0012
310	1,5-Hexadiene	C6H10	0.09951	0.0126	0.0012
312	MthCycPentadiene	C6H8	0.08413	0.0111	0.0011
420	1-Pentene-3-yne	C5H6	0.11211	0.0144	0.0014
502	Toluene	C7H8	0.12656	0.0179	0.0019
521	T-Butylbenzene	C10H14	0.07329	0.0091	0.0009
320	Dipropylene	C6H10	0.09896	0.0126	0.0012
520	Sec-Butylbenzene	C10H14	0.09714	0.0126	0.0013
313	1,4-Hexadiene	C6H10	0.08039	0.0096	0.0009
314	Dipropylene	C6H10	0.09432	0.0119	0.0012

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

316	DiCycPentadiene	C10H12	0.06075	0.0059	0.0004
333	1,5-CycOctadiene	C8H12	0.12818	0.0169	0.0017
701	Naphthalene	C10H8	0.12579	0.0178	0.0019
504	Ethylbenzene	C8H10	0.13041	0.019	0.0021
820	Indan	C9H10	0.16124	0.0255	0.0032
505	O-Xylene	C8H10	0.11965	0.0164	0.0017
612	P-Methylstyrene	C9H10	0.10944	0.0147	0.0015
330	DIISOCROTYL	C8H14	0.10053	0.0138	0.0015
507	P-Xylene	C8H10	0.10235	0.0134	0.0013
329	DIISOBUTENYL	C8H14	0.08068	0.0098	0.0009
506	M-Xylene	C8H10	0.10437	0.0138	0.0014
603	Methylstyrene	C9H10	0.10592	0.0145	0.0015
613	Alpha-MthStyrene	C9H10	0.10125	0.0135	0.0013
510	Isopropylbenzene	C9H12	0.10975	0.0154	0.0017
724	2-Methylindene	C10H10	0.11163	0.0159	0.0018
285	Vinylcyclohexene	C8H12	0.09278	0.0112	0.001
803	Indene	C9H8	0.11145	0.0155	0.0018
706	Tetralin	C10H12	0.17069	0.027	0.0034
511	O-Ethyltoluene	C9H12	0.11571	0.0161	0.0017
723	1-Methylindene	C10H10	0.06717	0.0077	0.0006
738	Fluorene	C13H10	0.09807	0.0134	0.0014
619	Tr-1PropenylBz	C9H10	0.11228	0.0154	0.0016
525	O-Diethylbenzene	C10H14	0.10799	0.015	0.0016
618	Propenyl Bz(cis)	C9H10	0.11442	0.0152	0.0015
602	O-Methylstyrene	C9H10	0.10216	0.014	0.0015
702	1-MthNaphthalene	C11H10	0.11958	0.0167	0.0017
509	N-Propylbenzene	C9H12	0.11536	0.016	0.0017
526	M-Diethylbenzene	C10H14	0.10277	0.014	0.0014
583	Cs-2-PhnButene-2	C10H12	0.09596	0.0124	0.0012
543	M-DiisopropylBz	C12H18	0.06874	0.0086	0.0008
584	Ts-2-PhnButene-2	C10H12	0.05656	0.0064	0.0005
580	1,2-DiC1-3C2-Bz	C10H14	0.11018	0.015	0.0015
704	1-EthNaphthalene	C12H12	0.10628	0.0148	0.0016
512	M-Ethyltoluene	C9H12	0.10464	0.0143	0.0014
522	1-Mth-2-iC3-Benz	C10H14	0.09498	0.0125	0.0012
513	P-Ethyltoluene	C9H12	0.10714	0.0143	0.0015
514	1,2,3-Mesitylene	C9H12	0.11762	0.0159	0.0016
614	M-Divinylbenzene	C10H10	0.10155	0.0134	0.0013
524	1-Mth-4-iC3-Benz	C10H14	0.09172	0.0119	0.0012
822	Gamma-Terpinene	C10H16	0.08868	0.0115	0.0011
821	Alpha-Terpinene	C10H16	0.07098	0.0084	0.0007
523	1-Mth-3-iC3-Benz	C10H14	0.08781	0.0113	0.0011
703	2-MthNaphthalene	C11H10	0.11256	0.0149	0.0016
557	CycHexylBenzene	C12H16	0.13444	0.021	0.0026
515	1,2,4-Mesitylene	C9H12	0.09961	0.0128	0.0012

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

519	Isobutylbenzene	C10H14	0.08248	0.0104	0.001
424	DiPhnAcetylene	C14H10	0.06227	0.0066	0.0005
544	P-DiisopropylBz	C12H18	0.08046	0.0108	0.0011
518	N-Butylbenzene	C10H14	0.11102	0.0152	0.0016
516	1,3,5-Mesitylene	C9H12	0.08791	0.0111	0.001
809	Acenaphthalene	C12H8	0.07273	0.0099	0.001
725	123-TriMthIndene	C12H14	0.07445	0.0093	0.0008
527	1,4-DiEthBenzene	C10H14	0.10867	0.015	0.0016
558	Diphenyl	C12H10	0.09517	0.0129	0.0013
576	2-Ethyl-m-Xylene	C10H14	0.10032	0.0132	0.0013
620	p-ISOPROPENYLSTY	C11H12	0.14671	0.0168	0.0016
585	o-PropylToluene	C10H14	0.10082	0.0131	0.0013
577	2-Ethyl-p-Xylene	C10H14	0.09305	0.0122	0.0012
579	4-Ethyl-o-Xylene	C10H14	0.09952	0.0131	0.0013
586	m-Propyltoluene	C10H14	0.09344	0.0122	0.0012
587	p-Propyltoluene	C10H14	0.09684	0.0126	0.0012
578	4-Ethyl-m-Xylene	C10H14	0.09682	0.0127	0.0012
575	5-Ethyl-m-Xylene	C10H14	0.08588	0.0107	0.001
530	Prehnitene	C10H14	0.11492	0.0153	0.0016
709	2,6-2Mth-Naphtha	C12H12	0.0997	0.0131	0.0013
715	2,7-2Mth-Naphtha	C12H12	0.10198	0.0137	0.0013
719	2-ETHYLNAPHTHALENE	C12H12	0.10667	0.0141	0.0014
621	p-tert-BUTYLSTY	C12H16	0.07514	0.0087	0.0008
532	1,2,4,5-TetMthBz	C10H14	0.09407	0.012	0.0011
531	1,2,3,5-TetMthBz	C10H14	0.09715	0.0125	0.0012
533	p-tert-BUTYL ET	C12H18	0.05556	0.0064	0.0005
567	N-Pentylbenzene	C11H16	0.10632	0.0142	0.0015
718	1-n-PROPYLNAPHTH	C13H14	0.08118	0.0098	0.0009
562	1,1-DiPhnEthane	C14H14	0.07224	0.0089	0.0008
616	4-ISOBUTYLSTYRE	C12H16	0.11681	0.0161	0.0017
260	1-Decene	C10H20	0.10809	0.0147	0.0015
735	Cis-Stilbene	C14H12	0.05658	0.0062	0.0005
568	Hexylbenzene	C12H18	0.10218	0.0135	0.0014
563	Diphenylmethane	C13H12	0.08708	0.0112	0.0011
564	1,2-DiPhnEthane	C14H14	0.09265	0.0118	0.0011
804	Anthracene	C14H10	0.12753	0.0171	0.0017
736	Trans-Stilbene	C14H12	0.10001	0.014	0.0014
805	Phenanthrene	C14H10	0.11705	0.0161	0.0017
713	1-ButNaphthalene	C14H16	0.08773	0.0116	0.0012
807	Pyrene	C16H10	0.09245	0.0117	0.0011
261	1-Undecene	C11H22	0.10537	0.0141	0.0015
581	23-2C1-23-2PhnC4	C18H22	0.03629	0.0034	0.0002
549	N-Heptylbenzene	C13H20	0.10077	0.0126	0.0013
710	1-PhnNaphthalene	C16H12	0.05296	0.0062	0.0005
566	2,4-Diphenyl-4-M	C18H20	0.05678	0.0059	0.0004

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

561	O-Terphenyl	C18H14	0.0266	0.0025	0.0002
569	N-Octylbenzene	C14H22	0.09659	0.0122	0.0012
565	Triphenylmethane	C19H16	0.03725	0.0038	0.0003
714	N-C6-Naphthalene	C16H20	0.08288	0.0108	0.0011
717	Fluoranthene	C16H10	0.07486	0.0086	0.0007
716	1-Hexyl-Tetralin	C16H24	0.06842	0.0084	0.0008
731	TriPhnEthylene	C20H16	0.05426	0.0057	0.0004
806	Chrysene	C18H12	0.11624	0.0172	0.002
588	1,1,2TriPhenEth	C20H18	0.02183	0.0019	0.0001
711	1-n-NonylNaphtha	C19H26	0.07976	0.0091	0.0008
570	N-Nonylbenzene	C15H24	0.09582	0.0119	0.0012
712	1-Decyl Naphtha	C20H28	0.07843	0.0088	0.0007
559	P-Terphenyl	C18H14	0.06993	0.0095	0.001
560	M-Terphenyl	C18H14	0.06042	0.0074	0.0007
589	TetraPhenylMetha	C25H20	0.04697	0.0048	0.0004
554	Decylbenzene	C16H26	0.09188	0.0115	0.0011
732	TetraPhnEthylene	C26H20	0.04907	0.0048	0.0003
574	N-Dodecylbenzene	C18H30	0.08616	0.0109	0.0011
571	N-Undecylbenzene	C17H28	0.08962	0.011	0.0011
572	Tridecylbenzene	C19H32	0.08461	0.0106	0.001
573	n-TETRADECYLBENZ	C20H34	0.07345	0.0089	0.0008
2575	n-PENTADECYLBENZ	C21H36	0.07203	0.0087	0.0008
2576	n-HEXADECYLBENZ	C22H38	0.07052	0.0086	0.0008
2577	n-HEPTADECYLBENZ	C23H40	0.06852	0.008	0.0007
2578	n-OCTADECYLBENZE	C24H42	0.06704	0.0077	0.0007

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

Dip ID	Halocarbons Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1544	Allyl Chloride	C3H5Cl	0.1107	0.0149	0.0015
1531	3-Chloropropyne	C3H3Cl	0.11489	0.0144	0.0013
1535	T-Butyl Chloride	C4H9Cl	0.10549	0.0138	0.0014
1530	Isopropyl Cl	C3H7Cl	0.2073	0.0353	0.0047
1572	O-DiCl-Benzene	C6H4Cl2	0.0943	0.0124	0.0012
1585	Propyl Chloride	C3H7Cl	0.12468	0.0182	0.0021
1684	Isopropyl Iodide	C3H7I	0.13953	0.0201	0.0022
1651	2-Bromopropane	C3H7Br	0.16279	0.025	0.003
1691	Iodobenzene	C6H5I	0.10126	0.0134	0.0013
1860	Fluorobenzene	C6H5F	0.11238	0.0147	0.0014

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

1571	Chlorobenzene	C6H5Cl	0.11795	0.0166	0.0018
1680	Bromobenzene	C6H5Br	0.09941	0.0129	0.0013
1526	1,2-DiCl-Propane	C3H6Cl2	0.08957	0.0113	0.001
1683	Propyl Iodide	C3H7I	0.20227	0.0323	0.0039
1536	2,3-DICHLOROBUT	C4H8Cl2	0.13973	0.0198	0.0022
2638	2-Bromobutane	C4H9Br	0.15201	0.0244	0.003
1586	1-Chlorobutane	C4H9Cl	0.11708	0.0166	0.0018
1573	M-DiCl-Benzene	C6H4Cl2	0.07829	0.0096	0.0009
2634	Benzotrifluoride	C7H5F3	0.09422	0.0136	0.0016
1574	P-DiCl-Benzene	C6H4Cl2	0.08064	0.0102	0.001
1650	1-Bromopropane	C3H7Br	0.23268	0.0393	0.0053
1587	2-Chlorobutane	C4H9Cl	0.18023	0.0281	0.0033
1678	M-Dibromobenzene	C6H4Br2	0.06349	0.0068	0.0005
1537	1,2-DiCl-Butane	C4H8Cl2	0.07538	0.0088	0.0008
1597	34-DiCl-1-Butene	C4H6Cl2	0.06277	0.008	0.0008
1577	O-Chlorotoluene	C7H7Cl	0.09798	0.0129	0.0013
1532	123-3Cl-Propane	C3H5Cl3	0.0631	0.0071	0.0006
1578	P-Chlorotoluene	C7H7Cl	0.1067	0.0145	0.0015
1562	Benzyl Chloride	C7H7Cl	0.0997	0.0135	0.0014
2661	P-Bromotoluene	C7H7Br	0.09188	0.0117	0.001
1508	1,4-DiCl-Butane	C4H8Cl2	0.11211	0.0155	0.0016
1655	1-Bromobutane	C4H9Br	0.2076	0.0328	0.0042
2652	Perfluoropropane	C3F8	0.21675	0.0402	0.0057
1505	2-Butylene DiCl	C4H6Cl2	0.10153	0.0144	0.0016
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	0.07658	0.0092	0.0008
1588	1-Chloropentane	C5H11Cl	0.11374	0.015	0.0015
1592	1,2,4-TriCl-Bz	C6H3Cl3	0.05923	0.0066	0.0005
1579	2,4-2Cl-Toluene	C7H6Cl2	0.07595	0.0095	0.0009
2593	1,3,5-TriCl-BZ	C6H3Cl3	0.05282	0.0057	0.0004
1697	1-Br-Naphthalene	C10H7Br	0.09433	0.0125	0.0013
1622	Perfluorobutane	C4F10	0.14314	0.0228	0.0028
1857	P-Cl-Benzo-TriF	C7H4ClF3	0.0527	0.0065	0.0006
1509	1,5-DiCl-Pentane	C5H10Cl2	0.11758	0.0165	0.0017
1589	1-Cl-Naphthalene	C10H7Cl	0.10221	0.0132	0.0014
1864	Perfluorobenzene	C6F6	0.0052	0.0002	0
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	0.03816	0.0044	0.0004
1667	1-Bromoheptane	C7H15Br	0.15693	0.0235	0.0027
1575	HexaCl-Benzene	C6Cl6	0.02679	0.0035	0.0004
2640	Freon 123B1	C2HBrClF3	0.05082	0.0059	0.0005
1504	Vinyl Chloride	C2H3Cl	0.18073	0.033	0.0053
1672	1,1-DiBr-Ethane	C2H4Br2	0.12937	0.0206	0.0026
1580	Acetylene DiCl	C2H2Cl2	0.18203	0.0307	0.0042
1692	Diiodomethane	CH2I2	0.29972	0.0541	0.0082
1698	Bromoform	CHBr3	0.09822	0.0125	0.0012
2687	Freon 13B1	CBrF3	0.0315	0.0033	0.0003

Table B.9 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using FOG (Continued)

1649	Tetrabromoethane	C2H2Br4	0.09215	0.012	0.0012
1503	Ethyl Chloride	C2H5Cl	0.1388	0.0211	0.0025
1641	Methyl Bromide	CH3Br	0.37682	0.0741	0.012
2688	Freon 12B2	CBr2F2	0.02132	0.0015	0.0001
1673	1,2-DiBr-Ethane	C2H4Br2	0.24476	0.0395	0.0047
2637	Dibromomethane	CH2Br2	0.25036	0.0439	0.0063
1612	Cl-2F-Ethylene	C2HClF2	0.15946	0.0262	0.0033
2639	Br-Cl-Methane	CH2BrCl	0.1218	0.0179	0.002
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	0.12426	0.0187	0.0024
1682	Ethyl Iodide	C2H5I	0.23489	0.0404	0.0054
2693	Perfluoroethane	C2F6	0.40364	0.0917	0.0171
1645	Ethyl Bromide	C2H5Br	0.27901	0.0505	0.0075
1619	111-3F-Ethane	C2H3F3	1.07677	0.3044	0.0772
2694	Vinyl Bromide	C2H3Br	0.12562	0.017	0.0017
1523	1,2-DiCl-Ethane	C2H4Cl2	0.07799	0.0098	0.0009
2527	1,3-DiCl-Propane	C3H6Cl2	0.09427	0.012	0.0012

TableB. 10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG.

Dip ID	Nitrates Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1761	Nitroethane	C2H5NO2	0.12339	0.0168	0.0018
1763	2-Nitropropane	C3H7NO2	0.06111	0.0065	0.0005
1762	1-Nitropropane	C3H7NO2	0.08658	0.0106	0.001
1779	P-Nitrotoluene	C7H7NO2	0.11795	0.0136	0.0013
1886	Nitrobenzene	C6H5NO2	0.11672	0.0138	0.0013
1778	O-Nitrotoluene	C7H7NO2	0.07857	0.0086	0.0007
1780	M-Nitrotoluene	C7H7NO2	0.10083	0.0114	0.0009
1891	O-Nitroanisole	C7H7NO3	0.13644	0.0193	0.0021
2740	M-Dinitrobenzene	C6H4N2O4	0.09363	0.0093	0.0007
2742	P-Dinitrobenzene	C6H4N2O4	0.08495	0.0081	0.0006
2741	O-Dinitrobenzene	C6H4N2O4	0.13681	0.0139	0.0011
2749	3,5-DiNitToluene	C7H6N2O4	0.07738	0.0079	0.0005
2743	DNT	C7H6N2O4	0.08158	0.0073	0.0004
2745	3,4-DiNitToluene	C7H6N2O4	0.1267	0.0128	0.0008
2744	2,6-DiNitToluene	C7H6N2O4	0.08158	0.0073	0.0004
2748	2,5-DiNitToluene	C7H6N2O4	0.08116	0.0073	0.0004
2746	1,3,5-TrinitroBz	C6H3N3O6	0.0556	0.0044	0.0003
2747	Trinitrotoluene	C7H5N3O6	0.03238	0.0021	0.0001

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Thiols Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1802	Ethyl Mercaptan	C2H6S	0.29667	0.0562	0.0087
1820	Dimethyl Sulfide	C2H6S	0.14928	0.0228	0.0028
1843	Thiacyclopentane	C4H8S	0.2225	0.0353	0.0044
1803	1-Propanethiol	C3H8S	0.23811	0.0424	0.0062
1805	Isobut Mercaptan	C4H10S	0.17836	0.0288	0.0037
6860	Ethylenedithiol	C2H6S2	0.37222	0.0746	0.0121
1811	Cyclohexanethiol	C6H12S	0.15062	0.0209	0.0022
1828	DiMth Disulfide	C2H6S2	0.15488	0.0241	0.003
1841	Butanethiol	C4H10S	0.20474	0.0342	0.0046
1814	Methylproylsulf	C4H10S	0.19062	0.0317	0.0042
2816	ETHYLtBUTYL SUL	C6H14S	0.09866	0.0131	0.0013
1818	Diethyl Sulfide	C4H10S	0.17	0.0266	0.0031
1812	Benzyl Mercaptan	C7H8S	0.14586	0.0224	0.0028
1838	T-OctylMercaptan	C8H18S	0.06108	0.0065	0.0005
1827	1-Pentanethiol	C5H12S	0.18246	0.0296	0.0038

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

2815	METHnBUTYL SULFD	C5H12S	0.11015	0.0143	0.0014
1824	DiethylDisulfide	C4H10S2	0.10677	0.0142	0.0014
1807	N-Hexylmercaptan	C6H14S	0.16535	0.0257	0.0031
6857	Dimercaptoethyl	C4H10OS2	0.24164	0.0411	0.0055
1839	1-Heptanethiol	C7H16S	0.15388	0.0234	0.0028
1829	DiProp Disulfide	C6H14S2	0.08713	0.0108	0.0009
1809	1-Octanethiol	C8H18S	0.14225	0.021	0.0024
1808	N-Nonanethiol	C9H20S	0.13268	0.0192	0.0023
1826	1-Decanethiol	C10H22S	0.12568	0.018	0.002
2838	tertDodecanThiol	C12H26S	0.06431	0.008	0.0007
1825	1-Undecanethiol	C11H24S	0.11841	0.0167	0.0019
1837	Dodecylthiol	C12H26S	0.11342	0.0146	0.0015

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Aldehydes Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1037	Methacrolein	C4H6O	0.09904	0.0115	0.0009
1002	Acetaldehyde	C2H4O	0.23697	0.0337	0.0039
1003	Propionaldehyde	C3H6O	0.16642	0.0231	0.0024
1041	Benzaldehyde	C7H6O	0.11341	0.0145	0.0014
1034	Acrolein	C3H4O	0.19207	0.0259	0.0027
1005	N-Butyraldehyde	C4H8O	0.13629	0.0178	0.0018
1036	Trans-2-Butenal	C4H6O	0.21146	0.0323	0.0038
1007	Valeraldehyde	C5H10O	0.1288	0.0168	0.0017
1006	Isobutyraldehyde	C4H8O	0.09489	0.0125	0.0012
1009	1-Hexanal	C6H12O	0.11998	0.0155	0.0015
1040	P-Tolualdehyde	C8H8O	0.10172	0.0138	0.0014
1016	2-Methylhexanal	C7H14O	0.08499	0.0105	0.001
1017	3-Methylhexanal	C7H14O	0.08951	0.0106	0.0009
1008	1-Heptanal	C7H14O	0.11728	0.0148	0.0014
1013	2-Ethylhexanal	C8H16O	0.07474	0.0091	0.0008
1010	1-Octanal	C8H16O	0.10887	0.0139	0.0013
1011	1-Nonanal	C9H18O	0.10549	0.013	0.0013
1020	1-Decanal	C10H20O	0.10248	0.0126	0.0012
1021	1-Undecanal	C11H22O	0.09939	0.0118	0.0012
1025	Dodecanal	C12H24O	0.09629	0.0116	0.0011
1026	1-Tridecanal	C13H26O	0.09341	0.0112	0.001
1014	1,2-Ethanedione	C2H2O2	0.05057	0.0055	0.0004
1044	1,4BenzDicarboxAldehy	C8H6O2	0.07254	0.0093	0.0009

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Epoxides Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1440	ISOBUTYLENE OXID	C4H8O	0.35802	0.0651	0.0093
1479	Tetrahydrofuran	C4H8O	0.3829	0.0731	0.0112
1477	2,5-Dihydrofuran	C4H6O	0.24368	0.0405	0.0051
1408	1-Methoxypropane	C4H10O	0.10126	0.0132	0.0013
1411	2-Methoxypropane	C4H10O	0.0896	0.0114	0.0011
1421	1,4-Dioxane	C4H8O2	0.32597	0.0548	0.0069
2422	1,3-DIOXANE	C4H8O2	0.35675	0.0638	0.0089
1426	2-Methoxybutane	C5H12O	0.06819	0.0081	0.0007
1413	1-Methoxybutane	C5H12O	0.09923	0.0128	0.0012
1461	Methoxybenzene	C7H8O	0.13078	0.0185	0.002
1448	1-Ethoxybutane	C6H14O	0.10345	0.0137	0.0013
1429	1-MethoxyPentane	C6H14O	0.12632	0.0174	0.0018
6885	Ethyl-3-Ethoxypr	C7H14O3	0.11031	0.0144	0.0014

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Ether Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1401	Dimethyl Ether	C2H6O	0.15099	0.022	0.0024
1407	MethylEthylEther	C3H8O	0.16661	0.0269	0.0034
1470	VinylMethylEther	C3H6O	0.09826	0.0131	0.0013
1405	MTBE	C5H12O	0.09658	0.0125	0.0012
1445	VinylEthyl Ether	C4H8O	0.11628	0.0157	0.0016
1402	Diethyl Ether	C4H10O	0.1209	0.0168	0.0018
1431	Methylal	C3H8O2	0.0651	0.0071	0.0006
1428	T-But EthylEther	C6H14O	0.08545	0.0109	0.001
1427	TAME	C6H14O	0.08625	0.0105	0.001
1410	Mth Isobut Ether	C5H12O	0.07828	0.0096	0.0009
1430	Eth-t-Pent-Ether	C7H16O	0.0758	0.0089	0.0007
1403	DiisopropylEther	C6H14O	0.04713	0.0044	0.0003
1415	Eth Propyl Ether	C5H12O	0.10824	0.0141	0.0015
1455	Dimethyl Acetal	C4H10O2	0.17376	0.026	0.0029
1446	Dipropyl Ether	C6H14O	0.09686	0.0122	0.0012
1447	Butyl VinylEther	C6H12O	0.10182	0.0137	0.0014
1462	EthylPhenylEther	C8H10O	0.12249	0.0174	0.0019
1406	Di-sec-But Ether	C8H18O	0.04695	0.0045	0.0003
1432	Acetal	C6H14O2	0.05368	0.0054	0.0004

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

1460	BenzylEthylEther	C9H12O	0.11478	0.0155	0.0015
1050	Paraldehyde	C6H12O3	0.03992	0.0032	0.0002
1404	Di-n-Butyl Ether	C8H18O	0.09125	0.0116	0.0011
1420	Anethole	C10H12O	0.10126	0.0133	0.0013
1456	DimethylCarbitol	C6H14O3	0.09617	0.0118	0.0011
1463	Dibenzyl Ether	C14H14O	0.06836	0.0102	0.0011
1425	Di-n-PentylEther	C10H22O	0.0901	0.0111	0.001
1458	Diethyl Carbitol	C8H18O3	0.08593	0.0103	0.0008
1412	Dihexyl Ether	C12H26O	0.08634	0.0118	0.0012
1454	Triglyme	C8H18O4	0.07439	0.0094	0.0009
1459	Dibutyl Carbitol	C12H26O3	0.07258	0.0076	0.0005
1424	Di-n-Octyl Ether	C16H34O	0.07163	0.0096	0.001
1457	Tetraglyme	C10H22O5	0.11967	0.0162	0.0015
1418	Dinonyl Ether	C18H38O	0.07436	0.0099	0.001
2432	ETHYLAL	C5H12O2	0.07623	0.0084	0.0006
2405	DIISOBUTYL ETHER	C8H18O	0.06513	0.0075	0.0006
2456	Ethyl Glyme	C6H14O2	0.09574	0.0126	0.0013
2417	ETHYLHEXYL ETHER	C8H18O	0.09874	0.0135	0.0014
2415	ETHYLISOPROPETH	C5H12O	0.07414	0.0082	0.0006

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	**Formate Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1301	Methyl Formate	C2H4O2	0.28781	0.0522	0.0076
1311	Vinyl Formate	C3H4O2	0.12912	0.02	0.0024
1302	Ethyl Formate	C3H6O2	0.17491	0.0272	0.0033
2306	t-Butyl Formate	C5H10O2	0.08605	0.0108	0.001
1303	Propyl Formate	C4H8O2	0.14019	0.0208	0.0025
2305	sec-ButylFormate	C5H10O2	0.08032	0.0103	0.001
2311	CYCLOHEXL FORMAT	C7H12O2	0.12256	0.0165	0.0017
1304	N-Butyl Formate	C5H10O2	0.11987	0.0168	0.0018
1305	Isobutyl Formate	C5H10O2	0.09179	0.0122	0.0011
2350	Benzyl Formate	C8H8O2	0.11884	0.0166	0.0018
2307	n-Hexyl Formate	C7H14O2	0.10523	0.0148	0.0016
1306	N-Pentyl Formate	C6H12O2	0.11363	0.0154	0.0016
2308	n-Heptyl Formate	C8H16O2	0.10248	0.0129	0.0012
1308	N-Octyl Formate	C9H18O2	0.09794	0.0114	0.0009
1309	n-Nonyl Formate	C10H20O2	0.08448	0.0109	0.001
1310	n-Decyl Formate	C11H22O2	0.08353	0.0109	0.001

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Ester Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1351	Mth Methacrylate	C5H8O2	0.11072	0.0145	0.0015
1312	Methyl Acetate	C3H6O2	0.34908	0.0645	0.0094
1331	Vinyl Propionate	C5H8O2	0.14746	0.0221	0.0025
1321	Vinyl Acetate	C4H6O2	0.12637	0.0178	0.0019
1352	Eth MthAcrylate	C6H10O2	0.11502	0.0145	0.0013
1322	MethylPropionate	C4H8O2	0.16558	0.0255	0.0031
1341	Methyl Acrylate	C4H6O2	0.22733	0.0369	0.0046
1313	Ethyl Acetate	C4H8O2	0.33673	0.0631	0.0095
1319	IsopropylAcetate	C5H10O2	0.12053	0.0166	0.0016
1332	Methyl Butyrate	C5H10O2	0.26877	0.0465	0.0064
1342	Ethyl Acrylate	C5H8O2	0.15475	0.0236	0.0027
1318	Allyl Acetate	C5H8O2	0.18443	0.0258	0.0026
1314	N-Propyl Acetate	C5H10O2	0.17953	0.0276	0.0034
1323	Ethyl Propionate	C5H10O2	0.17564	0.0276	0.0034
1360	I-But I-Butyrate	C8H16O2	0.08032	0.0098	0.0009
1320	Sec-ButylAcetate	C6H12O2	0.10412	0.0138	0.0013
1336	PropylI-Butyrate	C7H14O2	0.10359	0.0148	0.0016
1353	N-C3-Mthacrylate	C7H12O2	0.14468	0.0212	0.0025
1333	Ethyl Butyrate	C6H12O2	0.1436	0.0196	0.002
1347	EthylIsovalerate	C7H14O2	0.10886	0.0149	0.0015
1315	N-Butyl Acetate	C6H12O2	0.15946	0.0234	0.0027
1390	Methyl Benzoate	C8H8O2	0.13453	0.0181	0.0019
1388	ISOBUTYL MTHACR	C8H14O2	0.08216	0.0096	0.0008
1343	1-PropylAcrylate	C6H10O2	0.12803	0.0187	0.0021
1316	Isobutyl Acetate	C6H12O2	0.13525	0.0193	0.002
1344	N-Butyl Acrylate	C7H12O2	0.14033	0.0197	0.002
1357	Pentyl Acetate	C7H14O2	0.10424	0.0133	0.0013
1327	N-PropN-Butyrate	C7H14O2	0.12409	0.0171	0.0017
1324	N-PropPropionate	C6H12O2	0.14773	0.0218	0.0024
1291	Acetic Anhydride	C4H6O3	0.12441	0.0176	0.0019
1389	N-ButMthacrylate	C8H14O2	0.09284	0.012	0.0012
1359	Benzyl Acetate	C9H10O2	0.12717	0.0177	0.0019
1326	N-But Propionate	C7H14O2	0.13136	0.0192	0.0021
1391	Ethyl Benzoate	C9H10O2	0.12625	0.0171	0.0016
1897	CH3OC3H600CH3	C6H12O3	0.09812	0.0124	0.0011
1392	DiethylCarbonate	C5H10O3	0.15129	0.0199	0.0022
1385	N-But N-Butyrate	C8H16O2	0.11624	0.0152	0.0015
1317	IsopentylAcetate	C7H14O2	0.13051	0.0169	0.0017
1363	N-Hexyl Acetate	C8H16O2	0.16744	0.0257	0.003
1387	Ethylene Acetate	C6H10O4	0.265	0.0447	0.0074
1393	Diethyl Oxalate	C6H10O4	0.23396	0.0373	0.0047
1365	Butyl Benzoate	C11H14O2	0.10729	0.0143	0.0014
1361	I-C5 I-Valerate	C10H20O2	0.09014	0.0102	0.0007

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

1367	Heptyl Acetate	C9H18O2	0.1562	0.0238	0.0028
1346	N-Butyl Valerate	C9H18O2	0.11107	0.0156	0.0016
1358	2-C2-C6 Acetate	C10H20O2	0.08965	0.0105	0.0009
1394	Diethyl Malonate	C7H12O4	0.10998	0.0152	0.0015
1292	Propionyl Oxide	C6H10O3	0.11427	0.0158	0.0016
1364	Benzyl Benzoate	C14H12O2	0.11512	0.0136	0.0015
1381	2Mth p-Phthalate	C10H10O4	0.14838	0.0183	0.0015
1368	n-Octyl Acetate	C10H20O2	0.14354	0.0213	0.0024
1377	DiMthI-Phthalate	C10H10O4	0.16178	0.0195	0.0018
1896	Ethylene DiAcr	C8H10O4	0.17957	0.027	0.0029
1386	2-Ethylhexyl Acr	C11H20O2	0.07126	0.0085	0.0007
1395	Methyl Decanoate	C11H22O2	0.12036	0.0167	0.0018
1369	n-Nonyl Acetate	C11H22O2	0.11808	0.0174	0.002
1370	n-Decyl Acetate	C12H24O2	0.1203	0.0167	0.0019
1345	N-ButylNonanoate	C13H26O2	0.07025	0.0061	0.0004
1375	DiProp Phthalate	C14H18O4	0.07714	0.0094	0.0009
1376	Diisobutyl Phtha	C16H22O4	0.04525	0.0053	0.0005
1396	IsopropMyristate	C17H34O2	0.07774	0.0094	0.0009
1383	Butyl Stearate	C22H44O2	0.03971	0.0039	0.0003
1362	Methyl Oleate	C19H36O2	0.06927	0.0087	0.0008
1355	Diisooctyl Phtha	C24H38O4	0.05203	0.0056	0.0004
1382	DioctylTerephtha	C24H38O4	0.05411	0.0058	0.0004
1384	DIBUTYL SEBACATE	C18H34O4	0.07896	0.0105	0.001
1371	Diisodecyl Phtha	C28H46O4	0.0616	0.0052	0.0003
1354	DioctylPhthalate	C24H38O4	0.0195	0.0018	0.0001
2375	DiethylPhthalate	C12H14O4	0.10892	0.0153	0.0017
2388	Dipropyl Maleate	C10H16O4	0.09205	0.0126	0.0013
2381	Diallyl Maleate	C10H12O4	0.09638	0.0132	0.0014
2370	Glyceryl Triacet	C9H14O6	0.13783	0.0194	0.0021
2382	Dibutyl Maleate	C12H20O4	0.08702	0.0121	0.0013
2376	DibutylPhthalate	C16H22O4	0.06595	0.0081	0.0007
2353	CetylMthacrylate	C20H38O2	0.09101	0.0106	0.0008
2379	Dihexyl Adipate	C18H34O4	0.07896	0.0105	0.001
2321	T-Butyl Acetate	C6H12O2	0.09221	0.013	0.0015
2332	Methl.I-butyrate	C5H10O2	0.13236	0.0196	0.0023
2354	AllylMthacrylate	C7H10O2	0.09046	0.0116	0.0012
2364	CYCLOHEXL ACETAT	C8H14O2	0.10868	0.015	0.0015
2337	EthylIsobutyrate	C6H12O2	0.10818	0.0146	0.0014
2384	IsobutylAcrylate	C7H12O2	0.1027	0.0138	0.0014
2380	1,1-Diacetoxy C2	C6H10O4	0.17256	0.0265	0.0032
2392	n-PropylBenzoate	C10H12O2	0.1122	0.0143	0.0014
2377	DiMth Phthalate	C10H10O4	0.13709	0.0192	0.0019
2386	Diethyl Maleate	C8H12O4	0.13743	0.0186	0.0017
2385	Mth Dodecanoate	C13H26O2	0.11381	0.0151	0.0015
3379	Dioctyl Adipate	C22H42O4	0.09928	0.0081	0.0003

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

5886	Mth Acetoacetate	C5H8O3	0.11698	0.0168	0.0018
5884	Ethoxy Acetate	C6H12O3	0.16454	0.0241	0.0028
5887	EthAcetoAcetate	C6H10O3	0.13105	0.0187	0.0019
5885	Carbitol Acetate	C8H16O4	0.13374	0.0167	0.0014

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Ketone Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1096	Methyl Isopropen	C5H8O	0.08128	0.0098	0.0009
1079	Cyclopentanone	C5H8O	0.20603	0.0337	0.0042
1051	Acetone	C3H6O	0.19539	0.0317	0.004
1052	MEK	C4H8O	0.13656	0.02	0.0022
1065	Mesityl Oxide	C6H10O	0.07519	0.0091	0.0008
1066	T-But Mth Ketone	C6H12O	0.07032	0.0085	0.0008
1060	2-Pentanone	C5H10O	0.10595	0.0146	0.0015
1061	Mth iC3 Ketone	C5H10O	0.08124	0.0102	0.0009
1053	Diethyl Ketone	C5H10O	0.13968	0.0204	0.0021
1059	3-Hexanone	C6H12O	0.11338	0.0156	0.0017
1099	Diketene	C4H4O2	1.27761	0.3293	0.0696
1055	Sec-ButMthKetone	C6H12O	0.07126	0.0087	0.0007
1054	MIBK	C6H12O	0.07796	0.0095	0.0009
1095	EthIsopropKetone	C6H12O	0.09551	0.0131	0.0013
1063	2-Heptanone	C7H14O	0.09062	0.0117	0.0012
1064	5-Mth-2-Hexanone	C7H14O	0.08376	0.0107	0.001
1058	4-Heptanone	C7H14O	0.09609	0.0123	0.0012
1057	3-Heptanone	C7H14O	0.104	0.0145	0.0016
1076	2,4-Pentanedione	C5H8O2	0.04409	0.003	0.0001
1068	DiisobutylKetone	C9H18O	0.05985	0.0068	0.0006
1097	2-CycC6 CycC6one	C12H20O	0.07222	0.0087	0.0009
1083	2-Octanone	C8H16O	0.08547	0.011	0.001
1073	Dibutyl Ketone	C9H18O	0.08808	0.0111	0.0011
1062	2-Hexanone	C6H12O	0.09754	0.0129	0.0013
1077	Isophorone	C9H14O	0.10167	0.0121	0.001
1090	Acetophenone	C8H8O	0.10453	0.014	0.0014
1080	Cyclohexanone	C6H10O	0.17784	0.0267	0.0031
1074	2-Nonanone	C9H18O	0.08228	0.0105	0.001

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Hydrocarbons Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
404	DiMth-Acetylene	C4H6	0.13619	0.0215	0.0027
202	Propylene	C3H6	0.13192	0.0197	0.0023
412	2-Pentyne	C5H8	0.01325	0.001	0.0001
207	2-Methylpropene	C4H8	0.1195	0.0171	0.0019
204	1-Butene	C4H8	0.13179	0.0193	0.0022
205	Cis-2-Butene	C4H8	0.10803	0.0149	0.0016
402	Propyne	C3H4	0.19193	0.0337	0.0047
406	3-Hexyne	C6H10	0.08831	0.0115	0.0011
206	Trans-2-Butene	C4H8	0.09722	0.0127	0.0013
407	2-Hexyne	C6H10	0.09702	0.013	0.0014
231	33-2Mth-1-Butene	C6H12	0.0987	0.0131	0.0014
230	23-2Mth-1-Butene	C6H12	0.10503	0.0141	0.0014
229	2-Ethyl-1-Butene	C6H12	0.12008	0.0173	0.0019
8	I-Pentane	C5H12	0.12705	0.0182	0.002
14	2,2-DiMth-Butane	C6H14	0.14112	0.0207	0.0024
232	23-2Mth-2-Butene	C6H12	0.10089	0.0135	0.0014
213	3-Mth-1-Butene	C5H10	0.10633	0.0143	0.0015
212	2-Mth-1-Butene	C5H10	0.12302	0.0178	0.002
211	Trans-2-Pentene	C5H10	0.09904	0.0132	0.0013
210	Cis-2-Pentene	C5H10	0.10102	0.0136	0.0014
223	4-Mth-1-Pentene	C6H12	0.1049	0.0139	0.0014
221	2-Mth-1-Pentene	C6H12	0.11141	0.0154	0.0016
248	2-t-Butylpropene	C7H14	0.10574	0.0142	0.0014
227	Cs-4-Mth-2-C5H10	C6H12	0.07466	0.0089	0.0008
224	2-Mth-2-Pentene	C6H12	0.10431	0.0143	0.0015
403	1-Butyne	C4H6	0.13318	0.0207	0.0025
15	2,3-DiMth-Butane	C6H14	0.15005	0.0222	0.0025
214	2-Mth-2-Butene	C5H10	0.12031	0.017	0.0019
228	Ts-4-Mth-2-C5H10	C6H12	0.0806	0.01	0.0009
225	Cs-3-Mth-2-C5H10	C6H12	0.10515	0.0142	0.0015
218	Trans-2-Hexene	C6H12	0.09439	0.0123	0.0012
2226	3-METH-Tr-2Pente	C6H12	0.11454	0.0161	0.0017
222	3-Mth-1-Pentene	C6H12	0.09024	0.0113	0.0011
257	2-Diisobutylene	C8H16	0.08049	0.0102	0.001
256	1-Diisobutylene	C8H16	0.08882	0.011	0.001
217	Cis-2-Hexene	C6H12	0.09868	0.013	0.0013
2414	1-Heptyne	C7H12	0.10327	0.0138	0.0014
13	3-Methylpentane	C6H14	0.12995	0.0188	0.0021
219	Cis-3-Hexene	C6H12	0.09292	0.0121	0.0012
12	2-Methylpentane	C6H14	0.13912	0.0206	0.0023
220	Trans-3-Hexene	C6H12	0.09478	0.0126	0.0013
405	1-Pentyne	C5H8	0.11495	0.016	0.0017
209	1-Pentene	C5H10	0.12551	0.0179	0.002

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

11	N-Hexane	C6H14	0.15568	0.0238	0.0029
235	Cis-2-Heptene	C7H14	0.09725	0.0123	0.0011
249	Cis-3-Heptene	C7H14	0.09091	0.0114	0.0011
216	1-Hexene	C6H12	0.12243	0.0174	0.0018
239	3-Eth-1-Pentene	C7H14	0.08768	0.0115	0.0011
226	4-Mth-1-Hexene	C7H14	0.096	0.013	0.0013
240	3-Mth-1-Hexene	C7H14	0.08721	0.0114	0.0011
419	3-Mth-1-Butyne	C5H8	0.09215	0.0121	0.0013
233	2-Eth-1-Pentene	C7H14	0.11373	0.0153	0.0016
238	2-Mth-1-Hexene	C7H14	0.1074	0.0145	0.0015
416	1-Octyne	C8H14	0.09864	0.0132	0.0013
289	2,3Dimeth Hexene	C8H16	0.0785	0.0098	0.0009
234	1-Heptene	C7H14	0.11896	0.0166	0.0018
413	1-Hexyne	C6H10	0.10834	0.0148	0.0015
237	Trans-3-Heptene	C7H14	0.09033	0.0115	0.0011
236	Trans-2-Heptene	C7H14	0.09561	0.0121	0.0011
251	Trans-2-Octene	C8H16	0.09391	0.0116	0.001
279	Trans-4-Octene	C8H16	0.08762	0.0107	0.001
277	Trans-3-Octene	C8H16	0.09038	0.0111	0.001
2252	2Methl-1-Heptene	C8H16	0.10326	0.0134	0.0013
250	1-Octene	C8H16	0.11464	0.0158	0.0017
258	2-Ethyl-1-Hexene	C8H16	0.10526	0.014	0.0013
280	3-Octene	C8H16	0.08912	0.0109	0.001
278	4-Octene	C8H16	0.08855	0.0109	0.001
276	2-Octene	C8H16	0.09588	0.0118	0.0011
259	1-Nonene	C9H18	0.11126	0.0152	0.0016
262	1-Dodecene	C12H24	0.10283	0.0136	0.0014
263	1-Tridecene	C13H26	0.1001	0.0132	0.0013
264	1-Tetradecene	C14H28	0.09829	0.0128	0.0013
265	1-Pentadecene	C15H30	0.09636	0.0124	0.0012
266	1-Hexadecene	C16H32	0.09467	0.0121	0.0012
267	1-Octadecene	C18H36	0.09003	0.0112	0.0011
281	1-Heptadecene	C17H34	0.0921	0.0114	0.0011
284	1-Eicosene	C20H40	0.08814	0.0109	0.001
283	1-Nonadecene	C19H38	0.08876	0.0109	0.0011
3	Propane	C3H8	0.19112	0.0317	0.0042
4	I-Butane	C4H10	0.11879	0.0171	0.002
9	Neopentane	C5H12	0.12478	0.0177	0.0019
5	N-Butane	C4H10	0.17976	0.0288	0.0036
7	pentane	C5H12	0.16731	0.0263	0.0032
44	Hexamethylethane	C8H18	0.16473	0.0254	0.003
25	223-TriMthButane	C7H16	0.1506	0.022	0.0025
24	3,3-DiMthPentane	C7H16	0.13348	0.019	0.0021
51	2,2,3,3-4Mth-C5	C9H20	0.18202	0.0281	0.0034
21	2,2-DiMthPentane	C7H16	0.12632	0.018	0.002

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

42	2,3,3-TriMth-C5	C8H18	0.16216	0.024	0.0027
22	2,3-DiMthPentane	C7H16	0.12672	0.0179	0.0019
40	2,2,3-TriMth-C5	C8H18	0.12389	0.0172	0.0018
23	2,4-DiMthPentane	C7H16	0.11186	0.0153	0.0016
41	2,2,4-TriMth-C5	C8H18	0.10577	0.014	0.0014
39	3-Mth-3-Eth-C5	C8H18	0.13974	0.0199	0.0022
20	3-Ethylpentane	C7H16	0.12417	0.0176	0.0019
52	2,2,3,4-4Mth-C5	C9H20	0.12018	0.0162	0.0016
54	2334TetrMethPent	C9H20	0.16894	0.0251	0.0029
53	2,2,4,4-4Mth-C5	C9H20	0.11553	0.0156	0.0016
43	2,3,4-TriMth-C5	C8H18	0.12047	0.0164	0.0017
36	3,3-DiMth-Hexane	C8H18	0.11817	0.0163	0.0017
19	3-Methylhexane	C7H16	0.11837	0.0168	0.0018
18	2-Methylhexane	C7H16	0.12963	0.0189	0.0021
38	2-Mth-3-Eth-C5	C8H18	0.11459	0.0156	0.0016
190	2,2-2C1-3-C2-C5	C9H20	0.11089	0.0151	0.0015
32	2,2-DiMth-Hexane	C8H18	0.11672	0.0164	0.0018
37	3,4-DiMth-Hexane	C8H18	0.1063	0.0142	0.0015
50	3,3-DiEthPentane	C9H20	0.13853	0.0192	0.002
34	2,4-DiMth-Hexane	C8H18	0.09637	0.0126	0.0013
33	2,3-DiMth-Hexane	C8H18	0.11422	0.0157	0.0017
17	N-Heptane	C7H16	0.14579	0.0221	0.0026
49	244TriMethHexane	C9H20	0.1163	0.0157	0.0016
192	2,4-2C1-3-C2-C5	C9H20	0.10725	0.0141	0.0014
47	2,2,5-TriMth-C6	C9H20	0.09757	0.0127	0.0013
35	2,5-DiMth-Hexane	C8H18	0.10935	0.0149	0.0016
31	3-Ethylhexane	C8H18	0.11115	0.0153	0.0016
30	4-Methylheptane	C8H18	0.10875	0.015	0.0016
29	3-Methylheptane	C8H18	0.11273	0.0156	0.0017
28	2-Methylheptane	C8H18	0.12355	0.0176	0.0019
96	2,2-DiMthHeptane	C9H20	0.11059	0.015	0.0016
176	2,6-DiMthHeptane	C9H20	0.10582	0.0145	0.0015
27	N-Octane	C8H18	0.13789	0.0205	0.0024
94	3-Ethylheptane	C9H20	0.10416	0.014	0.0014
92	3-Methyloctane	C9H20	0.10772	0.0147	0.0015
93	4-Methyloctane	C9H20	0.10297	0.0138	0.0014
91	2-Methyloctane	C9H20	0.10525	0.0144	0.0015
72	2,2-DiMthOctane	C10H22	0.10572	0.0145	0.0015
2095	2,3Dimethloctane	C10H22	0.10386	0.0137	0.0014
2096	2,4Dimethloctane	C10H22	0.08319	0.0107	0.001
2098	2,6DimethlOctane	C10H22	0.09397	0.0123	0.0012
2097	2,5Dimethloctane	C10H22	0.08946	0.0114	0.0011
2099	2,7DimethlOctane	C10H22	0.10419	0.014	0.0014
46	N-Nonane	C9H20	0.13046	0.0191	0.0022
88	5-Methylnonane	C10H22	0.09718	0.0127	0.0013

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

85	3-Methylnonane	C10H22	0.10415	0.0141	0.0015
87	4-Methylnonane	C10H22	0.09868	0.0131	0.0013
86	2-Methylnonane	C10H22	0.11415	0.0159	0.0018
56	N-Decane	C10H22	0.12562	0.0181	0.002
63	N-Undecane	C11H24	0.12015	0.017	0.0019
64	N-Dodecane	C12H26	0.11589	0.0162	0.0018
65	N-Tridecane	C13H28	0.11144	0.0155	0.0017
66	N-Tetradecane	C14H30	0.10833	0.0148	0.0016
67	N-Pentadecane	C15H32	0.10519	0.0143	0.0015
68	N-Hexadecane	C16H34	0.10264	0.0137	0.0014
69	N-Heptadecane	C17H36	0.10098	0.0134	0.0014
70	N-Octadecane	C18H38	0.09691	0.0128	0.0013
71	N-Nonadecane	C19H40	0.09465	0.0123	0.0012
73	N-Eicosane	C20H42	0.09411	0.0121	0.0012
74	n-HENEICOSANE	C21H44	0.09207	0.0116	0.0011
75	n-DOCOSANE	C22H46	0.08986	0.011	0.0011
76	n-TRICOSANE	C23H48	0.08735	0.011	0.0011
77	n-Tetracosane	C24H50	0.08574	0.0108	0.001
78	n-PENTACOSANE	C25H52	0.08438	0.0103	0.001
79	n-HEXACOSANE	C26H54	0.08281	0.0102	0.001
81	n-Octacosane	C28H58	0.08004	0.0097	0.0009
2081	n-TRICONTANE	C30H62	0.07846	0.0091	0.0008
2082	n-Dotriacontane	C32H66	0.07432	0.0085	0.0007
2086	Hexatriacontane	C36H74	0.07204	0.0079	0.0006

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

	Cyclic Hydrocarbons				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
269	Cyclopentene	C5H8	0.14619	0.0221	0.0026
270	Cyclohexene	C6H10	0.16044	0.0243	0.0029
287	3MthCyclopentene	C6H10	0.07718	0.0103	0.001
286	1-MthCyclPentene	C6H10	0.12151	0.0184	0.0021
288	4MthCyclopenten	C6H10	0.08007	0.0108	0.0011
273	Cycloheptene	C7H12	0.15752	0.0237	0.0027
274	Cyclooctene	C8H14	0.15229	0.0226	0.0025
101	Cyclopropane	C3H6	0.1014	0.0134	0.0013
810	ADAMANTANE	C10H16	0.11853	0.015	0.0014
102	Cyclobutane	C4H8	0.13815	0.0198	0.0022
104	Cyclopentane	C5H10	0.18535	0.0294	0.0036

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

137	Cyclohexane	C6H12	0.17684	0.0281	0.0034
105	MthCyclopentane	C6H12	0.10721	0.0148	0.0015
146	Cs-1,4-2C1-CycC6	C8H16	0.07388	0.0092	0.0009
142	Cs-1,2-2C1-CycC6	C8H16	0.08556	0.011	0.0011
141	1,1-2C1-CycC6	C8H16	0.08294	0.0107	0.0011
145	Ts-1,3-2C1-CycC6	C8H16	0.07419	0.0093	0.0009
144	Cs-1,3-2C1-CycC6	C8H16	0.0657	0.0079	0.0007
147	Ts-1,4-2C1-CycC6	C8H16	0.06437	0.0076	0.0007
143	Ts-1,2-2C1-CycC6	C8H16	0.07213	0.0087	0.0008
138	MthCyclohexane	C7H14	0.10413	0.0142	0.0015
159	Cycloheptane	C7H14	0.25592	0.0443	0.0061
140	Ethylcyclohexane	C8H16	0.09378	0.0125	0.0013
154	Trans-Decalin	C10H18	0.1429	0.0205	0.0023
149	N-PropylCyc-C6	C9H18	0.07688	0.0098	0.001
109	Cs-1,2-2C1-CycC5	C7H14	0.08036	0.0103	0.001
110	Ts-1,2-2C1-CycC5	C7H14	0.06401	0.0077	0.0007
112	Ts-1,3-2C1-CycC5	C7H14	0.06385	0.0077	0.0007
107	Eth-Cyclopentane	C7H14	0.09275	0.0124	0.0013
114	N-PropCycPentane	C8H16	0.07774	0.01	0.001
108	1,1-DiMthCycC5	C7H14	0.07602	0.0098	0.001
111	Cs-1,3-2C1-CycC5	C7H14	0.06251	0.0075	0.0007
152	N-ButylCycHexane	C10H20	0.06572	0.0082	0.0008
160	Cyclooctane	C8H16	0.25705	0.0436	0.0059
153	Cis-Decalin	C10H18	0.1736	0.0263	0.0032
115	ISOPROPYLCYCLOPENTANE	C8H16	0.11655	0.0156	0.0016
150	Isopropyl-CycC6	C9H18	0.10753	0.0142	0.0014
116	1-C1-1-C2-CycC5	C8H16	0.07356	0.0094	0.0009
122	Butylcyclpentane	C9H18	0.0658	0.0083	0.0008
155	1,1-Bicyclohexyl	C12H22	0.15084	0.0214	0.0023
158	N-Decylcyclo-C6	C16H32	0.02979	0.0032	0.0003

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

	Aromatic Hydrocarbons				
Dip ID	**Name**	**Formula**	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
307	1,4-Pentadiene	C5H8	0.09983	0.0134	0.0014
306	1-ts3-Pentadiene	C5H8	0.12405	0.0176	0.0019
414	2-Methyl-1-Butenyne	C5H6	0.07485	0.0081	0.0006
305	Cs1,3-Pentadiene	C5H8	0.13257	0.0194	0.0022
309	Isoprene	C5H8	0.12389	0.0175	0.0019

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

421	1-Pentene-4-yne	C5H6	0.11358	0.014	0.0013
303	1,3-Butadiene	C4H6	0.15117	0.0233	0.0029
332	1,4-CyclHexadien	C6H8	0.11771	0.0177	0.002
501	Benzene	C6H6	0.1638	0.026	0.0033
315	Cyclopentadiene	C5H6	0.07815	0.0082	0.0005
319	Diisopropenyl	C6H10	0.11976	0.0167	0.0018
615	Ethynylbezene	C8H6	0.09209	0.0112	0.001
601	Styrene	C8H8	0.12677	0.0182	0.0021
331	1,3-CycHexadiene	C6H8	0.09549	0.0122	0.0012
310	1,5-Hexadiene	C6H10	0.10242	0.0133	0.0013
312	MthCycPentadiene	C6H8	0.08413	0.0111	0.0011
420	1-Pentene-3-yne	C5H6	0.11213	0.0144	0.0014
502	Toluene	C7H8	0.12656	0.0179	0.0019
521	T-Butylbenzene	C10H14	0.08284	0.0106	0.001
320	Dipropylene	C6H10	0.10938	0.0146	0.0014
520	Sec-Butylbenzene	C10H14	0.09713	0.0126	0.0013
313	1,4-Hexadiene	C6H10	0.08117	0.0098	0.0009
314	Dipropylene	C6H10	0.10436	0.0138	0.0014
316	DiCycPentadiene	C10H12	0.06075	0.0059	0.0004
333	1,5-CycOctadiene	C8H12	0.12818	0.0169	0.0017
701	Naphthalene	C10H8	0.1258	0.0178	0.0019
504	Ethylbenzene	C8H10	0.13042	0.019	0.0021
820	Indan	C9H10	0.16125	0.0255	0.0032
505	O-Xylene	C8H10	0.11964	0.0164	0.0017
612	P-Methylstyrene	C9H10	0.10945	0.0147	0.0015
330	DIISOCROTYL	C8H14	0.10792	0.0153	0.0017
507	P-Xylene	C8H10	0.10235	0.0134	0.0013
329	DIISOBUTENYL	C8H14	0.08068	0.0098	0.0009
506	M-Xylene	C8H10	0.10436	0.0138	0.0014
603	Methylstyrene	C9H10	0.10592	0.0145	0.0015
613	Alpha-MthStyrene	C9H10	0.10139	0.0136	0.0013
510	Isopropylbenzene	C9H12	0.12456	0.0181	0.0021
724	2-Methylindene	C10H10	0.11163	0.0159	0.0018
285	Vinylcyclohexene	C8H12	0.09278	0.0112	0.001
803	Indene	C9H8	0.11146	0.0155	0.0018
706	Tetralin	C10H12	0.17069	0.027	0.0034
511	O-Ethyltoluene	C9H12	0.1157	0.0161	0.0017
723	1-Methylindene	C10H10	0.06717	0.0077	0.0006
738	Fluorene	C13H10	0.09807	0.0134	0.0014
619	Tr-1PropenylBz	C9H10	0.11228	0.0154	0.0016
525	O-Diethylbenzene	C10H14	0.10799	0.015	0.0016
618	Propenyl Bz(cis)	C9H10	0.11442	0.0152	0.0015
602	O-Methylstyrene	C9H10	0.10216	0.014	0.0015
702	1-MthNaphthalene	C11H10	0.11957	0.0167	0.0017
509	N-Propylbenzene	C9H12	0.11537	0.016	0.0017

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

526	M-Diethylbenzene	C10H14	0.10277	0.014	0.0014
583	Cs-2-PhnButene-2	C10H12	0.09596	0.0124	0.0012
543	M-DiisopropylBz	C12H18	0.08546	0.0114	0.0011
584	Ts-2-PhnButene-2	C10H12	0.05674	0.0064	0.0005
580	1,2-DiC1-3C2-Bz	C10H14	0.11018	0.015	0.0015
704	1-EthNaphthalene	C12H12	0.10629	0.0148	0.0016
512	M-Ethyltoluene	C9H12	0.10463	0.0143	0.0014
522	1-Mth-2-iC3-Benz	C10H14	0.09497	0.0125	0.0012
513	P-Ethyltoluene	C9H12	0.10714	0.0143	0.0015
514	1,2,3-Mesitylene	C9H12	0.11763	0.0159	0.0016
614	M-Divinylbenzene	C10H10	0.10156	0.0134	0.0013
524	1-Mth-4-iC3-Benz	C10H14	0.10311	0.0138	0.0014
822	Gamma-Terpinene	C10H16	0.09938	0.0133	0.0013
821	Alpha-Terpinene	C10H16	0.0798	0.0098	0.0009
523	1-Mth-3-iC3-Benz	C10H14	0.09878	0.0131	0.0013
703	2-MthNaphthalene	C11H10	0.11255	0.0149	0.0016
557	CycHexylBenzene	C12H16	0.1142	0.017	0.002
515	1,2,4-Mesitylene	C9H12	0.09962	0.0128	0.0012
519	Isobutylbenzene	C10H14	0.09288	0.0121	0.0011
424	DiPhnAcetylene	C14H10	0.06227	0.0066	0.0005
544	P-DiisopropylBz	C12H18	0.09961	0.0141	0.0016
518	N-Butylbenzene	C10H14	0.11102	0.0152	0.0016
516	1,3,5-Mesitylene	C9H12	0.08791	0.0111	0.001
809	Acenaphthalene	C12H8	0.07272	0.0099	0.001
725	123-TriMthIndene	C12H14	0.07445	0.0093	0.0008
527	1,4-DiEthBenzene	C10H14	0.10867	0.015	0.0016
558	Diphenyl	C12H10	0.09516	0.0129	0.0013
576	2-Ethyl-m-Xylene	C10H14	0.10031	0.0132	0.0013
620	p-ISOPROPENYLSTY	C11H12	0.1467	0.0168	0.0016
585	o-PropylToluene	C10H14	0.10081	0.0131	0.0013
577	2-Ethyl-p-Xylene	C10H14	0.09305	0.0122	0.0012
579	4-Ethyl-o-Xylene	C10H14	0.09951	0.0131	0.0013
586	m-Propyltoluene	C10H14	0.09343	0.0122	0.0012
587	p-Propyltoluene	C10H14	0.09683	0.0126	0.0012
578	4-Ethyl-m-Xylene	C10H14	0.09681	0.0127	0.0012
575	5-Ethyl-m-Xylene	C10H14	0.08587	0.0107	0.001
530	Prehnitene	C10H14	0.11492	0.0153	0.0016
709	2,6-2Mth-Naphtha	C12H12	0.09969	0.0131	0.0013
715	2,7-2Mth-Naphtha	C12H12	0.10197	0.0137	0.0013
719	2-ETHYLNAPHTHALENE	C12H12	0.1012	0.0132	0.0013
621	p-tert-BUTYLSTY	C12H16	0.08362	0.0099	0.0009
532	1,2,4,5-TetMthBz	C10H14	0.09407	0.012	0.0011
531	1,2,3,5-TetMthBz	C10H14	0.09716	0.0125	0.0012
533	p-tert-BUTYL ET	C12H18	0.06209	0.0073	0.0006
567	N-Pentylbenzene	C11H16	0.10633	0.0142	0.0015

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

718	1-n-PROPYLNAPHTH	C13H14	0.08119	0.0098	0.0009
562	1,1-DiPhnEthane	C14H14	0.07224	0.0089	0.0008
616	4-ISOBUTYLSTYRE	C12H16	0.1287	0.0182	0.002
260	1-Decene	C10H20	0.1081	0.0147	0.0015
735	Cis-Stilbene	C14H12	0.05658	0.0062	0.0005
568	Hexylbenzene	C12H18	0.10218	0.0135	0.0014
563	Diphenylmethane	C13H12	0.08708	0.0112	0.0011
564	1,2-DiPhnEthane	C14H14	0.09264	0.0118	0.0011
804	Anthracene	C14H10	0.12188	0.0161	0.0016
736	Trans-Stilbene	C14H12	0.10001	0.014	0.0014
805	Phenanthrene	C14H10	0.11705	0.0161	0.0017
713	1-ButNaphthalene	C14H16	0.08772	0.0116	0.0012
807	Pyrene	C16H10	0.09244	0.0117	0.0011
261	1-Undecene	C11H22	0.10537	0.0141	0.0015
581	23-2C1-23-2PhnC4	C18H22	0.02502	0.0021	0.0001
549	N-Heptylbenzene	C13H20	0.10077	0.0126	0.0013
710	1-PhnNaphthalene	C16H12	0.05295	0.0062	0.0005
566	2,4-Diphenyl-4-M	C18H20	0.05677	0.0059	0.0004
561	O-Terphenyl	C18H14	0.0266	0.0025	0.0002
569	N-Octylbenzene	C14H22	0.09659	0.0122	0.0012
565	Triphenylmethane	C19H16	0.03725	0.0038	0.0003
714	N-C6-Naphthalene	C16H20	0.08288	0.0108	0.0011
717	Fluoranthene	C16H10	0.07485	0.0086	0.0007
716	1-Hexyl-Tetralin	C16H24	0.06841	0.0084	0.0008
731	TriPhnEthylene	C20H16	0.05426	0.0057	0.0004
806	Chrysene	C18H12	0.11625	0.0172	0.002
588	1,1,2TriPhenEth	C20H18	0.02183	0.0019	0.0001
711	1-n-NonylNaphtha	C19H26	0.07976	0.0091	0.0008
570	N-Nonylbenzene	C15H24	0.09581	0.0119	0.0012
712	1-Decyl Naphtha	C20H28	0.07843	0.0088	0.0007
559	P-Terphenyl	C18H14	0.06993	0.0095	0.001
560	M-Terphenyl	C18H14	0.06041	0.0074	0.0007
589	TetraPhenylMetha	C25H20	0.04697	0.0048	0.0004
554	Decylbenzene	C16H26	0.09188	0.0115	0.0011
732	TetraPhnEthylene	C26H20	0.04907	0.0048	0.0003
574	N-Dodecylbenzene	C18H30	0.08617	0.0109	0.0011
571	N-Undecylbenzene	C17H28	0.08962	0.011	0.0011
572	Tridecylbenzene	C19H32	0.08462	0.0106	0.001
573	n-TETRADECYLBENZ	C20H34	0.07345	0.0089	0.0008
2575	n-PENTADECYLBENZ	C21H36	0.07203	0.0087	0.0008
2576	n-HEXADECYLBENZ	C22H38	0.07052	0.0086	0.0008
2577	n-HEPTADECYLBENZ	C23H40	0.06852	0.008	0.0007
2578	n-OCTADECYLBENZE	C24H42	0.06704	0.0077	0.0007

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

Dip ID	Halocarbons Name	Formula	$P^{calc}_{760\,nnHg}$	$P^{calc}_{100\,nnHg}$	$P^{calc}_{10\,nnHg}$
1544	Allyl Chloride	C3H5Cl	0.11071	0.0149	0.0015
1531	3-Chloropropyne	C3H3Cl	0.11489	0.0144	0.0013
1535	T-Butyl Chloride	C4H9Cl	0.1055	0.0138	0.0014
1530	Isopropyl Cl	C3H7Cl	0.20733	0.0353	0.0047
1572	O-DiCl-Benzene	C6H4Cl2	0.0943	0.0124	0.0012
1585	Propyl Chloride	C3H7Cl	0.1247	0.0182	0.0021
1684	Isopropyl Iodide	C3H7I	0.13952	0.0201	0.0022
1651	2-Bromopropane	C3H7Br	0.16281	0.025	0.003
1691	Iodobenzene	C6H5I	0.10127	0.0134	0.0013
1860	Fluorobenzene	C6H5F	0.11238	0.0147	0.0014
1571	Chlorobenzene	C6H5Cl	0.11797	0.0166	0.0018
1680	Bromobenzene	C6H5Br	0.12488	0.0176	0.0019
1526	1,2-DiCl-Propane	C3H6Cl2	0.08958	0.0113	0.001
1683	Propyl Iodide	C3H7I	0.20227	0.0323	0.0039
1536	2,3-DICHLOROBUT	C4H8Cl2	0.13973	0.0198	0.0022
2638	2-Bromobutane	C4H9Br	0.15201	0.0244	0.003
1586	1-Chlorobutane	C4H9Cl	0.11709	0.0166	0.0018
1573	M-DiCl-Benzene	C6H4Cl2	0.07829	0.0096	0.0009
2634	Benzotrifluoride	C7H5F3	0.09421	0.0136	0.0016
1574	P-DiCl-Benzene	C6H4Cl2	0.08064	0.0102	0.001
1650	1-Bromopropane	C3H7Br	0.23267	0.0393	0.0053
1587	2-Chlorobutane	C4H9Cl	0.18023	0.0281	0.0033
1678	M-Dibromobenzene	C6H4Br2	0.09041	0.0112	0.001
1537	1,2-DiCl-Butane	C4H8Cl2	0.07538	0.0088	0.0008
1597	34-DiCl-1-Butene	C4H6Cl2	0.06277	0.008	0.0008
1577	O-Chlorotoluene	C7H7Cl	0.09798	0.0129	0.0013
1532	123-3Cl-Propane	C3H5Cl3	0.06311	0.0071	0.0006
1578	P-Chlorotoluene	C7H7Cl	0.10671	0.0145	0.0015
1562	Benzyl Chloride	C7H7Cl	0.09969	0.0135	0.0014
2661	P-Bromotoluene	C7H7Br	0.11256	0.0154	0.0015
1508	1,4-DiCl-Butane	C4H8Cl2	0.1121	0.0155	0.0016
1655	1-Bromobutane	C4H9Br	0.20763	0.0328	0.0042
2652	Perfluoropropane	C3F8	0.21678	0.0402	0.0057
1505	2-Butylene DiCl	C4H6Cl2	0.10152	0.0144	0.0016
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	0.07658	0.0092	0.0008
1588	1-Chloropentane	C5H11Cl	0.11373	0.015	0.0015
1592	1,2,4-TriCl-Bz	C6H3Cl3	0.05923	0.0066	0.0005
1579	2,4-2Cl-Toluene	C7H6Cl2	0.07596	0.0095	0.0009
2593	1,3,5-TriCl-BZ	C6H3Cl3	0.05282	0.0057	0.0004
1697	1-Br-Naphthalene	C10H7Br	0.10826	0.0152	0.0016
1622	Perfluorobutane	C4F10	0.14315	0.0228	0.0028
1857	P-Cl-Benzo-TriF	C7H4ClF3	0.0527	0.0065	0.0006
1509	1,5-DiCl-Pentane	C5H10Cl2	0.11757	0.0165	0.0017

Table B.10 Detailed Vapor Pressures for Different Organic Compounds Calculated by the Tihic et al. Approach using SOG (Continued)

1589	1-Cl-Naphthalene	C10H7Cl	0.10221	0.0132	0.0014
1864	Perfluorobenzene	C6F6	0.0052	0.0002	0
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	0.03817	0.0044	0.0004
1667	1-Bromoheptane	C7H15Br	0.15692	0.0235	0.0027
1575	HexaCl-Benzene	C6Cl6	0.02679	0.0035	0.0004
2640	Freon 123B1	C2HBrClF3	0.05082	0.0059	0.0005
1504	Vinyl Chloride	C2H3Cl	0.18076	0.033	0.0053
1672	1,1-DiBr-Ethane	C2H4Br2	0.12938	0.0206	0.0026
1580	Acetylene DiCl	C2H2Cl2	0.18205	0.0307	0.0042
1692	Diiodomethane	CH2I2	0.29973	0.0542	0.0082
1698	Bromoform	CHBr3	0.09821	0.0124	0.0012
2687	Freon 13B1	CBrF3	0.03151	0.0033	0.0003
1649	Tetrabromoethane	C2H2Br4	0.09216	0.012	0.0012
1503	Ethyl Chloride	C2H5Cl	0.13878	0.021	0.0025
1641	Methyl Bromide	CH3Br	0.37688	0.0741	0.012
2688	Freon 12B2	CBr2F2	0.02132	0.0015	0.0001
1673	1,2-DiBr-Ethane	C2H4Br2	0.24478	0.0395	0.0047
2637	Dibromomethane	CH2Br2	0.25034	0.0439	0.0062
1612	Cl-2F-Ethylene	C2HClF2	0.15946	0.0262	0.0033
2639	Br-Cl-Methane	CH2BrCl	0.1218	0.0179	0.002
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	0.12427	0.0187	0.0024
1682	Ethyl Iodide	C2H5I	0.23491	0.0404	0.0054
2693	Perfluoroethane	C2F6	0.40363	0.0917	0.0171
1645	Ethyl Bromide	C2H5Br	0.27902	0.0505	0.0075
1619	111-3F-Ethane	C2H3F3	1.0767	0.3044	0.0772
2694	Vinyl Bromide	C2H3Br	0.12562	0.017	0.0017
1523	1,2-DiCl-Ethane	C2H4Cl2	0.07798	0.0098	0.0009
2527	1,3-DiCl-Propane	C3H6Cl2	0.09428	0.012	0.0012

APPENDIX C.

BOILING TEMPERATURES AND THEIR ERRORS CALCULATED BY THE METHODS GIVEN IN CHAPTER III

Table C. 1 Detailed Boiling Temperature Errors for GC-PC-SAFT, GC-SAFT ans GC-ESD and also Tihic el at. Approach

	no. of Occ.	T AAD% 760 mmHg	T Bias% 760 mmHg	$100\ln(T^{calc}/T^{exp})$ 760 mmHg	ΔT 760 mmHg	$\lvert\Delta T\rvert$ 760 mmHg
	877	3.27	-1.25	-0.94	-4.17	14.17
PCSAFT	877	2.08	-0.33	-0.27	-2.05	9.08
ESD	877	2.27	-0.46	-0.35	-3.08	10.06
Tihic FOG	642	2.65	-0.44	-0.44	-0.42	10.95
Tihic SOG	665	2.56	-0.49	-0.50	-0.71	10.59
	no. of Occ.	T AAD% 100 mmHg	T Bias% 100mmHg	$100\ln(T^{calc}/T^{exp})$ 100mmHg	ΔT 100mmHg	$\lvert\Delta T\rvert$ 100mmHg
SAFT	877	3.41	-1.84	-1.56	-5.88	12.20
PCSAFT	877	2.02	-0.09	-0.02	-0.84	7.12
ESD	877	2.12	0.01	0.13	-0.64	7.61
Tihic FOG	642	2.80	-0.46	-0.49	-0.23	9.85
Tihic SOG	665	2.68	-0.50	-0.53	-0.46	9.45
	no. of Occ.	T AAD% 10mmHg	T Bias% 10mmHg	$100\ln(T^{calc}/T^{exp})$ 10mmHg	ΔT 10mmHg	$\lvert\Delta T\rvert$ 10mmHg
SAFT	877	3.66	-2.18	-1.92	-6.20	11.08
PCSAFT	877	2.18	0.18	0.24	0.13	6.45
ESD	877	2.24	0.32	0.44	0.74	6.73
Tihic FOG	642	2.96	-0.43	-0.48	0.04	9.03
Tihic SOG	665	2.81	-0.47	-0.51	-0.16	8.59

Table C. 2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg

	Alcohols				
Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1181	Phenol	C6H6O	455.08	393.94	345.26
1182	O-Cresol	C7H8O	464.04	400.30	350.10
1183	M-Cresol	C7H8O	475.27	411.75	361.10
1176	2,6-Xylenol	C8H10O	474.19	406.98	354.05
1111	2-Mth-2-Butanol	C5H12O	375.14	328.53	290.71
1178	3,5-Xylenol	C8H10O	494.89	428.78	376.60
1133	2-Octanol	C8H18O	452.75	393.24	347.71
2885	4-HYDROXYSTYREN	C8H8O	501.97	434.77	380.44
1197	P-t-Butylphenol	C10H14O	512.96	443.37	389.86
1172	2,4-Xylenol	C8H10O	483.80	417.66	365.23
1184	P-Cresol	C7H8O	474.91	411.61	361.89
1151	Cyclohexanol	C6H12O	433.99	378.40	334.95
1170	2,3-Xylenol	C8H10O	490.08	423.00	369.35
1187	P-Ethyl Phenol	C8H10O	491.52	426.58	373.45
2859	P-Methoxyphenol	C7H8O2	517.64	450.61	398.41
1121	2-Ethylhexanol	C8H18O	457.76	397.91	352.37
1179	PropargylAlcohol	C3H4O	387.06	334.19	290.75
1123	3-Mth-1-Butanol	C5H12O	404.06	354.49	314.15
2196	P-t-Amylphenol	C11H16O	535.74	462.19	403.67
1174	2,5-Xylenol	C8H10O	483.98	418.22	364.39
1115	2-Hexanol	C6H14O	413.06	360.65	318.24
1152	1-MthCycHexanol	C7H14O	441.51	375.67	325.68
4854	Guaiacol	C7H8O2	478.51	411.69	360.93
1107	Sec-Butanol	C4H10O	372.77	326.91	289.60
1167	Allyl Alcohol	C3H6O	369.98	322.63	283.92
1130	4-Mth-2-Pentanol	C6H14O	404.83	351.43	308.07
1177	3,4-Xylenol	C8H10O	500.12	433.47	379.89
1114	1-Hexanol	C6H14O	430.78	376.58	333.38
1106	Isobutanol	C4H10O	380.83	334.77	297.46
1125	1-Heptanol	C7H16O	449.63	392.42	348.09
1105	N-Butanol	C4H10O	390.83	342.89	303.84
1109	1-Pentanol	C5H12O	410.83	359.07	317.66
1132	1-Octanol	C8H18O	468.52	408.25	361.49
1113	T-Butylcarbinol	C5H12O	386.36	337.69	298.93
1137	1-Undecanol	C11H24O	518.56	451.14	398.96
1108	Tert-Butanol	C4H10O	355.62	312.59	277.96
1103	N-Propanol	C3H8O	370.34	324.84	287.15
1134	1-Nonanol	C9H20O	486.50	423.21	374.53
2195	P-t-Octylphenol	C14H22O	563.32	486.05	424.88
1102	Ethanol	C2H6O	351.46	307.47	270.63
1124	3-Mth-2-Butanol	C5H12O	384.51	336.53	299.46
1136	1-Decanol	C10H22O	503.83	437.73	386.95
1140	Dodecanol	C12H26O	537.34	466.08	411.52
1104	Isopropanol	C3H8O	355.50	311.87	275.51

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1110	2-Pentanol	C5H12O	392.16	343.96	304.95
1120	3-Pentanol	C5H12O	388.65	339.65	300.99
1112	2-Mth-1-Butanol	C5H12O	401.70	352.68	312.45
1154	Ts-2-Mth-CycC6OH	C7H14O	440.05	381.30	332.56
1153	Cs-2-Mth-CycC6OH	C7H14O	438.29	378.25	329.62
1156	Ts-3-Mth-CycC6OH	C7H14O	447.01	390.02	343.66
1157	Cs-4-Mth-CycC6OH	C7H14O	444.04	387.10	340.76
2197	P-Cumylphenol	C15H16O	608.49	528.00	463.16
1180	Benzyl Alcohol	C7H8O	477.72	415.05	365.00
1158	Ts-4-Mth-CycC6OH	C7H14O	444.38	388.12	342.37
1155	Cs-3-Mth-CycC6OH	C7H14O	446.45	390.29	344.18
1168	2-Phn-2-Propanol	C9H12O	474.83	411.02	358.30
1141	1-Tridecanol	C13H28O	553.65	479.98	423.44
1147	2-Eth-1-Butanol	C6H14O	419.64	364.89	323.04
1117	2-Mth-1-Pentanol	C6H14O	421.41	367.05	324.56
2115	2-Phenylethanol	C8H10O	491.98	426.47	372.37
1142	1-Tetradecanol	C14H30O	568.99	492.99	434.50
2118	1-PHN-1-PROPANOL	C9H12O	491.90	424.87	370.27
2119	1-PHN-2-PROPANOL	C9H12O	492.81	426.03	371.64
1126	2-Heptanol	C7H16O	432.38	374.86	330.78
1143	1-Pentadecanol	C15H32O	583.78	506.13	446.43
1129	Isoheptanol	C7H16O	445.02	389.36	344.01
2117	2,6-DiMth-4-C7OH	C9H20O	450.60	393.59	347.44
1144	1-Hexadecanol	C16H34O	597.62	518.22	456.86
1145	Heptadecanol	C17H36O	610.84	530.09	467.17
1199	Nonylphenol	C15H24O	590.45	515.53	455.78
1146	1-Octadecanol	C18H38O	624.00	541.45	477.08
1135	2-Nonanol	C9H20O	471.35	407.76	358.44
1149	1-Nonadecanol	C19H40O	634.84	550.69	485.10
1139	Isodecanol	C10H22O	492.02	431.02	381.39
1148	1-Eicosanol	C20H42O	645.53	560.61	494.73
2198	Dinonylphenol	C24H42O	735.10	644.52	571.12
1159	Menthol	C10H20O	489.41	423.78	369.57
1202	DiethyleneGlycol	C4H10O3	518.09	453.49	402.15
1245	1,3-Benzenediol	C6H6O2	549.35	483.52	429.02
1186	P-Hydroquinone	C6H6O2	558.82	490.57	433.24
1244	1,2-Benzenediol	C6H6O2	518.36	449.42	391.68
1219	2MTH,13PROPNDIO	C4H10O2	487.24	427.66	378.30
1212	1,3-Propanediol	C3H8O2	487.26	426.78	376.15
1235	P-t-But-Catechol	C10H14O2	558.15	488.22	431.30
1203	Triglycol	C6H14O4	561.53	488.61	431.56
1198	Bisphenol A	C15H16O2	633.93	567.09	512.37
1238	2,3-Butanediol	C4H10O2	453.66	400.60	354.84
1211	1,2-Propanediol	C3H8O2	460.87	404.96	358.00
2219	2,4-PENTANEDIOL	C5H12O2	474.16	416.96	367.89
1215	1,4-Butynediol	C4H6O2	511.37	456.68	410.44

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1214	Neopentyl Glycol	C5H12O2	477.08	423.41	377.36
1221	1,3-Butanediol	C4H10O2	481.36	422.72	374.47
1220	1,2-Butanediol	C4H10O2	469.63	412.14	365.00
1240	Ts2-C4H8-14-Diol	C4H8O2	499.23	445.29	399.43
1239	Cis-Butenediol	C4H8O2	508.05	448.49	397.48
1241	1,4-Butanediol	C4H10O2	500.98	443.85	395.23
1222	Hexylene Glycol	C6H14O2	470.63	416.77	370.07
1213	Dipropylene Gly	C6H14O3	505.42	442.87	388.25
1242	1,5-Pentanediol	C5H12O2	512.46	454.95	404.76
1243	1,6-Hexanediol	C6H14O2	526.29	464.35	410.53
1204	TetraC2H4 Glycol	C8H18O5	602.48	528.43	468.40
6886	C6H4(COOC2H4OH)2	C12H14O6	683.23	613.90	554.88
1248	123-Benzenetriol	C6H6O3	581.53	511.73	450.56
1231	Glycerol	C3H8O3	560.86	494.81	439.83
1247	Hexaglycerol	C6H14O3	562.09	500.91	446.92
1246	Pentaerythritol	C5H12O4	630.96	577.02	529.01
1250	Sorbitol	C6H14O6	704.20	644.49	591.63
1249	Inositol	C6H12O6	690.95	634.71	584.45

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Amines

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1742	Ethyleneimine	C2H5N	329.16	283.11	246.24
1745	Piperidine	C5H11N	379.48	322.45	277.10
2726	Propyleneimine	C3H7N	334.23	284.71	245.36
1766	Pyrrolidine	C4H9N	359.63	307.63	266.47
1719	Isopropylamine	C3H9N	304.95	260.64	226.04
1711	N-Propylamine	C3H9N	320.74	274.38	237.20
1726	Sec-Butylamine	C4H11N	336.27	285.69	245.80
1704	Ethylamine	C2H7N	289.92	248.27	215.18
1702	Dimethylamine	C2H7N	280.22	240.41	208.91
1710	Diethylamine	C4H11N	328.88	279.48	240.22
1740	Allylamine	C3H7N	326.68	279.80	242.32
1712	N-Butylamine	C4H11N	350.61	299.68	259.39
1794	HexMthyleneimine	C6H13N	411.46	350.79	304.15
1729	Cyclohexylamine	C6H13N	407.38	345.95	298.05
1714	Isobutylamine	C4H11N	340.92	291.21	251.95
2853	Acetamide	C2H5NO	494.66	429.84	377.69
2731	N-C1-CycC6-Amine	C7H15N	422.12	360.82	312.41
1743	Diisopropylamine	C6H15N	357.12	302.85	264.49

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1796	N,N-DiMthAniline	C8H11N	466.59	398.81	343.80
1792	Aniline	C6H7N	457.03	393.14	341.75
1713	N-Pentylamine	C5H13N	377.54	322.75	279.21
1733	Benzylamine	C7H9N	457.27	392.38	341.16
1737	M-Toluidine	C7H9N	476.47	409.67	357.43
3796	N-Ethylaniline	C8H11N	476.27	409.41	357.08
1878	2-Methacrylamide	C4H7NO	488.50	421.80	367.95
1736	O-Toluidine	C7H9N	473.37	406.12	353.77
2739	Diallylamine	C6H11N	384.12	329.70	286.43
2706	Hexylamine	C6H15N	405.62	346.60	299.75
2724	O-Ethylaniline	C8H11N	482.95	415.92	362.12
1707	Dipropylamine	C6H15N	381.78	325.48	280.51
1738	P-Toluidine	C7H9N	473.57	407.33	354.85
1795	N-Methylaniline	C7H9N	468.70	402.09	348.68
1718	Diisobutylamine	C8H19N	412.51	352.29	303.75
1879	Acrylamide	C3H5NO	513.66	440.90	387.35
2707	1-Aminoheptane	C7H17N	429.83	367.09	316.93
2730	DiCycHexylAmine	C12H23N	528.82	448.17	387.27
2787	P-Aminodiphenyl	C12H11N	610.37	525.17	455.64
1744	Dibutylamine	C8H19N	432.17	369.15	319.66
2708	1-Octylamine	C8H19N	452.78	387.97	336.07
2791	2,6-DiEthAniline	C10H15N	508.83	442.72	387.19
2709	1-Nonylamine	C9H21N	475.36	407.63	353.47
2710	1-Decylamine	C10H23N	493.41	424.00	368.90
3722	Diamylamine	C10H23N	476.41	411.74	360.37
3724	Undecylamine	C11H25N	514.73	440.95	383.34
2712	Dodecylamine	C12H27N	532.34	457.98	398.99
1720	Tetradecylamine	C14H31N	564.66	487.49	426.12
2752	Piperazine	C4H10N2	419.41	362.07	315.77
1752	Propylenediamine	C3H10N2	392.47	339.28	296.33
1741	Ethylenediamine	C2H8N2	390.30	337.37	294.56
2725	O-Aminoaniline	C6H8N2	530.14	460.53	403.66
2750	P-Aminoaniline	C6H8N2	540.33	469.67	412.13
2727	M-Aminoaniline	C6H8N2	559.77	483.59	420.33
1750	AEP	C6H15N3	493.55	426.89	373.54
1732	Toluene Diamine	C7H10N2	557.22	484.62	425.09
1731	hexamethyleneDiamine	C6H16N2	472.75	406.05	351.10
3750	P-Benzidine	C12H12N2	674.76	589.32	519.80

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Nitrilies

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1773	Propionitrile	C3H5N	370.81	314.33	270.05

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1782	Butyronitrile	C4H7N	390.52	332.20	286.48
2720	Allyl Cyanide	C4H5N	391.65	333.49	287.34
1783	Valeronitrile	C5H9N	414.05	352.02	303.58
3874	Benzyl Cyanide	C8H7N	506.34	434.75	376.44
1786	Hexanenitrile	C6H11N	436.71	372.46	320.46
1776	Succinonitrile	C4H4N2	540.52	467.92	409.56
1781	Glutaronitrile	C5H6N2	559.22	478.21	413.11
2735	14-2Cyano-2-C4H8	C6H6N2	547.43	475.60	417.66
1777	Adiponitrile	C6H8N2	567.80	490.70	427.49

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Silanes

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
3985	Dimethyl Silane	C2H8Si	253.39	211.70	180.48
3984	Methyl Silane	CH6Si	216.06	179.79	151.49
3986	Trimethyl Silane	C3H10Si	279.92	234.18	198.93
1984	TetraMth Silane	C4H12Si	299.78	251.92	215.02
2994	TETRAETHYL Si	C8H20Si	426.48	361.46	309.86
1965	HexMthDisiloxane	C6H18OSi2	373.64	316.56	271.53
1966	6C1Cyc3Siloxane	C6H18O3Si3	408.31	347.80	300.58
1988	8C1Cyc4Siloxane	C8H24O4Si4	448.36	383.74	334.13
3991	DecaMethcyclpenS	C10H30O5Si5	483.89	414.46	359.00
3992	DodecaMethCyHexS	C12H36O6Si6	517.84	444.16	385.99

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Imines

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1767	N-MthPyrrolidine	C5H11N	352.38	297.97	255.31
2797	3-Methylpyridine	C6H7N	417.30	355.27	306.68
1797	2-Methylpyridine	C6H7N	402.50	342.82	296.02
2799	4-Methylpyridine	C6H7N	418.43	356.31	307.59
1753	N,N-DiEthAniline	C10H15N	489.22	420.35	365.53
1754	N-Methylpyrrole	C5H7N	386.09	329.19	284.68
3740	Acridine	C13H9N	618.96	529.23	458.16

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Tert-N

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1703	Trimethylamine	C3H9N	276.23	232.51	199.25
2856	DiMth Acetamide	C4H9NO	439.10	375.90	325.27
1706	Triethylamine	C6H15N	361.78	306.41	263.05
2716	Tributylamine	C12H27N	487.53	420.94	368.07
2719	Tripropylamine	C9H21N	429.83	372.81	326.81
3723	Triamylamine	C15H33N	516.45	448.78	394.45

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Nitrate

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1761	Nitroethane	C2H5NO2	387.13	330.22	285.74
1763	2-Nitropropane	C3H7NO2	393.36	334.69	288.85
1762	1-Nitropropane	C3H7NO2	404.49	344.93	298.00
1779	P-Nitrotoluene	C7H7NO2	511.98	436.67	380.40
1886	Nitrobenzene	C6H5NO2	483.78	412.65	357.40
1778	O-Nitrotoluene	C7H7NO2	495.39	423.85	366.97
1780	M-Nitrotoluene	C7H7NO2	505.42	431.63	372.86
1891	O-Nitroanisole	C7H7NO3	546.59	473.67	414.83
2740	M-Dinitrobenzene	C6H4N2O4	575.20	493.66	430.70
2742	P-Dinitrobenzene	C6H4N2O4	571.07	489.71	426.59
2741	O-Dinitrobenzene	C6H4N2O4	592.07	505.65	439.77
2749	3,5-DiNitToluene	C7H6N2O4	588.03	507.57	440.39
2743	DNT	C7H6N2O4	590.30	505.33	437.05
2745	3,4-DiNitToluene	C7H6N2O4	610.03	522.20	449.71
2744	2,6-DiNitToluene	C7H6N2O4	590.30	505.33	437.05
2748	2,5-DiNitToluene	C7H6N2O4	590.08	505.22	435.38
2746	1,3,5-TrinitroBz	C6H3N3O6	629.90	543.34	479.91
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	743.00	654.80	582.43
2747	Trinitrotoluene	C7H5N3O6	624.67	538.16	470.33

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Thiols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1802	Ethyl Mercaptan	C2H6S	308.16	260.59	223.31
1820	Dimethyl Sulfide	C2H6S	310.51	262.70	225.66
1843	Thiacyclopentane	C4H8S	394.29	334.27	287.35

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1803	1-Propanethiol	C3H8S	340.79	288.65	248.13
1805	Isobut Mercaptan	C4H10S	361.62	306.05	262.89
6860	Ethylenedithiol	C2H6S2	419.47	357.39	308.03
1811	Cyclohexanethiol	C6H12S	431.83	365.27	313.58
1828	DiMth Disulfide	C2H6S2	382.87	324.74	279.37
1841	Butanethiol	C4H10S	371.39	314.64	270.63
1814	Methylproylsulf	C4H10S	368.67	312.65	268.96
2816	ETHYLtBUTYL SUL	C6H14S	393.57	333.07	286.27
1818	Diethyl Sulfide	C4H10S	365.27	309.37	264.77
1812	Benzyl Mercaptan	C7H8S	472.38	402.79	348.87
1838	T-OctylMercaptan	C8H18S	428.64	361.83	309.95
1827	1-Pentanethiol	C5H12S	399.71	339.46	292.52
2815	METHnBUTYL SULFD	C5H12S	393.57	333.07	286.27
1824	DiethylDisulfide	C4H10S2	427.15	362.88	312.85
1807	N-Hexylmercaptan	C6H14S	425.66	361.83	312.00
6857	Dimercaptoethyl	C4H10OS2	489.95	420.30	364.99
1839	1-Heptanethiol	C7H16S	450.18	383.45	331.64
1829	DiProp Disulfide	C6H14S2	468.84	399.59	343.51
1809	1-Octanethiol	C8H18S	472.24	402.78	348.58
1808	N-Nonanethiol	C9H20S	492.80	421.25	366.33
1826	1-Decanethiol	C10H22S	512.41	438.95	381.48
2838	tertDodecanThiol	C12H26S	515.60	443.00	385.78
1825	1-Undecanethiol	C11H24S	530.32	455.20	396.97
1837	Dodecylthiol	C12H26S	547.72	468.28	408.12

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Aldehydes

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1037	Methacrolein	C4H6O	341.16	289.06	248.08
1002	Acetaldehyde	C2H4O	294.21	248.71	214.25
1003	Propionaldehyde	C3H6O	321.15	272.89	235.06
1041	Benzaldehyde	C7H6O	451.81	385.29	332.79
1034	Acrolein	C3H4O	325.89	275.57	236.47
1005	N-Butyraldehyde	C4H8O	348.03	295.69	255.12
1036	Trans-2-Butenal	C4H6O	375.45	320.82	277.39
1007	Valeraldehyde	C5H10O	376.15	320.31	276.80
1006	Isobutyraldehyde	C4H8O	337.47	288.66	249.96
1009	1-Hexanal	C6H12O	401.29	342.46	296.73
1040	P-Tolualdehyde	C8H8O	477.57	410.40	356.80
1016	2-Methylhexanal	C7H14O	415.36	355.95	308.81
1017	3-Methylhexanal	C7H14O	417.15	356.12	307.02

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1008	1-Heptanal	C7H14O	426.03	363.62	314.32
1013	2-Ethylhexanal	C8H16O	434.21	372.91	324.36
1010	1-Octanal	C8H16O	447.05	383.04	332.81
1011	1-Nonanal	C9H18O	468.08	400.81	349.96
1020	1-Decanal	C10H20O	487.83	418.61	365.42
1021	1-Undecanal	C11H22O	506.27	434.29	380.31
1025	Dodecanal	C12H24O	523.55	450.38	393.07
1026	1-Tridecanal	C13H26O	539.88	465.37	407.19
1014	1,2-Ethanedione	C2H2O2	323.77	279.74	244.12
1044	1,4BenzDicarboxAldehy	C8H6O2	519.56	450.71	395.13

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Epoxides

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1440	ISOBUTYLENE OXID	C4H8O	324.88	273.44	233.20
1478	Furan	C4H4O	304.45	258.66	222.72
1479	Tetrahydrofuran	C4H8O	339.12	287.67	247.19
1443	1,3-Propylene Ox	C3H6O	321.06	272.03	233.19
1477	2,5-Dihydrofuran	C4H6O	338.89	288.05	247.33
1471	1,2-Epoxybutane	C4H8O	336.73	285.45	244.97
1408	1-Methoxypropane	C4H10O	312.00	264.39	227.61
1442	1,2-Propylene Ox	C3H6O	307.63	261.08	224.85
1411	2-Methoxypropane	C4H10O	304.00	257.45	220.95
1421	1,4-Dioxane	C4H8O2	374.52	318.71	273.91
1422	Trioxane	C3H6O3	387.57	332.86	288.98
2422	1,3-DIOXANE	C4H8O2	377.97	322.71	278.73
1426	2-Methoxybutane	C5H12O	332.41	282.18	242.74
1413	1-Methoxybutane	C5H12O	343.13	291.31	250.70
1461	Methoxybenzene	C7H8O	426.98	364.49	315.21
1448	1-Ethoxybutane	C6H14O	365.24	310.72	267.80
1429	1-MethoxyPentane	C6H14O	371.93	316.15	272.38
6885	Ethyl-3-Ethoxypr	C7H14O3	441.29	378.85	329.36

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Ether

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1401	Dimethyl Ether	C2H6O	248.37	209.93	179.59
1407	MethylEthylEther	C3H8O	280.32	238.42	205.61

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1470	VinylMethylEther	C3H6O	278.71	236.65	203.38
1405	MTBE	C5H12O	328.24	277.76	238.33
1445	VinylEthyl Ether	C4H8O	308.68	261.62	224.72
1402	Diethyl Ether	C4H10O	307.54	260.73	224.62
1431	Methylal	C3H8O2	315.10	268.41	231.97
1428	T-But EthylEther	C6H14O	346.02	293.51	252.46
1427	TAME	C6H14O	359.43	304.30	261.48
1410	Mth Isobut Ether	C5H12O	331.83	281.60	242.18
1430	Eth-t-Pent-Ether	C7H16O	374.68	317.58	272.49
1403	DiisopropylEther	C6H14O	341.61	289.34	247.59
1415	Eth Propyl Ether	C5H12O	336.84	285.32	246.28
1455	Dimethyl Acetal	C4H10O2	357.60	305.65	264.37
1446	Dipropyl Ether	C6H14O	363.10	308.27	265.50
1447	Butyl VinylEther	C6H12O	366.91	312.89	270.46
1462	EthylPhenylEther	C8H10O	442.97	378.96	328.68
1406	Di-sec-But Ether	C8H18O	394.09	335.49	290.03
1432	Acetal	C6H14O2	376.62	320.74	276.63
1460	BenzylEthylEther	C9H12O	458.46	391.86	338.53
1050	Paraldehyde	C6H12O3	397.29	341.19	296.65
1404	Di-n-Butyl Ether	C8H18O	414.00	353.52	306.00
1420	Anethole	C10H12O	508.84	436.85	379.73
1456	DimethylCarbitol	C6H14O3	435.78	375.19	326.99
1463	Dibenzyl Ether	C14H14O	561.29	490.14	431.57
1425	Di-n-PentylEther	C10H22O	459.65	393.24	339.75
1458	Diethyl Carbitol	C8H18O3	461.83	398.18	346.16
1412	Dihexyl Ether	C12H26O	498.73	431.26	377.53
1454	Triglyme	C8H18O4	489.42	426.59	375.80
1459	Dibutyl Carbitol	C12H26O3	528.78	455.49	394.77
1424	Di-n-Octyl Ether	C16H34O	559.96	487.95	430.13
1457	Tetraglyme	C10H22O5	548.96	479.76	421.77
1418	Dinonyl Ether	C18H38O	591.27	516.13	455.67
2432	ETHYLAL	C5H12O2	360.76	306.71	263.88
2405	DIISOBUTYL ETHER	C8H18O	395.56	336.91	291.08
2456	Ethyl Glyme	C6H14O2	394.28	338.32	294.23
2417	ETHYLHEXYL ETHER	C8H18O	416.84	357.17	310.13
2415	ETHYLISOPROPETH	C5H12O	326.30	276.83	238.03

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Dip ID	Formate Name	Formula	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1301	Methyl Formate	C2H4O2	304.94	260.19	224.77
1311	Vinyl Formate	C3H4O2	320.23	274.46	237.77

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1302	Ethyl Formate	C3H6O2	327.58	278.93	240.48
2306	t-Butyl Formate	C5H10O2	355.80	302.02	259.81
1303	Propyl Formate	C4H8O2	354.15	302.17	261.66
2305	sec-ButylFormate	C5H10O2	366.83	313.08	270.29
2311	CYCLOHEXL FORMAT	C7H12O2	435.37	370.63	320.34
1304	N-Butyl Formate	C5H10O2	379.33	323.75	279.80
1305	Isobutyl Formate	C5H10O2	371.12	316.90	272.93
2350	Benzyl Formate	C8H8O2	476.23	408.42	354.44
2307	n-Hexyl Formate	C7H14O2	428.32	367.70	319.61
1306	N-Pentyl Formate	C6H12O2	405.34	346.12	300.03
2308	n-Heptyl Formate	C8H16O2	451.30	385.41	332.87
1308	N-Octyl Formate	C9H18O2	471.94	401.94	346.22
1309	n-Nonyl Formate	C10H20O2	487.01	419.27	364.14
1310	n-Decyl Formate	C11H22O2	506.22	437.01	380.40

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

	Ester				
Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1351	Mth Methacrylate	C5H8O2	373.20	318.32	275.80
1312	Methyl Acetate	C3H6O2	330.20	282.12	243.93
1331	Vinyl Propionate	C5H8O2	368.45	315.17	272.89
1321	Vinyl Acetate	C4H6O2	345.85	295.53	255.39
1352	Eth MthAcrylate	C6H10O2	390.30	331.82	285.50
1322	MethylPropionate	C4H8O2	352.61	301.45	261.16
1341	Methyl Acrylate	C4H6O2	353.64	301.08	259.50
1313	Ethyl Acetate	C4H8O2	350.35	299.60	259.44
1319	IsopropylAcetate	C5H10O2	361.67	308.72	266.24
1332	Methyl Butyrate	C5H10O2	375.80	321.16	278.18
1342	Ethyl Acrylate	C5H8O2	372.55	318.40	275.02
1318	Allyl Acetate	C5H8O2	377.44	320.64	275.36
1314	N-Propyl Acetate	C5H10O2	374.59	320.23	277.83
1323	Ethyl Propionate	C5H10O2	372.48	318.44	276.10
1360	I-But I-Butyrate	C8H16O2	420.69	359.38	311.51
1320	Sec-ButylAcetate	C6H12O2	384.91	329.07	284.25
1336	PropylI-Butyrate	C7H14O2	408.43	350.66	304.82
1353	N-C3-Mthacrylate	C7H12O2	413.97	352.65	305.49
1333	Ethyl Butyrate	C6H12O2	394.53	335.64	289.05
1347	EthylIsovalerate	C7H14O2	407.71	349.00	301.88
1315	N-Butyl Acetate	C6H12O2	399.16	341.37	296.28
1390	Methyl Benzoate	C8H8O2	472.46	403.97	350.53
1388	ISOBUTYL MTHACR	C8H14O2	428.38	365.03	315.30

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1343	1-PropylAcrylate	C6H10O2	392.46	336.45	292.06
1316	Isobutyl Acetate	C6H12O2	389.55	333.22	288.19
1344	N-Butyl Acrylate	C7H12O2	420.58	358.31	308.72
1357	Pentyl Acetate	C7H14O2	420.86	359.51	312.10
1327	N-PropN-Butyrate	C7H14O2	415.97	355.58	307.39
1324	N-PropPropionate	C6H12O2	395.55	338.17	292.40
1291	Acetic Anhydride	C4H6O3	412.64	355.28	309.47
1389	N-ButMthacrylate	C8H14O2	436.05	373.67	324.07
1359	Benzyl Acetate	C9H10O2	487.08	418.29	363.70
1326	N-But Propionate	C7H14O2	418.08	358.63	311.39
1391	Ethyl Benzoate	C9H10O2	486.73	416.39	359.29
1897	CH3OC3H600CH3	C6H12O3	419.17	360.43	313.41
1392	DiethylCarbonate	C5H10O3	399.97	341.13	296.92
1385	N-But N-Butyrate	C8H16O2	438.29	374.43	324.26
1317	IsopentylAcetate	C7H14O2	414.81	353.25	306.25
1363	N-Hexyl Acetate	C8H16O2	444.35	381.23	331.09
1387	Ethylene Acetate	C6H10O4	463.66	401.65	356.36
1393	Diethyl Oxalate	C6H10O4	458.53	395.13	344.76
1365	Butyl Benzoate	C11H14O2	523.03	449.52	390.00
1361	I-C5 I-Valerate	C10H20O2	467.24	398.20	341.82
1367	Heptyl Acetate	C9H18O2	465.50	400.41	348.28
1346	N-Butyl Valerate	C9H18O2	459.63	395.58	343.93
1358	2-C2-C6 Acetate	C10H20O2	473.31	405.05	351.52
1394	Diethyl Malonate	C7H12O4	471.81	407.91	355.72
1292	Propionyl Oxide	C6H10O3	440.30	379.15	330.02
1364	Benzyl Benzoate	C14H12O2	595.94	508.94	445.85
1381	2Mth p-Phthalate	C10H10O4	560.84	480.90	415.22
1368	n-Octyl Acetate	C10H20O2	484.36	417.12	363.11
1377	DiMthI-Phthalate	C10H10O4	554.91	472.34	409.07
1896	Ethylene DiAcr	C8H10O4	503.04	434.40	378.14
1386	2-Ethylhexyl Acr	C11H20O2	489.53	421.02	364.91
1395	Methyl Decanoate	C11H22O2	505.13	435.23	379.93
1369	n-Nonyl Acetate	C11H22O2	497.05	429.88	376.18
1370	n-Decyl Acetate	C12H24O2	517.48	446.44	391.53
1345	N-ButylNonanoate	C13H26O2	520.04	440.57	380.63
1375	DiProp Phthalate	C14H18O4	590.72	512.25	449.25
1376	Diisobutyl Phtha	C16H22O4	592.97	517.83	457.29
1396	IsopropMyristate	C17H34O2	588.47	510.19	447.85
1383	Butyl Stearate	C22H44O2	623.05	542.62	478.02
1362	Methyl Oleate	C19H36O2	617.42	539.72	476.71
1355	Diisooctyl Phtha	C24H38O4	693.73	607.03	537.18
1382	DioctylTerephtha	C24H38O4	698.22	610.70	539.88
1384	DIBUTYL SEBACATE	C18H34O4	622.42	546.77	484.46
1371	Diisodecyl Phtha	C28H46O4	739.70	639.93	557.88
1354	DioctylPhthalate	C24H38O4	656.95	578.29	514.71
2375	DiethylPhthalate	C12H14O4	566.87	492.76	433.44

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

2388	Dipropyl Maleate	C10H16O4	521.06	453.21	398.89
2381	Diallyl Maleate	C10H12O4	520.46	453.62	399.57
2370	Glyceryl Triacet	C9H14O6	532.47	465.15	410.59
2382	Dibutyl Maleate	C12H20O4	553.35	483.44	426.90
2376	DibutylPhthalate	C16H22O4	612.97	534.14	469.75
2353	CetylMthacrylate	C20H38O2	641.46	556.04	484.03
2379	Dihexyl Adipate	C18H34O4	622.42	546.77	484.46
2321	T-Butyl Acetate	C6H12O2	369.46	316.12	274.88
2332	Methl.I-butyrate	C5H10O2	365.73	312.31	270.26
2354	AllylMthacrylate	C7H10O2	412.71	353.28	307.08
2364	CYCLOHEXL ACETAT	C8H14O2	447.54	383.08	331.84
2337	EthylIsobutyrate	C6H12O2	383.24	326.79	281.76
2384	IsobutylAcrylate	C7H12O2	410.17	350.97	303.99
2380	1,1-Diacetoxy C2	C6H10O4	441.80	380.89	332.45
2392	n-PropylBenzoate	C10H12O2	504.08	430.83	373.26
2387	Dimethyl Maleate	C6H8O4	477.77	412.63	360.38
2377	DiMth Phthalate	C10H10O4	557.21	482.39	421.00
2386	Diethyl Maleate	C8H12O4	498.36	429.46	372.87
2385	Mth Dodecanoate	C13H26O2	540.39	466.25	407.78
3379	Dioctyl Adipate	C22H42O4	690.06	589.00	503.47
5886	Mth Acetoacetate	C5H8O3	444.69	383.80	335.13
5884	Ethoxy Acetate	C6H12O3	429.76	369.95	322.62
5887	EthAcetoAcetate	C6H10O3	454.44	391.58	340.17
5885	Carbitol Acetate	C8H16O4	490.61	422.67	366.85

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Ketone

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1096	Methyl Isopropen	C5H8O	371.46	315.56	271.49
1079	Cyclopentanone	C5H8O	403.70	343.60	295.98
1051	Acetone	C3H6O	329.29	280.02	240.95
1052	MEK	C4H8O	352.49	299.85	258.21
1065	Mesityl Oxide	C6H10O	402.67	343.34	296.51
1066	T-But Mth Ketone	C6H12O	379.21	322.16	277.58
1060	2-Pentanone	C5H10O	375.18	319.69	275.98
1061	Mth iC3 Ketone	C5H10O	367.23	312.28	268.30
1053	Diethyl Ketone	C5H10O	374.90	319.16	274.39
1059	3-Hexanone	C6H12O	396.65	338.23	292.54
1099	Diketene	C4H4O2	399.34	343.12	296.96
1055	Sec-ButMthKetone	C6H12O	390.82	332.93	286.42
1054	MIBK	C6H12O	389.29	331.22	286.40

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1095	EthIsopropKetone	C6H12O	386.88	330.62	285.71
1063	2-Heptanone	C7H14O	424.21	362.31	313.79
1064	5-Mth-2-Hexanone	C7H14O	417.93	356.76	309.00
1058	4-Heptanone	C7H14O	417.31	355.69	307.43
1057	3-Heptanone	C7H14O	420.21	359.77	312.32
1076	2,4-Pentanedione	C5H8O2	413.51	345.26	291.78
1068	DiisobutylKetone	C9H18O	441.10	376.93	327.03
1097	2-CycC6 CycC6one	C12H20O	537.49	460.44	403.62
1083	2-Octanone	C8H16O	446.29	382.06	330.88
1073	Dibutyl Ketone	C9H18O	461.60	395.21	343.23
1062	2-Hexanone	C6H12O	400.69	341.65	295.58
1077	Isophorone	C9H14O	488.38	413.78	354.29
1090	Acetophenone	C8H8O	475.42	406.57	351.80
1080	Cyclohexanone	C6H10O	428.57	363.99	313.44
1074	2-Nonanone	C9H18O	467.45	401.02	347.62

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Alcohol-Ethers

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
2862	2-Butoxyethanol	C6H14O2	444.19	383.50	335.51
4857	butyl carbitol	C8H18O3	504.29	435.18	382.31
2898	2-Chloroethanol	C2H5ClO	401.71	348.53	303.64
2864	Carbitol	C6H14O3	475.02	411.23	360.38
3854	Methyl propasol	C4H10O2	393.54	339.17	294.65
2860	2-Methoxyethanol	C3H8O2	397.67	342.77	299.38
2854	DiacetoneAlcohol	C6H12O2	441.03	380.30	330.11
2861	2-Ethoxyethanol	C4H10O2	408.44	352.05	307.67
2889	HydroxyAcetone	C3H6O2	418.75	361.61	314.86
3856	1tButoxy2Propnol	C7H16O2	417.20	364.53	321.71
3858	PROPGLYC2tBUTYL	C7H16O2	417.20	364.53	321.71
4855	2-Propoxyethanol	C5H12O2	424.60	364.89	319.77
4849	Acetovanillone	C9H10O3	570.86	500.62	443.05
5883	Ethyl Lactate	C5H10O3	427.67	367.35	315.95
6883	2-HydroxyEth Acr	C5H8O3	483.80	423.93	373.86
2863	Methyl Carbitol	C5H12O3	466.53	404.52	354.05
3855	Dowanol DPM	C7H16O3	461.12	398.21	346.15
3857	TriPropGlymEthlE	C10H22O4	515.74	454.53	402.26

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
404	DiMth-Acetylene	C4H6	300.15	254.51	218.57
202	Propylene	C3H6	225.50	189.09	160.92
412	2-Pentyne	C5H8	329.28	278.48	239.75
207	2-Methylpropene	C4H8	266.07	223.62	191.07
204	1-Butene	C4H8	266.87	224.25	191.36
205	Cis-2-Butene	C4H8	276.78	233.25	199.55
402	Propyne	C3H4	249.92	212.16	182.28
406	3-Hexyne	C6H10	354.57	300.24	257.22
206	Trans-2-Butene	C4H8	273.98	230.43	196.76
407	2-Hexyne	C6H10	357.65	302.95	260.85
231	33-2Mth-1-Butene	C6H12	314.39	264.29	226.17
230	23-2Mth-1-Butene	C6H12	328.79	277.16	237.27
229	2-Ethyl-1-Butene	C6H12	337.67	285.68	244.96
8	I-Pentane	C5H12	301.00	253.00	215.97
14	2,2-DiMth-Butane	C6H14	322.82	271.16	231.91
232	23-2Mth-2-Butene	C6H12	346.36	293.26	251.87
213	3-Mth-1-Butene	C5H10	293.18	246.27	210.24
212	2-Mth-1-Butene	C5H10	304.30	256.68	219.73
211	Trans-2-Pentene	C5H10	309.49	261.17	223.75
210	Cis-2-Pentene	C5H10	310.07	261.77	224.35
223	4-Mth-1-Pentene	C6H12	326.96	275.33	235.59
221	2-Mth-1-Pentene	C6H12	335.25	283.18	243.01
248	2-t-Butylpropene	C7H14	350.88	295.71	253.18
227	Cs-4-Mth-2-C5H10	C6H12	329.52	278.05	238.40
224	2-Mth-2-Pentene	C6H12	340.46	288.09	247.41
403	1-Butyne	C4H6	281.21	238.59	205.24
15	2,3-DiMth-Butane	C6H14	331.08	278.59	238.17
214	2-Mth-2-Butene	C5H10	311.65	262.87	225.19
228	Ts-4-Mth-2-C5H10	C6H12	331.81	280.20	240.34
225	Cs-3-Mth-2-C5H10	C6H12	340.82	288.10	247.05
218	Trans-2-Hexene	C6H12	341.03	288.41	247.69
2226	3-METH-Tr-2Pente	C6H12	343.59	290.81	249.82
222	3-Mth-1-Pentene	C6H12	327.39	275.39	235.50
257	2-Diisobutylene	C8H16	378.04	320.10	275.29
256	1-Diisobutylene	C8H16	374.68	315.87	270.82
217	Cis-2-Hexene	C6H12	342.02	289.16	247.71
2414	1-Heptyne	C7H12	373.08	316.81	272.54
13	3-Methylpentane	C6H14	336.34	283.80	243.05
219	Cis-3-Hexene	C6H12	339.61	287.03	246.25
12	2-Methylpentane	C6H14	333.36	281.29	240.73
220	Trans-3-Hexene	C6H12	340.24	287.84	247.11
405	1-Pentyne	C5H8	313.37	265.05	227.44
209	1-Pentene	C5H10	303.09	255.25	218.25
11	N-Hexane	C6H14	341.88	288.89	248.34

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

235	Cis-2-Heptene	C7H14	371.56	314.05	269.28
249	Cis-3-Heptene	C7H14	368.93	311.91	267.95
216	1-Hexene	C6H12	336.50	284.39	243.51
239	3-Eth-1-Pentene	C7H14	357.24	302.63	260.05
226	4-Mth-1-Hexene	C7H14	359.89	304.85	261.81
240	3-Mth-1-Hexene	C7H14	357.06	302.34	260.09
419	3-Mth-1-Butyne	C5H8	302.18	255.33	219.39
233	2-Eth-1-Pentene	C7H14	367.08	310.28	266.78
238	2-Mth-1-Hexene	C7H14	365.11	308.97	265.26
416	1-Octyne	C8H14	399.30	340.05	293.38
289	2,3Dimeth Hexene	C8H16	383.56	325.38	280.00
234	1-Heptene	C7H14	366.85	310.57	267.01
413	1-Hexyne	C6H10	344.49	291.94	251.09
237	Trans-3-Heptene	C7H14	368.71	312.17	268.18
236	Trans-2-Heptene	C7H14	370.99	313.77	269.37
251	Trans-2-Octene	C8H16	398.08	336.92	289.33
279	Trans-4-Octene	C8H16	395.37	334.73	287.95
277	Trans-3-Octene	C8H16	396.47	335.60	288.38
2252	2Methl-1-Heptene	C8H16	392.35	332.19	285.05
250	1-Octene	C8H16	394.38	334.70	288.41
258	2-Ethyl-1-Hexene	C8H16	393.04	333.18	285.86
280	3-Octene	C8H16	395.97	335.15	287.76
278	4-Octene	C8H16	395.74	335.16	287.47
276	2-Octene	C8H16	398.82	337.45	289.65
259	1-Nonene	C9H18	419.95	357.31	308.60
262	1-Dodecene	C12H24	486.55	416.39	361.12
263	1-Tridecene	C13H26	505.84	433.70	377.49
264	1-Tetradecene	C14H28	524.31	450.15	392.39
265	1-Pentadecene	C15H30	541.65	465.65	406.44
266	1-Hexadecene	C16H32	558.11	480.53	419.92
267	1-Octadecene	C18H36	587.79	507.35	444.95
281	1-Heptadecene	C17H34	573.24	493.80	432.46
284	1-Eicosene	C20H40	615.84	533.31	468.43
283	1-Nonadecene	C19H38	601.98	520.28	457.15
3	Propane	C3H8	231.08	193.57	164.63
4	I-Butane	C4H10	261.24	219.09	186.96
9	Neopentane	C5H12	282.61	236.43	200.63
5	N-Butane	C4H10	272.62	228.98	195.27
7	pentane	C5H12	309.20	260.56	223.03
44	Hexamethylethane	C8H18	379.39	319.77	273.70
25	223-TriMthButane	C7H16	354.00	297.61	254.31
24	3,3-DiMthPentane	C7H16	359.21	302.43	258.55
51	2,2,3,3-4Mth-C5	C9H20	413.43	348.87	299.05
21	2,2-DiMthPentane	C7H16	352.36	296.99	254.45
42	2,3,3-TriMth-C5	C8H18	387.88	326.97	279.99
22	2,3-DiMthPentane	C7H16	362.92	306.43	262.63

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

40	2,2,3-TriMth-C5	C8H18	382.95	323.06	276.95
23	2,4-DiMthPentane	C7H16	353.59	298.51	256.03
41	2,2,4-TriMth-C5	C8H18	372.25	313.80	268.80
39	3-Mth-3-Eth-C5	C8H18	391.42	330.25	283.04
20	3-Ethylpentane	C7H16	366.51	309.95	266.26
52	2,2,3,4-4Mth-C5	C9H20	406.18	342.79	293.87
54	2334TetrMethPent	C9H20	414.70	350.11	300.27
53	2,2,4,4-4Mth-C5	C9H20	395.42	333.31	285.49
43	2,3,4-TriMth-C5	C8H18	386.61	326.55	280.06
36	3,3-DiMth-Hexane	C8H18	385.11	325.29	279.21
19	3-Methylhexane	C7H16	364.83	308.79	265.02
18	2-Methylhexane	C7H16	363.03	307.28	263.83
38	2-Mth-3-Eth-C5	C8H18	388.79	328.87	282.58
190	2,2-2C1-3-C2-C5	C9H20	406.93	344.57	296.00
32	2,2-DiMth-Hexane	C8H18	379.94	321.37	276.20
37	3,4-DiMth-Hexane	C8H18	390.85	330.82	284.41
50	3,3-DiEthPentane	C9H20	419.32	354.22	303.80
34	2,4-DiMth-Hexane	C8H18	382.57	323.73	278.37
33	2,3-DiMth-Hexane	C8H18	388.67	329.08	282.99
17	N-Heptane	C7H16	371.55	315.02	271.06
49	244TriMethHexane	C9H20	403.80	341.22	292.86
192	2,4-2C1-3-C2-C5	C9H20	409.78	346.93	298.12
47	2,2,5-TriMth-C6	C9H20	397.41	336.19	289.13
35	2,5-DiMth-Hexane	C8H18	382.30	323.68	278.43
31	3-Ethylhexane	C8H18	391.63	332.03	285.89
30	4-Methylheptane	C8H18	390.83	331.51	285.57
29	3-Methylheptane	C8H18	392.15	332.52	286.30
28	2-Methylheptane	C8H18	390.75	331.49	285.39
96	2,2-DiMthHeptane	C9H20	405.90	343.78	295.78
176	2,6-DiMthHeptane	C9H20	408.38	347.13	299.38
27	N-Octane	C8H18	398.84	338.92	292.27
94	3-Ethylheptane	C9H20	416.03	353.58	304.88
92	3-Methyloctane	C9H20	417.31	354.68	306.17
93	4-Methyloctane	C9H20	415.59	353.13	304.69
91	2-Methyloctane	C9H20	416.42	354.18	305.92
72	2,2-DiMthOctane	C10H22	430.06	365.84	315.52
2095	2,3Dimethloctane	C10H22	437.45	371.84	320.99
2096	2,4Dimethloctane	C10H22	428.90	365.35	315.74
2098	2,6DimethlOctane	C10H22	433.54	369.12	318.59
2097	2,5Dimethloctane	C10H22	431.66	367.15	317.12
2099	2,7DimethlOctane	C10H22	433.14	368.54	318.17
46	N-Nonane	C9H20	423.81	361.00	312.10
88	5-Methylnonane	C10H22	438.23	373.06	322.98
85	3-Methylnonane	C10H22	440.95	375.78	324.98
87	4-Methylnonane	C10H22	438.83	373.85	322.90
86	2-Methylnonane	C10H22	440.18	375.21	325.16

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

56	N-Decane	C10H22	447.46	381.94	330.79
63	N-Undecane	C11H24	469.09	401.10	348.20
64	N-Dodecane	C12H26	489.52	419.29	364.50
65	N-Tridecane	C13H28	508.44	436.51	380.17
66	N-Tetradecane	C14H30	526.62	452.74	394.83
67	N-Pentadecane	C15H32	543.65	468.26	408.82
68	N-Hexadecane	C16H34	559.92	482.69	422.01
69	N-Heptadecane	C17H36	575.66	497.23	435.27
70	N-Octadecane	C18H38	589.43	509.94	447.03
71	N-Nonadecane	C19H40	603.26	522.39	458.50
73	N-Eicosane	C20H42	617.25	535.05	469.89
74	n-HENEICOSANE	C21H44	629.84	546.28	480.61
75	n-DOCOSANE	C22H46	641.73	556.54	489.95
76	n-TRICOSANE	C23H48	652.87	568.31	500.91
77	n-Tetracosane	C24H50	663.97	578.78	510.38
78	n-PENTACOSANE	C25H52	674.74	588.08	519.40
79	n-HEXACOSANE	C26H54	684.93	598.14	528.82
81	n-Octacosane	C28H58	704.27	616.17	545.10
2081	n-TRICONTANE	C30H62	722.86	632.56	559.61
2082	n-Dotriacontane	C32H66	738.48	647.61	573.88
2086	Hexatriacontane	C36H74	770.21	676.92	599.72

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Cyclic Hydrocarbons

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
269	Cyclopentene	C5H8	317.53	267.77	229.02
270	Cyclohexene	C6H10	356.03	300.63	257.95
287	3MthCyclopentene	C6H10	337.94	285.84	245.01
286	1-MthCyclPentene	C6H10	348.47	294.84	252.78
288	4MthCyclopenten	C6H10	339.10	286.83	245.85
273	Cycloheptene	C7H12	387.85	328.32	281.29
274	Cyclooctene	C8H14	416.40	353.17	303.04
101	Cyclopropane	C3H6	240.35	201.80	171.64
810	ADAMANTANE	C10H16	460.93	385.36	327.25
102	Cyclobutane	C4H8	285.68	240.23	204.89
104	Cyclopentane	C5H10	322.42	271.76	232.32
137	Cyclohexane	C6H12	353.93	298.64	255.45
105	MthCyclopentane	C6H12	344.96	290.95	248.56
146	Cs-1,4-2C1-CycC6	C8H16	397.46	335.43	287.60
142	Cs-1,2-2C1-CycC6	C8H16	402.88	339.97	291.48
141	1,1-2C1-CycC6	C8H16	392.70	330.78	283.21

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

145	Ts-1,3-2C1-CycC6	C8H16	397.61	335.69	287.95
144	Cs-1,3-2C1-CycC6	C8H16	393.25	331.69	284.28
147	Ts-1,4-2C1-CycC6	C8H16	392.52	330.74	283.18
143	Ts-1,2-2C1-CycC6	C8H16	396.59	334.17	286.09
138	MthCyclohexane	C7H14	373.88	315.21	270.30
159	Cycloheptane	C7H14	391.98	331.11	284.06
140	Ethylcyclohexane	C8H16	404.93	342.20	293.70
154	Trans-Decalin	C10H18	460.04	388.84	334.07
149	N-PropylCyc-C6	C9H18	429.85	364.15	313.28
109	Cs-1,2-2C1-CycC5	C7H14	372.68	314.61	269.85
110	Ts-1,2-2C1-CycC5	C7H14	365.01	308.01	264.11
112	Ts-1,3-2C1-CycC5	C7H14	364.93	307.86	263.95
107	Eth-Cyclopentane	C7H14	376.50	318.12	273.05
114	N-PropCycPentane	C8H16	404.08	342.29	294.43
108	1,1-DiMthCycC5	C7H14	361.02	304.23	260.75
111	Cs-1,3-2C1-CycC5	C7H14	364.24	307.38	262.91
152	N-ButylCycHexane	C10H20	454.10	385.66	332.55
160	Cyclooctane	C8H16	424.27	358.85	308.23
153	Cis-Decalin	C10H18	468.93	396.56	341.17
115	ISOPROPYLCYCLOPENTANE	C8H16	399.49	337.66	289.53
150	Isopropyl-CycC6	C9H18	427.65	361.87	311.01
116	1-C1-1-C2-CycC5	C8H16	394.61	333.30	285.87
122	Butylcyclpentane	C9H18	429.51	364.90	314.71
155	1,1-Bicyclohexyl	C12H22	511.56	433.90	373.50
158	N-Decylcyclo-C6	C16H32	571.08	490.29	427.25

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Aromatic Hydrocarbons

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
307	1,4-Pentadiene	C5H8	299.09	252.24	215.98
306	1-ts3-Pentadiene	C5H8	315.17	266.10	227.99
414	2-Methyl-1-Butenyne	C5H6	305.22	255.92	218.11
305	Cs1,3-Pentadiene	C5H8	317.21	268.17	230.07
309	Isoprene	C5H8	307.20	258.97	221.57
421	1-Pentene-4-yne	C5H6	315.41	264.75	226.03
303	1,3-Butadiene	C4H6	268.58	226.00	193.20
332	1,4-CyclHexadien	C6H8	360.38	307.14	264.53
501	Benzene	C6H6	353.28	299.31	257.37
315	Cyclopentadiene	C5H6	314.57	262.42	220.89
319	Diisopropenyl	C6H10	341.97	288.91	247.78
615	Ethynylbezene	C8H6	416.06	352.25	302.03

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

601	Styrene	C8H8	418.60	355.37	306.53
331	1,3-CycHexadiene	C6H8	353.44	298.76	256.28
310	1,5-Hexadiene	C6H10	332.47	279.93	239.09
312	MthCycPentadiene	C6H8	346.20	293.50	252.01
420	1-Pentene-3-yne	C5H6	332.42	279.47	239.21
502	Toluene	C7H8	383.83	325.14	279.27
521	T-Butylbenzene	C10H14	442.41	375.53	323.89
320	Dipropylene	C6H10	356.93	302.21	259.43
520	Sec-Butylbenzene	C10H14	446.69	378.89	327.39
313	1,4-Hexadiene	C6H10	338.39	285.65	244.84
314	Dipropylene	C6H10	355.38	300.95	259.05
316	DiCycPentadiene	C10H12	443.07	374.81	321.05
333	1,5-CycOctadiene	C8H12	423.12	359.83	310.30
701	Naphthalene	C10H8	491.01	417.39	359.56
504	Ethylbenzene	C8H10	409.32	347.23	298.89
820	Indan	C9H10	451.00	382.94	329.92
505	O-Xylene	C8H10	417.44	354.41	305.24
612	P-Methylstyrene	C9H10	445.82	379.07	326.95
330	DIISOCROTYL	C8H14	408.37	348.14	301.42
507	P-Xylene	C8H10	411.52	349.11	300.44
329	DIISOBUTENYL	C8H14	387.79	328.61	282.34
506	M-Xylene	C8H10	412.25	349.95	301.20
603	Methylstyrene	C9H10	444.50	378.53	326.57
613	Alpha-MthStyrene	C9H10	439.01	373.20	321.20
510	Isopropylbenzene	C9H12	425.57	361.30	311.54
724	2-Methylindene	C10H10	479.06	408.26	352.77
285	Vinylcyclohexene	C8H12	400.94	338.10	290.11
803	Indene	C9H8	455.93	386.69	334.10
706	Tetralin	C10H12	480.79	408.84	352.72
511	O-Ethyltoluene	C9H12	438.34	372.75	321.48
723	1-Methylindene	C10H10	471.90	401.64	346.33
738	Fluorene	C13H10	570.38	487.14	421.59
619	Tr-1PropenylBz	C9H10	451.46	384.44	331.71
525	O-Diethylbenzene	C10H14	456.56	388.81	335.88
618	Propenyl Bz(cis)	C9H10	452.23	384.10	330.09
602	O-Methylstyrene	C9H10	443.05	377.75	326.46
702	1-MthNaphthalene	C11H10	517.48	441.21	380.51
509	N-Propylbenzene	C9H12	432.35	367.19	316.32
526	M-Diethylbenzene	C10H14	454.51	386.80	333.89
583	Cs-2-PhnButene-2	C10H12	467.95	398.35	343.86
543	M-DiisopropylBz	C12H18	476.40	406.53	351.61
584	Ts-2-PhnButene-2	C10H12	447.24	380.86	328.86
580	1,2-DiC1-3C2-Bz	C10H14	467.10	398.21	344.20
704	1-EthNaphthalene	C12H12	531.31	453.89	393.30
512	M-Ethyltoluene	C9H12	434.32	369.52	318.14
522	1-Mth-2-iC3-Benz	C10H14	451.37	383.79	329.95

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

513	P-Ethyltoluene	C9H12	435.26	369.56	318.67
514	1,2,3-Mesitylene	C9H12	449.30	382.35	329.43
614	M-Divinylbenzene	C10H10	473.00	402.61	346.87
524	1-Mth-4-iC3-Benz	C10H14	449.96	382.38	329.99
822	Gamma-Terpinene	C10H16	456.51	388.96	335.91
821	Alpha-Terpinene	C10H16	447.77	380.68	328.27
523	1-Mth-3-iC3-Benz	C10H14	448.22	381.11	328.27
703	2-MthNaphthalene	C11H10	514.66	437.62	378.51
557	CycHexylBenzene	C12H16	512.97	439.28	381.43
515	1,2,4-Mesitylene	C9H12	442.67	376.54	324.52
519	Isobutylbenzene	C10H14	445.94	379.17	326.31
424	DiPhnAcetylene	C14H10	573.69	488.79	422.04
544	P-DiisopropylBz	C12H18	482.94	412.82	357.90
518	N-Butylbenzene	C10H14	456.54	388.52	335.43
516	1,3,5-Mesitylene	C9H12	437.83	372.82	321.62
809	Acenaphthalene	C12H8	543.30	465.26	403.62
725	123-TriMthIndene	C12H14	508.72	434.07	373.83
527	1,4-DiEthBenzene	C10H14	456.82	388.84	335.91
558	Diphenyl	C12H10	528.05	451.73	391.70
576	2-Ethyl-m-Xylene	C10H14	463.21	394.69	341.15
620	p-ISOPROPENYLSTY	C11H12	514.97	431.76	371.15
585	o-PropylToluene	C10H14	458.04	389.45	336.04
577	2-Ethyl-p-Xylene	C10H14	460.15	392.45	338.55
579	4-Ethyl-o-Xylene	C10H14	462.88	394.51	340.96
586	m-Propyltoluene	C10H14	454.96	387.41	334.58
587	p-Propyltoluene	C10H14	456.40	388.44	335.31
578	4-Ethyl-m-Xylene	C10H14	461.76	393.62	339.53
575	5-Ethyl-m-Xylene	C10H14	456.93	388.94	335.89
530	Prehnitene	C10H14	478.16	407.87	353.25
709	2,6-2Mth-Naphtha	C12H12	535.48	457.48	395.11
715	2,7-2Mth-Naphtha	C12H12	536.54	458.72	395.95
719	2-ETHYLNAPHTHALENE	C12H12	531.48	452.27	390.50
621	p-tert-BUTYLSTY	C12H16	499.72	424.06	365.80
532	1,2,4,5-TetMthBz	C10H14	469.86	400.91	346.46
531	1,2,3,5-TetMthBz	C10H14	471.18	402.13	347.81
533	p-tert-BUTYL ET	C12H18	485.00	413.40	357.28
567	N-Pentylbenzene	C11H16	478.66	407.79	353.11
718	1-n-PROPYLNAPHTH	C13H14	546.09	465.27	402.66
562	1,1-DiPhnEthane	C14H14	546.18	467.40	405.22
616	4-ISOBUTYLSTYRE	C12H16	524.00	447.60	387.49
260	1-Decene	C10H20	443.66	378.41	327.50
735	Cis-Stilbene	C14H12	553.58	473.65	410.97
568	Hexylbenzene	C12H18	499.29	426.20	369.54
563	Diphenylmethane	C13H12	537.75	459.89	398.94
564	1,2-DiPhnEthane	C14H14	553.68	473.50	410.50
804	Anthracene	C14H10	614.71	523.17	450.81

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

736	Trans-Stilbene	C14H12	579.99	499.57	434.84
805	Phenanthrene	C14H10	610.01	521.00	450.75
713	1-ButNaphthalene	C14H16	562.27	482.11	419.04
807	Pyrene	C16H10	667.91	569.96	492.98
261	1-Undecene	C11H22	465.83	397.97	345.35
581	23-2C1-23-2PhnC4	C18H22	589.13	503.12	436.53
549	N-Heptylbenzene	C13H20	519.61	443.02	384.42
710	1-PhnNaphthalene	C16H12	607.55	522.46	454.92
566	2,4-Diphenyl-4-M	C18H20	613.49	524.76	455.66
561	O-Terphenyl	C18H14	609.32	524.11	457.80
569	N-Octylbenzene	C14H22	537.37	459.67	399.80
565	Triphenylmethane	C19H16	632.57	544.62	474.92
714	N-C6-Naphthalene	C16H20	594.97	512.14	446.57
717	Fluoranthene	C16H10	656.03	557.99	479.79
716	1-Hexyl-Tetralin	C16H24	578.42	497.00	432.91
731	TriPhnEthylene	C20H16	669.60	576.28	502.36
806	Chrysene	C18H12	714.66	616.55	538.48
588	1,1,2TriPhenEth	C20H18	621.93	535.78	467.65
711	1-n-NonylNaphtha	C19H26	639.53	548.90	477.61
570	N-Nonylbenzene	C15H24	555.56	475.61	414.49
712	1-Decyl Naphtha	C20H28	652.68	560.48	487.97
559	P-Terphenyl	C18H14	655.33	568.13	498.12
560	M-Terphenyl	C18H14	647.82	559.51	488.47
589	TetraPhenylMetha	C25H20	742.82	641.14	560.67
554	Decylbenzene	C16H26	571.14	490.53	427.99
732	TetraPhnEthylene	C26H20	760.52	657.41	575.47
574	N-Dodecylbenzene	C18H30	600.45	518.35	453.41
571	N-Undecylbenzene	C17H28	586.57	504.18	440.51
572	Tridecylbenzene	C19H32	614.57	531.04	465.16
573	n-TETRADECYLBENZ	C20H34	627.08	542.76	475.77
2575	n-PENTADECYLBENZ	C21H36	639.58	554.55	486.65
2576	n-HEXADECYLBENZ	C22H38	651.43	566.08	497.55
2577	n-HEPTADECYLBENZ	C23H40	662.34	575.01	505.44
2578	n-OCTADECYLBENZE	C24H42	673.10	584.71	514.41

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Halocarbons

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1544	Allyl Chloride	C3H5Cl	318.43	268.69	230.04
1595	2-Chloropropene	C3H5Cl	295.90	248.69	211.84
1531	3-Chloropropyne	C3H3Cl	331.00	278.90	238.12
1561	6Cl-1,3Butadiene	C4Cl6	486.25	414.57	359.07

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1535	T-Butyl Chloride	C4H9Cl	323.65	272.32	232.50
1583	Chloroprene	C4H5Cl	332.54	279.74	239.05
1530	Isopropyl Cl	C3H7Cl	308.80	261.02	223.39
1572	O-DiCl-Benzene	C6H4Cl2	453.52	385.53	332.30
1585	Propyl Chloride	C3H7Cl	319.70	270.54	232.30
1684	Isopropyl Iodide	C3H7I	363.03	305.78	261.48
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	401.38	341.83	296.01
1651	2-Bromopropane	C3H7Br	332.56	280.75	240.37
1691	Iodobenzene	C6H5I	461.67	391.65	336.87
1860	Fluorobenzene	C6H5F	358.34	303.81	260.78
1571	Chlorobenzene	C6H5Cl	405.11	343.54	295.04
1680	Bromobenzene	C6H5Br	429.02	363.86	313.07
1526	1,2-DiCl-Propane	C3H6Cl2	369.23	312.58	268.04
1683	Propyl Iodide	C3H7I	375.61	316.97	270.84
1576	Benzotrichloride	C7H5Cl3	487.02	411.46	352.48
1536	2,3-DICHLOROBUT	C4H8Cl2	392.36	332.18	285.62
2638	2-Bromobutane	C4H9Br	364.56	310.11	267.02
1586	1-Chlorobutane	C4H9Cl	351.58	297.85	256.09
1573	M-DiCl-Benzene	C6H4Cl2	446.11	378.68	325.36
2634	Benzotrifluoride	C7H5F3	375.23	318.74	275.34
1574	P-DiCl-Benzene	C6H4Cl2	447.27	380.19	327.75
1650	1-Bromopropane	C3H7Br	344.14	290.99	249.79
1587	2-Chlorobutane	C4H9Cl	341.23	287.99	246.28
2653	8F-2-Butene	C4F8	270.19	227.50	194.52
1678	M-Dibromobenzene	C6H4Br2	491.12	416.66	358.70
1537	1,2-DiCl-Butane	C4H8Cl2	392.36	332.18	285.62
1597	34-DiCl-1-Butene	C4H6Cl2	388.32	332.17	288.48
1577	O-Chlorotoluene	C7H7Cl	432.14	367.18	316.22
1532	123-3Cl-Propane	C3H5Cl3	430.26	366.16	315.56
1578	P-Chlorotoluene	C7H7Cl	435.49	370.26	319.63
1562	Benzyl Chloride	C7H7Cl	453.46	386.56	333.29
2661	P-Bromotoluene	C7H7Br	457.71	389.31	334.05
1508	1,4-DiCl-Butane	C4H8Cl2	427.94	364.73	314.74
1655	1-Bromobutane	C4H9Br	375.16	317.00	272.43
1599	BenzylDichloride	C7H6Cl2	486.78	411.81	352.23
2652	Perfluoropropane	C3F8	236.56	199.50	170.19
1505	2-Butylene DiCl	C4H6Cl2	429.63	366.27	316.21
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	425.81	363.02	313.40
1588	1-Chloropentane	C5H11Cl	381.58	322.49	276.56
2654	OctaF-CycButane	C4F8	267.20	226.94	195.29
1592	1,2,4-TriCl-Bz	C6H3Cl3	486.17	413.48	354.75
1579	2,4-2Cl-Toluene	C7H6Cl2	474.48	404.89	349.76
2593	1,3,5-TriCl-BZ	C6H3Cl3	481.59	409.50	351.31
1697	1-Br-Naphthalene	C10H7Br	554.42	473.99	410.23
1622	Perfluorobutane	C4F10	271.08	229.72	197.51
1857	P-Cl-Benzo-TriF	C7H4ClF3	411.96	350.93	302.91

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

1509	1,5-DiCl-Pentane	C5H10Cl2	456.16	389.59	336.79
1589	1-Cl-Naphthalene	C10H7Cl	533.05	453.30	392.33
1582	6ClCycPentadiene	C5Cl6	512.63	436.59	376.69
1864	Perfluorobenzene	C6F6	353.38	301.66	260.80
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	451.42	386.08	334.45
1667	1-Bromoheptane	C7H15Br	452.05	385.16	332.64
1575	HexaCl-Benzene	C6Cl6	582.34	509.39	452.57
2640	Freon 123B1	C2HBrClF3	323.44	273.78	235.77
1504	Vinyl Chloride	C2H3Cl	259.13	219.55	189.18
1672	1,1-DiBr-Ethane	C2H4Br2	381.16	325.95	282.00
1580	Acetylene DiCl	C2H2Cl2	333.35	282.49	242.93
1692	Diiodomethane	CH2I2	455.37	386.43	333.47
1698	Bromoform	CHBr3	422.33	358.67	308.64
2687	Freon 13B1	CBrF3	215.32	180.48	153.32
2690	Br-3F-Ethylene	C2BrF3	270.85	228.02	194.55
1649	Tetrabromoethane	C2H2Br4	516.92	442.90	384.30
2686	Freon 12B1	CBrClF2	269.14	226.21	193.04
1503	Ethyl Chloride	C2H5Cl	285.44	241.15	206.50
2641	Br-TriCl-Methane	CBrCl3	378.15	319.15	272.68
1641	Methyl Bromide	CH3Br	276.72	233.70	200.11
2688	Freon 12B2	CBr2F2	296.18	248.47	212.47
1696	DiCl-F-Methane	CHCl2F	281.89	239.02	205.66
2545	2,3-DiCl-Propene	C3H4Cl2	366.49	312.47	270.93
1673	1,2-DiBr-Ethane	C2H4Br2	404.37	342.33	292.83
2637	Dibromomethane	CH2Br2	370.09	314.86	271.56
1542	TetraCl-Ethylene	C2Cl4	394.24	334.33	287.00
1541	TriCl-Ethylene	C2HCl3	359.99	304.87	261.10
1527	111-TriCl-Ethane	C2H3Cl3	347.26	293.23	251.49
1612	Cl-2F-Ethylene	C2HClF2	254.57	215.44	184.45
1617	Ethyl Fluoride	C2H5F	235.54	198.64	169.64
2639	Br-Cl-Methane	CH2BrCl	341.19	290.15	249.51
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	320.78	271.29	233.54
1682	Ethyl Iodide	C2H5I	345.23	291.43	248.95
1522	1,1-DiCl-Ethane	C2H4Cl2	330.17	280.16	240.70
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	264.01	222.93	191.05
1525	Hexachloroethane	C2Cl6	457.62	389.45	337.32
1528	1112-4Cl-Ethane	C2H2Cl4	403.33	342.23	294.93
1590	Penta-Cl-Ethane	C2HCl5	433.29	366.15	315.21
1529	1122-4Cl-Ethane	C2H2Cl4	418.43	356.92	307.83
2693	Perfluoroethane	C2F6	194.95	163.40	138.48
1611	Freon 114B2	C2Br2F4	320.35	270.54	232.30
2692	Cl-PentaF-Ethane	C2ClF5	234.00	197.07	168.35
2655	122-3Cl-112-3FC2	C2Cl3F3	320.71	271.00	232.16
1609	12-2Cl-1122-4FC2	C2Cl2F4	276.76	233.36	199.59
2526	1,1-DiCl-Propane	C3H6Cl2	361.23	306.37	263.62
1645	Ethyl Bromide	C2H5Br	311.27	263.14	225.88

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

2658	1112-4Cl-22-2FC2	C2Cl4F2	364.78	309.47	266.68
1619	111-3F-Ethane	C2H3F3	225.88	190.70	163.33
1524	1,1,2-3Cl-Ethane	C2H3Cl3	387.32	329.17	283.16
1640	1,1-DiF-Ethane	C2H4F2	249.12	211.32	181.65
2691	Genetron 1113	C2ClF3	244.78	206.89	177.33
1591	Vinylidene DiCl	C2H2Cl2	304.76	257.75	221.79
1614	Difluoromethane	CH2F2	221.46	188.38	162.17
2694	Vinyl Bromide	C2H3Br	288.96	242.73	206.43
1694	Refrigerant 123	C2HCl2F3	300.96	255.09	219.45
1523	1,2-DiCl-Ethane	C2H4Cl2	356.82	303.00	261.00
2656	1122-4Cl-12-2FC2	C2Cl4F2	365.82	309.52	265.99
2527	1,3-DiCl-Propane	C3H6Cl2	393.34	333.77	287.64

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

Acids

Dip ID	**Name**	**Formula**	$T_{b,760\,mmHg}^{Exp}$	$T_{b,100\,mmHg}^{Exp}$	$T_{b,10\,mmHg}^{Exp}$
1277	Acrylic Acid	C3H4O2	414.34	312.16	358.60
1274	Ts-Crotonic Acid	C4H6O2	458.44	353.03	400.12
1279	Oleic Acid	C18H34O2	633.19	496.34	558.23
1278	Methacrylic Acid	C4H6O2	434.38	332.13	377.64
2271	Cinnamic Acid	C9H8O2	573.54	448.71	503.60
1266	n-UNDECANOIC ACI	C11H22O2	557.13	432.16	487.14
1282	O-Toluic Acid	C8H8O2	532.64	408.93	464.40
2283	IBUPROFEN	C13H18O2	580.85	451.32	510.95
1261	Isovaleric Acid	C5H10O2	449.44	345.66	392.30
1264	1,4-CychexDicarboxAcid	C8H12O4	669.49	529.24	592.86
1283	P-Toluic Acid	C8H8O2	548.59	421.12	478.32
1257	3-MthButyricAcid	C5H10O2	450.52	343.36	391.32
1288	Isophthalic Acid	C8H6O4	753.30	598.42	668.90
2282	PyromelliticAcid	C10H6O8	722.37	595.05	654.11
2871	4CarboxAcidBzldhyde	C8H6O3	702.50	547.17	617.25
1256	N-Butyric Acid	C4H8O2	436.74	335.59	381.00
1276	Stearic Acid	C18H36O2	647.86	501.64	564.88
1285	Adipic Acid	C6H10O4	610.62	479.08	538.65
1273	Cs-Crotonic Acid	C4H6O2	445.37	340.39	387.49
4851	Diglycolic Acid	C4H6O5	610.36	486.41	542.98
1286	Maleic Acid	C4H4O4	565.31	449.09	502.10
2277	Citraconic Acid	C5H6O4	607.36	478.37	536.92
2278	Itaconic Acid	C5H6O4	601.34	473.57	531.55

Table C.2 Experimental Boiling Temperatures at 760, 100, and 10 mmHg (Continued)

2281	Glutaric Acid	C5H8O4	595.28	470.76	527.21
1271	TetradecylicAcid	C14H28O2	598.99	464.89	523.16
1259	N-Nonanoic Acid	C9H18O2	529.06	409.76	462.65
1280	Linoleic Acid	C18H32O2	628.39	492.07	553.40
1260	Isobutyric Acid	C4H8O2	427.38	327.44	371.79
2268	Fumaric Acid	C4H4O4	563.34	447.87	500.19
1287	Phthalic Acid	C8H6O4	598.27	475.06	531.15
1289	TerephthalicAcid	C8H6O4	832.54	661.66	739.06
2280	Succinic Acid	C4H6O4	591.25	469.03	524.71
1270	Tridecanoic Acid	C13H26O2	585.29	454.76	511.42
1254	N-Decanoic Acid	C10H20O2	542.94	423.22	476.78
2270	Suberic Acid	C8H14O4	625.21	492.65	553.43
2255	Linolenic Acid	C18H30O2	632.17	495.25	556.80
1262	N-Hexanoic Acid	C6H12O2	478.69	371.49	419.51
4852	Levulinic Acid	C5H8O3	530.13	410.13	464.06
2275	Sebacic Acid	C10H18O4	641.91	505.77	567.53
1255	Oxalic Acid	C2H2O4	569.16	452.77	506.00
2259	PentadecylicAcid	C15H30O2	611.86	474.03	533.59
2266	NonadecanoicAcid	C19H38O2	658.93	509.53	574.07
2269	Pimelic Acid	C7H12O4	615.33	487.35	545.39
1252	Acetic Acid	C2H4O2	391.16	290.53	335.62
3268	Malonic Acid	C3H4O4	579.89	459.96	514.68
2279	2-EthButyricAcid	C6H12O2	467.04	356.61	406.00
1265	N-Octanoic Acid	C8H16O2	512.76	398.66	449.34
2258	NeopentanoicAcid	C5H10O2	436.88	339.35	382.13
2257	Azelaic Acid	C9H16O4	633.70	498.88	559.59
1281	Benzoic Acid	C7H6O2	522.08	405.36	458.20
1269	Dodecanoic Acid	C12H24O2	571.79	444.90	500.18
2261	Heptanoic Acid	C7H14O2	496.08	384.73	434.49
1258	N-Valeric Acid	C5H10O2	458.91	353.76	400.90
2265	HeptadecylicAcid	C17H34O2	635.47	492.74	554.91
2267	N-Eicosanic Acid	C20H40O2	670.05	518.25	583.86
1253	Propionic Acid	C3H6O2	414.29	314.01	359.47
5877	Ascorbic Acid	C6H8O6	637.11	539.27	585.46
1272	HexadecanoicAcid	C16H32O2	623.95	483.23	544.17

Table C. 3 Boiling Temperatures Calculated by the GC-PC-SAFT method.

Alcohols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1181	Phenol	C6H6O	437.32	384.53	342.09
1182	O-Cresol	C7H8O	458.89	403.16	358.50
1183	M-Cresol	C7H8O	458.87	403.14	358.48
1176	2,6-Xylenol	C8H10O	479.24	420.85	374.13
1111	2-Mth-2-Butanol	C5H12O	394.87	343.26	301.98
1178	3,5-Xylenol	C8H10O	479.20	420.81	374.09
1133	2-Octanol	C8H18O	463.17	402.08	354.10
2885	4-HYDROXYSTYREN	C8H8O	489.24	428.82	380.56
1197	P-t-Butylphenol	C10H14O	506.32	445.60	396.82
1172	2,4-Xylenol	C8H10O	479.22	420.83	374.10
1184	P-Cresol	C7H8O	458.69	402.95	358.31
1151	Cyclohexanol	C6H12O	436.86	378.92	332.96
1170	2,3-Xylenol	C8H10O	474.98	417.10	370.79
1187	P-Ethyl Phenol	C8H10O	474.98	417.09	370.79
2859	P-Methoxyphenol	C7H8O2	480.38	425.21	380.41
1121	2-Ethylhexanol	C8H18O	463.15	402.06	354.09
1179	PropargylAlcohol	C3H4O	369.69	321.14	281.81
1123	3-Mth-1-Butanol	C5H12O	401.57	349.43	307.77
2196	P-t-Amylphenol	C11H16O	521.77	459.13	408.78
1174	2,5-Xylenol	C8H10O	479.20	420.80	374.08
1115	2-Hexanol	C6H14O	423.04	367.78	323.95
1152	1-MthCycHexanol	C7H14O	447.40	387.89	340.93
4854	Guaiacol	C7H8O2	480.42	425.25	380.46
1107	Sec-Butanol	C4H10O	379.17	330.22	290.74
1167	Allyl Alcohol	C3H6O	360.77	313.94	275.80
1130	4-Mth-2-Pentanol	C6H14O	420.79	364.76	320.36
1177	3,4-Xylenol	C8H10O	479.19	420.79	374.07
1114	1-Hexanol	C6H14O	425.82	371.14	327.72
1106	Isobutanol	C4H10O	379.13	330.19	290.72
1125	1-Heptanol	C7H16O	445.96	388.33	342.79
1105	N-Butanol	C4H10O	382.72	334.36	295.35
1109	1-Pentanol	C5H12O	404.76	353.19	311.94
1132	1-Octanol	C8H18O	465.25	404.83	357.25
1113	T-Butylcarbinol	C5H12O	394.81	343.21	301.94
1137	1-Undecanol	C11H24O	518.38	450.74	397.60
1108	Tert-Butanol	C4H10O	372.10	323.65	284.55
1103	N-Propanol	C3H8O	359.51	314.46	277.75
1134	1-Nonanol	C9H20O	483.73	420.69	371.17
2195	P-t-Octylphenol	C14H22O	559.44	491.33	436.65
1102	Ethanol	C2H6O	334.85	293.21	258.89
1124	3-Mth-2-Butanol	C5H12O	399.11	346.15	303.86
1136	1-Decanol	C10H22O	501.41	435.97	384.58
1140	Dodecanol	C12H26O	534.55	464.90	410.12
1104	Isopropanol	C3H8O	355.46	309.76	272.54
1110	2-Pentanol	C5H12O	401.65	349.50	307.82

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1120	3-Pentanol	C5H12O	401.63	349.48	307.80
1112	2-Mth-1-Butanol	C5H12O	401.58	349.44	307.77
1154	Ts-2-Mth-CycC6OH	C7H14O	447.37	387.86	340.91
1153	Cs-2-Mth-CycC6OH	C7H14O	447.37	387.87	340.91
1156	Ts-3-Mth-CycC6OH	C7H14O	447.34	387.84	340.89
1157	Cs-4-Mth-CycC6OH	C7H14O	447.35	387.85	340.90
2197	P-Cumylphenol	C15H16O	590.90	521.46	465.06
1180	Benzyl Alcohol	C7H8O	465.06	405.93	358.92
1158	Ts-4-Mth-CycC6OH	C7H14O	447.35	387.85	340.90
1155	Cs-3-Mth-CycC6OH	C7H14O	447.34	387.84	340.89
1168	2-Phn-2-Propanol	C9H12O	496.14	431.07	379.84
1141	1-Tridecanol	C13H28O	550.02	478.54	422.23
1147	2-Eth-1-Butanol	C6H14O	423.01	367.75	323.93
1117	2-Mth-1-Pentanol	C6H14O	423.00	367.74	323.92
2115	2-Phenylethanol	C8H10O	484.83	419.38	367.97
1142	1-Tetradecanol	C14H30O	564.83	491.69	433.96
2118	1-PHN-1-PROPANOL	C9H12O	501.32	435.92	384.38
2119	1-PHN-2-PROPANOL	C9H12O	501.31	435.92	384.38
1126	2-Heptanol	C7H16O	443.53	385.27	339.33
1143	1-Pentadecanol	C15H32O	578.98	504.34	445.28
1129	Isoheptanol	C7H16O	443.49	385.23	339.30
2117	2,6-DiMth-4-C7OH	C9H20O	479.75	414.12	362.99
1144	1-Hexadecanol	C16H34O	592.58	516.57	456.29
1145	Heptadecanol	C17H36O	605.60	528.35	466.95
1199	Nonylphenol	C15H24O	581.94	511.06	454.06
1146	1-Octadecanol	C18H38O	618.08	539.71	477.26
1135	2-Nonanol	C9H20O	481.97	418.19	368.23
1149	1-Nonadecanol	C19H40O	630.05	550.66	487.24
1139	Isodecanol	C10H22O	499.99	433.72	381.88
1148	1-Eicosanol	C20H42O	641.58	561.26	496.95
2198	Dinonylphenol	C24H42O	679.39	600.91	536.63
1159	Menthol	C10H20O	508.04	430.17	369.99

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Amines

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1742	Ethyleneimine	C2H5N	294.06	248.98	213.74
1745	Piperidine	C5H11N	395.90	335.40	288.37
1766	Pyrrolidine	C4H9N	364.77	308.77	265.22

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1719	Isopropylamine	C3H9N	306.73	259.04	222.17
1711	N-Propylamine	C3H9N	329.75	278.73	239.18
1726	Sec-Butylamine	C4H11N	339.28	286.95	246.47
1704	Ethylamine	C2H7N	295.28	249.32	213.65
1702	Dimethylamine	C2H7N	285.96	243.30	209.99
1710	Diethylamine	C4H11N	351.87	298.63	257.25
1740	Allylamine	C3H7N	327.13	274.03	233.08
1712	N-Butylamine	C4H11N	360.95	305.60	262.66
1794	HexMthyleneimine	C6H13N	424.72	360.21	310.04
1729	Cyclohexylamine	C6H13N	415.45	351.10	301.29
1714	Isobutylamine	C4H11N	354.17	298.04	254.80
2853	Acetamide	C2H5NO	497.39	421.96	362.44
2731	N-C1-CycC6-Amine	C7H15N	429.39	365.86	316.26
1743	Diisopropylamine	C6H15N	360.13	310.44	271.07
1796	N,N-DiMthAniline	C8H11N	503.02	434.43	379.77
1792	Aniline	C6H7N	457.50	393.46	342.61
1713	N-Pentylamine	C5H13N	389.41	330.30	284.40
1733	Benzylamine	C7H9N	462.90	396.17	343.63
1737	M-Toluidine	C7H9N	481.23	414.75	361.86
3796	N-Ethylaniline	C8H11N	475.12	407.90	354.81
1878	2-Methacrylamide	C4H7NO	564.52	476.66	407.92
1736	O-Toluidine	C7H9N	481.23	414.75	361.86
2739	Diallylamine	C6H11N	411.40	345.56	294.96
2706	Hexylamine	C6H15N	415.55	353.16	304.62
2724	O-Ethylaniline	C8H11N	498.26	430.15	375.90
1707	Dipropylamine	C6H15N	406.34	346.04	299.01
1738	P-Toluidine	C7H9N	481.23	414.75	361.86
1795	N-Methylaniline	C7H9N	448.09	385.27	335.51
1718	Diisobutylamine	C8H19N	447.28	378.93	326.06
1879	Acrylamide	C3H5NO	547.81	461.66	394.09
2707	1-Aminoheptane	C7H17N	439.69	374.41	323.52
2730	DiCycHexylAmine	C12H23N	507.05	438.52	384.02
2787	P-Aminodiphenyl	C12H11N	578.82	507.31	449.18
1744	Dibutylamine	C8H19N	452.98	387.16	335.63
2708	1-Octylamine	C8H19N	462.11	394.27	341.27
2791	2,6-DiEthAniline	C10H15N	533.18	462.02	405.13
2709	1-Nonylamine	C9H21N	483.01	412.88	357.99
2710	1-Decylamine	C10H23N	502.57	430.40	373.79
3722	Diamylamine	C10H23N	493.59	423.38	368.18
3724	Undecylamine	C11H25N	520.94	446.94	388.77
2712	Dodecylamine	C12H27N	538.25	462.60	403.00
1720	Tetradecylamine	C14H31N	570.08	491.58	429.50
2752	Piperazine	C4H10N2	421.82	357.20	307.06
1752	Propylenediamine	C3H10N2	378.57	318.64	272.55
1741	Ethylenediamine	C2H8N2	369.62	310.88	265.52

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

2725	O-Aminoaniline	C6H8N2	528.04	460.53	405.86
2750	P-Aminoaniline	C6H8N2	528.03	460.53	405.86
2727	M-Aminoaniline	C6H8N2	528.03	460.52	405.86
1750	AEP	C6H15N3	504.32	426.28	366.00
1732	Toluene Diamine	C7H10N2	546.88	477.57	421.39
1731	hexamethyleneDiamine	C6H16N2	480.66	407.47	350.76
3750	P-Benzidine	C12H12N2	624.94	552.42	492.72

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Silanes

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
3985	Dimethyl Silane	C2H8Si	248.95	209.01	178.31
3984	Methyl Silane	CH6Si	216.08	180.96	153.91
3986	Trimethyl Silane	C3H10Si	279.47	235.32	201.37
1984	TetraMth Silane	C4H12Si	307.34	259.53	222.72
2994	TETRAETHYL Si	C8H20Si	411.24	350.82	303.76
1965	HexMthDisiloxane	C6H18OSi2	377.78	324.14	282.07
1966	6C1Cyc3Siloxane	C6H18O3Si3	395.82	345.00	304.20
1988	8C1Cyc4Siloxane	C8H24O4Si4	437.87	384.67	341.41
3991	DecaMethcyclpenS	C10H30O5Si5	470.93	416.59	371.76
3992	DodecaMethCyHexS	C12H36O6Si6	497.74	443.11	397.22

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Imines

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1767	N-MthPyrrolidine	C5H11N	354.59	298.25	254.69
2797	3-Methylpyridine	C6H7N	413.73	350.67	301.51
1797	2-Methylpyridine	C6H7N	413.73	350.67	301.51
2799	4-Methylpyridine	C6H7N	413.73	350.67	301.51
1753	N,N-DiEthAniline	C10H15N	481.17	412.92	359.14
1754	N-Methylpyrrole	C5H7N	393.75	324.23	271.04
3740	Acridine	C13H9N	579.82	508.52	450.49

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Tert-N

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1703	Trimethylamine	C3H9N	296.97	246.47	207.78
2856	DiMth Acetamide	C4H9NO	412.22	345.34	293.72
1706	Triethylamine	C6H15N	363.73	308.09	264.96
2716	Tributylamine	C12H27N	497.02	426.53	371.15
2719	Tripropylamine	C9H21N	437.24	372.98	322.83
3723	Triamylamine	C15H33N	547.11	472.00	412.60

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Nitrate

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1761	Nitroethane	C2H5NO2	384.16	329.05	285.39
1763	2-Nitropropane	C3H7NO2	393.42	335.21	289.53
1762	1-Nitropropane	C3H7NO2	409.88	351.47	305.22
1779	P-Nitrotoluene	C7H7NO2	500.10	422.23	361.76
1886	Nitrobenzene	C6H5NO2	478.56	401.95	342.60
1778	O-Nitrotoluene	C7H7NO2	500.10	422.23	361.76
1780	M-Nitrotoluene	C7H7NO2	500.10	422.23	361.76
1891	O-Nitroanisole	C7H7NO3	504.42	435.22	380.07
2740	M-Dinitrobenzene	C6H4N2O4	602.20	506.40	432.06
2742	P-Dinitrobenzene	C6H4N2O4	602.20	506.40	432.06
2741	O-Dinitrobenzene	C6H4N2O4	602.20	506.40	432.06
2749	3,5-DiNitToluene	C7H6N2O4	611.21	516.50	442.86
2743	DNT	C7H6N2O4	611.21	516.50	442.86
2745	3,4-DiNitToluene	C7H6N2O4	611.21	516.50	442.86
2744	2,6-DiNitToluene	C7H6N2O4	611.21	516.50	442.86
2748	2,5-DiNitToluene	C7H6N2O4	611.21	516.50	442.86
2746	1,3,5-TrinitroBz	C6H3N3O6	724.12	609.53	520.48
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	791.71	688.82	606.25
2747	Trinitrotoluene	C7H5N3O6	720.54	609.33	522.77

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Thiols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1802	Ethyl Mercaptan	C2H6S	306.13	256.71	218.46
1820	Dimethyl Sulfide	C2H6S	309.69	262.08	224.87
1843	Thiacyclopentane	C4H8S	377.22	320.40	275.90
1803	1-Propanethiol	C3H8S	339.49	285.66	244.00
1805	Isobut Mercaptan	C4H10S	363.98	305.14	259.86
6860	Ethylenedithiol	C2H6S2	409.91	341.99	289.71
1811	Cyclohexanethiol	C6H12S	439.10	370.88	318.06
1828	DiMth Disulfide	C2H6S2	409.91	341.99	289.71
1841	Butanethiol	C4H10S	369.65	311.98	267.30
1814	Methylproylsulf	C4H10S	369.65	311.98	267.30
2816	ETHYLtBUTYL SUL	C6H14S	403.11	342.12	294.68
1818	Diethyl Sulfide	C4H10S	364.57	310.36	267.91
1812	Benzyl Mercaptan	C7H8S	469.68	401.39	347.71
1838	T-OctylMercaptan	C8H18S	459.12	388.71	334.24
1827	1-Pentanethiol	C5H12S	397.18	336.13	288.76
2815	METHnBUTYL SULFD	C5H12S	397.08	338.12	291.98
1824	DiethylDisulfide	C4H10S2	436.34	372.87	322.96
1807	N-Hexylmercaptan	C6H14S	422.50	358.46	308.68
6857	Dimercaptoethyl	C4H10OS2	513.90	428.77	363.48
1839	1-Heptanethiol	C7H16S	445.93	379.23	327.27
1829	DiProp Disulfide	C6H14S2	479.64	411.26	357.36
1809	1-Octanethiol	C8H18S	467.72	398.64	344.73
1808	N-Nonanethiol	C9H20S	488.07	416.87	361.17
1826	1-Decanethiol	C10H22S	507.15	434.04	376.72
2838	tertDodecanThiol	C12H26S	537.25	459.18	398.16
1825	1-Undecanethiol	C11H24S	525.10	450.26	391.47
1837	Dodecylthiol	C12H26S	542.03	465.63	405.49

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Aldehydes

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1037	Methacrolein	C4H6O	339.40	285.78	244.35
1002	Acetaldehyde	C2H4O	276.94	234.88	202.06
1003	Propionaldehyde	C3H6O	312.06	264.69	227.82
1041	Benzaldehyde	C7H6O	447.48	383.76	333.40
1034	Acrolein	C3H4O	306.77	258.09	220.38

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1005	N-Butyraldehyde	C4H8O	343.97	292.05	251.62
1036	Trans-2-Butenal	C4H6O	344.57	290.02	247.86
1007	Valeraldehyde	C5H10O	373.11	317.24	273.70
1006	Isobutyraldehyde	C4H8O	335.92	283.58	243.11
1009	1-Hexanal	C6H12O	399.89	340.57	294.27
1040	P-Tolualdehyde	C8H8O	471.87	405.64	353.19
1016	2-Methylhexanal	C7H14O	420.61	357.20	307.94
1017	3-Methylhexanal	C7H14O	420.61	357.20	307.94
1008	1-Heptanal	C7H14O	424.62	362.26	313.50
1013	2-Ethylhexanal	C8H16O	444.48	378.25	326.68
1010	1-Octanal	C8H16O	447.57	382.51	331.55
1011	1-Nonanal	C9H18O	468.97	401.50	348.56
1020	1-Decanal	C10H20O	488.99	419.37	364.63
1021	1-Undecanal	C11H22O	507.78	436.22	379.85
1025	Dodecanal	C12H24O	525.48	452.18	394.32
1026	1-Tridecanal	C13H26O	542.19	467.31	408.09
1014	1,2-Ethanedione	C2H2O2	329.28	279.34	240.42
1044	1,4BenzDicarboxAldehy	C8H6O2	513.19	445.74	391.53

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Epoxides

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1440	ISOBUTYLENE OXID	C4H8O	301.01	249.70	210.28
1479	Tetrahydrofuran	C4H8O	327.93	274.67	233.45
1477	2,5-Dihydrofuran	C4H6O	338.83	284.59	242.59
1408	1-Methoxypropane	C4H10O	319.61	273.25	236.74
1411	2-Methoxypropane	C4H10O	310.22	263.90	227.65
1421	1,4-Dioxane	C4H8O2	365.05	303.82	256.62
2422	1,3-DIOXANE	C4H8O2	365.05	303.82	256.62
1426	2-Methoxybutane	C5H12O	339.57	289.38	250.08
1413	1-Methoxybutane	C5H12O	347.47	297.48	258.09
1461	Methoxybenzene	C7H8O	419.53	361.98	316.12
1448	1-Ethoxybutane	C6H14O	374.23	316.58	271.88
1429	1-MethoxyPentane	C6H14O	374.23	316.58	271.88
6885	Ethyl-3-Ethoxypr	C7H14O3	457.93	388.63	334.73

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Ether

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1401	Dimethyl Ether	C2H6O	256.85	219.17	189.41
1407	MethylEthylEther	C3H8O	278.57	233.50	198.64
1470	VinylMethylEther	C3H6O	281.64	238.89	205.43
1405	MTBE	C5H12O	329.55	280.20	241.67
1445	VinylEthyl Ether	C4H8O	310.11	258.01	218.00
1402	Diethyl Ether	C4H10O	313.64	263.79	225.23
1431	Methylal	C3H8O2	324.13	278.79	242.73
1428	T-But EthylEther	C6H14O	358.15	300.22	255.75
1427	TAME	C6H14O	357.52	304.59	263.21
1410	Mth Isobut Ether	C5H12O	339.57	289.38	250.08
1430	Eth-t-Pent-Ether	C7H16O	386.98	325.54	278.27
1403	DiisopropylEther	C6H14O	347.12	292.44	250.27
1415	Eth Propyl Ether	C5H12O	345.34	291.33	249.53
1455	Dimethyl Acetal	C4H10O2	352.51	293.70	248.53
1446	Dipropyl Ether	C6H14O	374.23	316.58	271.88
1447	Butyl VinylEther	C6H12O	374.89	314.66	268.30
1462	EthylPhenylEther	C8H10O	449.73	384.25	332.81
1406	Di-sec-But Ether	C8H18O	401.84	340.47	292.93
1432	Acetal	C6H14O2	409.47	341.54	289.57
1460	BenzylEthylEther	C9H12O	472.78	398.76	341.54
1050	Paraldehyde	C6H12O3	392.22	328.83	280.10
1404	Di-n-Butyl Ether	C8H18O	425.24	361.51	311.90
1420	Anethole	C10H12O	489.42	426.30	375.44
1456	DimethylCarbitol	C6H14O3	426.03	365.94	318.43
1463	Dibenzyl Ether	C14H14O	588.05	503.92	437.74
1425	Di-n-PentylEther	C10H22O	469.18	400.62	347.02
1458	Diethyl Carbitol	C8H18O3	501.93	421.64	359.95
1412	Dihexyl Ether	C12H26O	507.67	435.21	378.31
1454	Triglyme	C8H18O4	496.63	426.06	370.47
1459	Dibutyl Carbitol	C12H26O3	574.57	488.21	421.19
1424	Di-n-Octyl Ether	C16H34O	572.48	494.21	432.23
1457	Tetraglyme	C10H22O5	650.36	542.81	460.73
1418	Dinonyl Ether	C18H38O	600.19	519.74	455.79
2432	ETHYLAL	C5H12O2	383.15	320.68	272.66
2405	DIISOBUTYL ETHER	C8H18O	418.13	351.78	300.78
2456	Ethyl Glyme	C6H14O2	410.91	345.22	294.64
2417	ETHYLHEXYL ETHER	C8H18O	425.24	361.51	311.90
2415	ETHYLISOPROPETH	C5H12O	325.31	274.94	235.89

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Formate

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1301	Methyl Formate	C2H4O2	293.35	247.89	212.46
1311	Vinyl Formate	C3H4O2	322.25	270.65	230.73
1302	Ethyl Formate	C3H6O2	325.90	276.03	237.16
2306	t-Butyl Formate	C5H10O2	367.61	310.27	265.93
1303	Propyl Formate	C4H8O2	355.61	301.86	259.94
2305	sec-ButylFormate	C5H10O2	377.02	319.06	274.09
2311	CYCLOHEXL FORMAT	C7H12O2	443.01	375.74	323.45
1304	N-Butyl Formate	C5H10O2	382.88	325.70	281.06
1305	Isobutyl Formate	C5H10O2	377.02	319.06	274.09
2350	Benzyl Formate	C8H8O2	475.27	408.46	355.60
2307	n-Hexyl Formate	C7H14O2	431.43	368.50	319.20
1306	N-Pentyl Formate	C6H12O2	408.06	347.84	300.75
2308	n-Heptyl Formate	C8H16O2	453.21	387.85	336.55
1308	N-Octyl Formate	C9H18O2	473.60	406.04	352.93
1309	n-Nonyl Formate	C10H20O2	492.73	423.20	368.43
1310	n-Decyl Formate	C11H22O2	510.76	439.44	383.15

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Ester

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1351	Mth Methacrylate	C5H8O2	374.20	320.78	278.56
1312	Methyl Acetate	C3H6O2	325.43	280.01	243.84
1331	Vinyl Propionate	C5H8O2	369.67	312.32	267.78
1321	Vinyl Acetate	C4H6O2	349.12	299.10	259.54
1352	Eth MthAcrylate	C6H10O2	395.86	335.06	287.82
1322	MethylPropionate	C4H8O2	352.65	303.64	264.64
1341	Methyl Acrylate	C4H6O2	344.28	289.60	247.24
1313	Ethyl Acetate	C4H8O2	341.69	290.11	249.78
1319	IsopropylAcetate	C5H10O2	371.66	319.06	277.43
1332	Methyl Butyrate	C5H10O2	370.25	314.97	271.74
1342	Ethyl Acrylate	C5H8O2	374.42	315.92	270.56
1318	Allyl Acetate	C5H8O2	375.80	322.34	280.05
1314	N-Propyl Acetate	C5H10O2	377.88	325.66	284.11
1323	Ethyl Propionate	C5H10O2	370.25	314.97	271.74
1360	I-But I-Butyrate	C8H16O2	441.53	374.08	321.80
1320	Sec-ButylAcetate	C6H12O2	396.13	340.50	296.46

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1336	PropylI-Butyrate	C7H14O2	420.93	357.50	308.13
1353	N-C3-Mthacrylate	C7H12O2	417.40	353.98	304.62
1333	Ethyl Butyrate	C6H12O2	396.52	337.98	292.15
1347	EthylIsovalerate	C7H14O2	416.76	354.30	305.62
1315	N-Butyl Acetate	C6H12O2	401.37	346.27	302.42
1390	Methyl Benzoate	C8H8O2	463.18	402.13	353.08
1388	ISOBUTYL MTHACR	C8H14O2	447.40	378.25	324.76
1343	1-PropylAcrylate	C6H10O2	397.35	336.57	289.31
1316	Isobutyl Acetate	C6H12O2	396.13	340.50	296.46
1344	N-Butyl Acrylate	C7H12O2	425.13	361.38	311.61
1357	Pentyl Acetate	C7H14O2	423.33	365.63	319.69
1327	N-PropN-Butyrate	C7H14O2	420.82	359.38	311.21
1324	N-PropPropionate	C6H12O2	396.52	337.98	292.15
1291	Acetic Anhydride	C4H6O3	408.87	352.70	307.84
1389	N-ButMthacrylate	C8H14O2	449.39	381.83	329.25
1359	Benzyl Acetate	C9H10O2	478.16	411.43	358.55
1326	N-But Propionate	C7H14O2	420.82	359.38	311.21
1391	Ethyl Benzoate	C9H10O2	489.68	421.13	366.85
1897	CH3OC3H600CH3	C6H12O3	419.89	363.02	317.63
1392	DiethylCarbonate	C5H10O3	404.39	341.82	293.23
1385	N-But N-Butyrate	C8H16O2	443.41	379.38	329.09
1317	IsopentylAcetate	C7H14O2	418.93	360.59	314.36
1363	N-Hexyl Acetate	C8H16O2	447.25	382.34	331.44
1387	Ethylene Acetate	C6H10O4	446.56	389.12	342.75
1393	Diethyl Oxalate	C6H10O4	447.29	381.77	330.36
1365	Butyl Benzoate	C11H14O2	526.41	454.03	396.57
1361	I-C5 I-Valerate	C10H20O2	480.89	409.74	354.26
1367	Heptyl Acetate	C9H18O2	468.24	401.03	348.23
1346	N-Butyl Valerate	C9H18O2	464.51	398.15	345.94
1358	2-C2-C6 Acetate	C10H20O2	479.16	414.14	362.43
1394	Diethyl Malonate	C7H12O4	473.41	404.45	350.34
1292	Propionyl Oxide	C6H10O3	451.91	387.03	335.85
1364	Benzyl Benzoate	C14H12O2	599.37	515.86	449.78
1381	2Mth p-Phthalate	C10H10O4	532.33	470.03	418.83
1368	n-Octyl Acetate	C10H20O2	487.91	418.64	364.11
1377	DiMthI-Phthalate	C10H10O4	548.81	477.76	420.57
1896	Ethylene DiAcr	C8H10O4	515.21	435.56	373.87
1386	2-Ethylhexyl Acr	C11H20O2	511.26	435.72	376.84
1395	Methyl Decanoate	C11H22O2	502.87	432.51	376.97
1369	n-Nonyl Acetate	C11H22O2	506.40	435.26	379.17
1370	n-Decyl Acetate	C12H24O2	523.84	451.01	393.47
1345	N-ButylNonanoate	C13H26O2	536.96	463.33	404.99
1375	DiProp Phthalate	C14H18O4	605.25	528.98	467.37
1376	Diisobutyl Phtha	C16H22O4	632.80	551.75	486.56
1396	IsopropMyristate	C17H34O2	599.37	518.65	454.52

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1383	Butyl Stearate	C22H44O2	654.62	571.88	505.23
1362	Methyl Oleate	C19H36O2	630.53	546.77	480.05
1355	Diisooctyl Phtha	C24H38O4	715.03	628.80	558.60
1382	DioctylTerephtha	C24H38O4	710.06	626.55	558.16
1384	DIBUTYL SEBACATE	C18H34O4	641.00	557.50	490.67
1371	Diisodecyl Phtha	C28H46O4	747.88	660.25	588.38
1354	DioctylPhthalate	C24H38O4	715.03	628.80	558.60
2375	DiethylPhthalate	C12H14O4	572.03	499.47	440.87
2388	Dipropyl Maleate	C10H16O4	545.61	465.79	403.35
2381	Diallyl Maleate	C10H12O4	560.94	474.17	407.02
2370	Glyceryl Triacet	C9H14O6	529.07	464.42	411.79
2382	Dibutyl Maleate	C12H20O4	578.53	495.84	430.90
2376	DibutylPhthalate	C16H22O4	629.74	551.47	488.11
2353	CetylMthacrylate	C20H38O2	642.48	557.76	490.16
2379	Dihexyl Adipate	C18H34O4	641.00	557.50	490.67
2321	T-Butyl Acetate	C6H12O2	386.97	327.03	280.61
2332	Methl.I-butyrate	C5H10O2	368.38	311.30	267.03
2354	AllylMthacrylate	C7H10O2	430.94	362.67	310.01
2364	CYCLOHEXL ACETAT	C8H14O2	459.98	390.55	336.51
2337	EthylIsobutyrate	C6H12O2	395.74	335.29	288.33
2384	IsobutylAcrylate	C7H12O2	424.36	358.01	306.74
2380	1,1-Diacetoxy C2	C6H10O4	454.57	385.38	331.56
2392	n-PropylBenzoate	C10H12O2	508.60	438.04	382.10
2377	DiMth Phthalate	C10H10O4	532.33	470.03	418.83
2386	Diethyl Maleate	C8H12O4	508.51	432.23	372.80
2385	Mth Dodecanoate	C13H26O2	536.96	463.33	404.99
3379	Dioctyl Adipate	C22H42O4	699.20	606.65	532.90
5886	Mth Acetoacetate	C5H8O3	433.11	369.36	319.28
5884	Ethoxy Acetate	C6H12O3	428.64	368.15	320.31
5887	EthAcetoAcetate	C6H10O3	456.37	389.87	337.59
5885	Carbitol Acetate	C8H16O4	500.03	428.89	372.83

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Ketone

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1096	Methyl Isopropen	C5H8O	379.01	320.34	274.70
1079	Cyclopentanone	C5H8O	389.84	332.27	287.00
1051	Acetone	C3H6O	321.34	272.69	234.53
1052	MEK	C4H8O	352.11	299.33	257.97

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1065	Mesityl Oxide	C6H10O	408.10	346.38	298.23
1066	T-But Mth Ketone	C6H12O	393.17	333.00	286.23
1060	2-Pentanone	C5H10O	380.21	323.81	279.59
1061	Mth iC3 Ketone	C5H10O	374.63	317.35	272.73
1053	Diethyl Ketone	C5H10O	377.59	322.48	279.13
1059	3-Hexanone	C6H12O	403.03	344.76	298.89
1099	Diketene	C4H4O2	346.07	291.28	248.62
1055	Sec-ButMthKetone	C6H12O	401.62	341.00	293.72
1054	MIBK	C6H12O	401.62	341.00	293.72
1095	EthIsopropKetone	C6H12O	398.20	339.08	292.82
1063	2-Heptanone	C7H14O	429.98	367.51	318.45
1064	5-Mth-2-Hexanone	C7H14O	426.49	362.90	313.25
1058	4-Heptanone	C7H14O	426.63	365.53	317.39
1057	3-Heptanone	C7H14O	426.63	365.53	317.39
1076	2,4-Pentanedione	C5H8O2	442.39	377.65	326.69
1068	DiisobutylKetone	C9H18O	464.60	396.28	342.86
1097	2-CycC6 CycC6one	C12H20O	549.50	469.96	407.57
1083	2-Octanone	C8H16O	452.22	387.21	336.07
1073	Dibutyl Ketone	C9H18O	469.16	403.27	351.21
1062	2-Hexanone	C6H12O	406.06	346.45	299.68
1077	Isophorone	C9H14O	466.77	397.89	344.01
1090	Acetophenone	C8H8O	473.60	407.39	354.86
1080	Cyclohexanone	C6H10O	417.76	356.37	308.13
1074	2-Nonanone	C9H18O	472.99	405.69	352.68

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Alcohol-Ethers

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
2862	2-Butoxyethanol	C6H14O2	455.59	394.77	346.85
4857	butyl carbitol	C8H18O3	527.07	453.85	396.95
2898	2-Chloroethanol	C2H5ClO	392.73	342.27	301.45
2864	Carbitol	C6H14O3	491.15	422.86	369.48
3854	Methyl propasol	C4H10O2	401.01	350.38	309.75
2860	2-Methoxyethanol	C3H8O2	382.69	335.72	297.67
2854	DiacetoneAlcohol	C6H12O2	465.89	404.37	355.83
2861	2-Ethoxyethanol	C4H10O2	413.75	358.97	315.23
2889	HydroxyAcetone	C3H6O2	410.40	358.70	317.01
3856	1tButoxy2Propnol	C7H16O2	470.94	404.82	353.19
3858	PROPGLYC2tBUTYL	C7H16O2	450.68	389.71	341.87

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

4855	2-Propoxyethanol	C5H12O2	435.14	377.29	331.44
4849	Acetovanillone	C9H10O3	549.40	488.42	438.27
5883	Ethyl Lactate	C5H10O3	448.13	388.75	341.75
6883	2-HydroxyEth Acr	C5H8O3	459.00	397.28	348.54
2863	Methyl Carbitol	C5H12O3	472.31	406.62	355.01
3855	Dowanol DPM	C7H16O3	491.51	427.01	376.29
3857	TriPropGlymEthlE	C10H22O4	571.48	494.41	434.12

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
404	DiMth-Acetylene	C4H6	298.86	253.36	217.84
202	Propylene	C3H6	236.95	198.60	168.87
412	2-Pentyne	C5H8	384.87	328.23	283.89
207	2-Methylpropene	C4H8	271.87	228.33	194.65
204	1-Butene	C4H8	274.56	230.83	196.97
205	Cis-2-Butene	C4H8	276.74	232.34	198.01
402	Propyne	C3H4	247.83	207.32	176.05
406	3-Hexyne	C6H10	358.53	305.16	263.45
206	Trans-2-Butene	C4H8	276.74	232.34	198.01
407	2-Hexyne	C6H10	358.53	305.16	263.45
231	33-2Mth-1-Butene	C6H12	320.22	268.15	228.19
230	23-2Mth-1-Butene	C6H12	329.44	276.52	235.82
229	2-Ethyl-1-Butene	C6H12	337.95	285.51	244.88
8	I-Pentane	C5H12	304.39	257.06	220.39
14	2,2-DiMth-Butane	C6H14	324.51	274.03	234.99
232	23-2Mth-2-Butene	C6H12	340.99	289.42	249.26
213	3-Mth-1-Butene	C5H10	298.35	249.74	212.36
212	2-Mth-1-Butene	C5H10	306.47	258.18	220.82
211	Trans-2-Pentene	C5H10	311.22	262.11	224.12
210	Cis-2-Pentene	C5H10	311.22	262.11	224.12
223	4-Mth-1-Pentene	C6H12	331.60	278.60	237.78
221	2-Mth-1-Pentene	C6H12	337.95	285.51	244.88
248	2-t-Butylpropene	C7H14	349.64	293.60	250.55
227	Cs-4-Mth-2-C5H10	C6H12	334.40	280.62	239.24
224	2-Mth-2-Pentene	C6H12	341.18	288.76	248.07
403	1-Butyne	C4H6	284.92	239.20	203.91
15	2,3-DiMth-Butane	C6H14	326.30	274.63	234.81
214	2-Mth-2-Butene	C5H10	310.32	261.96	224.47
228	Ts-4-Mth-2-C5H10	C6H12	334.40	280.62	239.24

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

225	Cs-3-Mth-2-C5H10	C6H12	341.18	288.76	248.07
218	Trans-2-Hexene	C6H12	342.54	289.32	248.10
2226	3-METH-Tr-2Pente	C6H12	341.18	288.76	248.07
222	3-Mth-1-Pentene	C6H12	331.60	278.60	237.78
257	2-Diisobutylene	C8H16	381.02	321.59	275.74
256	1-Diisobutylene	C8H16	378.51	318.90	273.00
217	Cis-2-Hexene	C6H12	342.54	289.32	248.10
2414	1-Heptyne	C7H12	377.22	319.48	274.72
13	3-Methylpentane	C6H14	335.17	283.79	243.92
219	Cis-3-Hexene	C6H12	342.54	289.32	248.10
12	2-Methylpentane	C6H14	335.17	283.79	243.92
220	Trans-3-Hexene	C6H12	342.54	289.32	248.10
405	1-Pentyne	C5H8	318.57	268.30	229.47
209	1-Pentene	C5H10	308.80	260.38	222.88
11	N-Hexane	C6H14	343.49	292.35	252.40
235	Cis-2-Heptene	C7H14	371.16	314.33	270.23
249	Cis-3-Heptene	C7H14	371.16	314.33	270.23
216	1-Hexene	C6H12	339.98	287.45	246.72
239	3-Eth-1-Pentene	C7H14	361.77	304.93	261.08
226	4-Mth-1-Hexene	C7H14	361.77	304.93	261.08
240	3-Mth-1-Hexene	C7H14	361.77	304.93	261.08
419	3-Mth-1-Butyne	C5H8	308.77	258.16	219.34
233	2-Eth-1-Pentene	C7H14	366.74	310.64	267.11
238	2-Mth-1-Hexene	C7H14	366.74	310.64	267.11
416	1-Octyne	C8H14	403.04	342.20	294.94
289	2,3Dimeth Hexene	C8H16	387.73	327.53	281.03
234	1-Heptene	C7H14	368.52	312.37	268.77
413	1-Hexyne	C6H10	349.19	294.95	252.98
237	Trans-3-Heptene	C7H14	371.16	314.33	270.23
236	Trans-2-Heptene	C7H14	371.16	314.33	270.23
251	Trans-2-Octene	C8H16	397.49	337.45	290.79
279	Trans-4-Octene	C8H16	397.49	337.45	290.79
277	Trans-3-Octene	C8H16	397.49	337.45	290.79
2252	2Methl-1-Heptene	C8H16	393.22	333.89	287.77
250	1-Octene	C8H16	394.79	335.45	289.26
258	2-Ethyl-1-Hexene	C8H16	393.22	333.89	287.77
280	3-Octene	C8H16	397.49	337.45	290.79
278	4-Octene	C8H16	397.49	337.45	290.79
276	2-Octene	C8H16	397.49	337.45	290.79
259	1-Nonene	C9H18	419.11	356.91	308.41
262	1-Dodecene	C12H24	482.62	413.54	359.32
263	1-Tridecene	C13H26	501.23	430.29	374.49
264	1-Tetradecene	C14H28	518.78	446.15	388.91
265	1-Pentadecene	C15H30	535.37	461.21	402.64
266	1-Hexadecene	C16H32	551.09	475.54	415.75

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

267	1-Octadecene	C18H36	580.23	502.26	440.30
281	1-Heptadecene	C17H34	566.02	489.21	428.29
284	1-Eicosene	C20H40	606.70	526.72	462.91
283	1-Nonadecene	C19H38	593.77	514.75	451.83
3	Propane	C3H8	248.62	210.39	180.54
4	I-Butane	C4H10	270.76	228.05	194.98
9	Neopentane	C5H12	292.54	246.33	210.64
5	N-Butane	C4H10	282.86	239.78	206.19
7	pentane	C5H12	314.43	267.07	230.13
44	Hexamethylethane	C8H18	364.72	307.18	262.94
25	223-TriMthButane	C7H16	345.97	291.27	249.17
24	3,3-DiMthPentane	C7H16	353.80	299.57	257.54
51	2,2,3,3-4Mth-C5	C9H20	391.77	330.98	284.10
21	2,2-DiMthPentane	C7H16	353.80	299.57	257.54
42	2,3,3-TriMth-C5	C8H18	374.39	316.16	271.24
22	2,3-DiMthPentane	C7H16	356.20	300.71	257.86
40	2,2,3-TriMth-C5	C8H18	374.39	316.16	271.24
23	2,4-DiMthPentane	C7H16	356.20	300.71	257.86
41	2,2,4-TriMth-C5	C8H18	374.39	316.16	271.24
39	3-Mth-3-Eth-C5	C8H18	380.76	323.21	278.51
20	3-Ethylpentane	C7H16	363.45	308.48	265.75
52	2,2,3,4-4Mth-C5	C9H20	395.31	332.99	285.11
54	2334TetrMethPent	C9H20	395.31	332.99	285.11
53	2,2,4,4-4Mth-C5	C9H20	391.77	330.98	284.10
43	2,3,4-TriMth-C5	C8H18	377.58	317.89	271.99
36	3,3-DiMth-Hexane	C8H18	380.76	323.21	278.51
19	3-Methylhexane	C7H16	363.45	308.48	265.75
18	2-Methylhexane	C7H16	363.45	308.48	265.75
38	2-Mth-3-Eth-C5	C8H18	383.63	324.77	279.21
190	2,2-2C1-3-C2-C5	C9H20	400.53	339.18	291.73
32	2,2-DiMth-Hexane	C8H18	380.76	323.21	278.51
37	3,4-DiMth-Hexane	C8H18	383.63	324.77	279.21
50	3,3-DiEthPentane	C9H20	405.70	345.19	298.09
34	2,4-DiMth-Hexane	C8H18	383.63	324.77	279.21
33	2,3-DiMth-Hexane	C8H18	383.63	324.77	279.21
17	N-Heptane	C7H16	370.34	315.83	273.19
49	244TriMethHexane	C9H20	400.53	339.18	291.73
192	2,4-2C1-3-C2-C5	C9H20	404.10	341.26	292.82
47	2,2,5-TriMth-C6	C9H20	400.53	339.18	291.73
35	2,5-DiMth-Hexane	C8H18	383.63	324.77	279.21
31	3-Ethylhexane	C8H18	389.53	331.38	286.09
30	4-Methylheptane	C8H18	389.53	331.38	286.09
29	3-Methylheptane	C8H18	389.53	331.38	286.09
28	2-Methylheptane	C8H18	389.53	331.38	286.09
96	2,2-DiMthHeptane	C9H20	405.70	345.19	298.09

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

176	2,6-DiMthHeptane	C9H20	408.92	347.08	299.09
27	N-Octane	C8H18	395.23	337.72	292.65
94	3-Ethylheptane	C9H20	413.72	352.73	305.13
92	3-Methyloctane	C9H20	413.72	352.73	305.13
93	4-Methyloctane	C9H20	413.72	352.73	305.13
91	2-Methyloctane	C9H20	413.72	352.73	305.13
72	2,2-DiMthOctane	C10H22	428.87	365.72	316.46
2095	2,3Dimethloctane	C10H22	432.38	367.87	317.70
2096	2,4Dimethloctane	C10H22	432.38	367.87	317.70
2098	2,6DimethlOctane	C10H22	432.38	367.87	317.70
2097	2,5Dimethloctane	C10H22	432.38	367.87	317.70
2099	2,7DimethlOctane	C10H22	432.38	367.87	317.70
46	N-Nonane	C9H20	418.41	358.20	310.93
88	5-Methylnonane	C10H22	436.24	372.71	323.02
85	3-Methylnonane	C10H22	436.24	372.71	323.02
87	4-Methylnonane	C10H22	436.24	372.71	323.02
86	2-Methylnonane	C10H22	436.24	372.71	323.02
56	N-Decane	C10H22	440.07	377.43	328.16
63	N-Undecane	C11H24	460.38	395.55	344.46
64	N-Dodecane	C12H26	479.49	412.66	359.91
65	N-Tridecane	C13H28	497.51	428.88	374.60
66	N-Tetradecane	C14H30	514.55	444.28	388.59
67	N-Pentadecane	C15H32	530.70	458.94	401.95
68	N-Hexadecane	C16H34	546.05	472.91	414.73
69	N-Heptadecane	C17H36	560.65	486.26	426.97
70	N-Octadecane	C18H38	574.57	499.03	438.71
71	N-Nonadecane	C19H40	587.86	511.27	450.00
73	N-Eicosane	C20H42	600.58	523.02	460.86
74	n-HENEICOSANE	C21H44	612.75	534.31	471.32
75	n-DOCOSANE	C22H46	624.42	545.17	481.40
76	n-TRICOSANE	C23H48	635.63	555.63	491.14
77	n-Tetracosane	C24H50	646.40	565.72	500.56
78	n-PENTACOSANE	C25H52	656.77	575.46	509.66
79	n-HEXACOSANE	C26H54	666.75	584.88	518.48
81	n-Octacosane	C28H58	685.66	602.79	535.30
2081	n-TRICONTANE	C30H62	703.28	619.60	551.15
2082	n-Dotriacontane	C32H66	719.77	635.42	566.12
2086	Hexatriacontane	C36H74	749.75	664.48	593.75

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Cyclic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
269	Cyclopentene	C5H8	324.56	272.31	231.88
270	Cyclohexene	C6H10	358.69	301.63	257.50
287	3MthCyclopentene	C6H10	343.69	288.28	245.55
286	1-MthCyclPentene	C6H10	354.34	299.00	256.07
288	4MthCyclopenten	C6H10	343.69	288.28	245.55
273	Cycloheptene	C7H12	390.04	328.68	281.22
274	Cyclooctene	C8H14	419.04	353.82	303.34
101	Cyclopropane	C3H6	256.48	216.36	185.00
810	ADAMANTANE	C10H16	451.51	380.44	325.59
102	Cyclobutane	C4H8	293.79	248.09	212.47
104	Cyclopentane	C5H10	328.23	277.54	238.08
137	Cyclohexane	C6H12	360.07	304.90	261.97
105	MthCyclopentane	C6H12	346.05	292.42	250.81
146	Cs-1,4-2C1-CycC6	C8H16	392.23	331.94	285.23
142	Cs-1,2-2C1-CycC6	C8H16	392.23	331.94	285.23
141	1,1-2C1-CycC6	C8H16	390.96	331.47	285.27
145	Ts-1,3-2C1-CycC6	C8H16	392.23	331.94	285.23
144	Cs-1,3-2C1-CycC6	C8H16	392.23	331.94	285.23
147	Ts-1,4-2C1-CycC6	C8H16	392.23	331.94	285.23
143	Ts-1,2-2C1-CycC6	C8H16	392.23	331.94	285.23
138	MthCyclohexane	C7H14	376.54	318.72	273.84
159	Cycloheptane	C7H14	389.61	330.41	284.33
140	Ethylcyclohexane	C8H16	402.95	341.92	294.47
154	Trans-Decalin	C10H18	459.02	389.06	334.77
149	N-PropylCyc-C6	C9H18	427.34	363.46	313.70
109	Cs-1,2-2C1-CycC5	C7H14	362.95	306.61	262.99
110	Ts-1,2-2C1-CycC5	C7H14	362.95	306.61	262.99
112	Ts-1,3-2C1-CycC5	C7H14	362.95	306.61	262.99
107	Eth-Cyclopentane	C7H14	374.71	317.45	272.97
114	N-PropCycPentane	C8H16	401.04	340.58	293.52
108	1,1-DiMthCycC5	C7H14	362.10	306.49	263.35
111	Cs-1,3-2C1-CycC5	C7H14	362.95	306.61	262.99
152	N-ButylCycHexane	C10H20	449.98	383.57	331.72
160	Cyclooctane	C8H16	417.14	354.29	305.34
153	Cis-Decalin	C10H18	459.02	389.06	334.77
115	ISOPROPYLCYCLOPENTANE	C8H16	396.23	334.74	287.18
150	Isopropyl-CycC6	C9H18	423.76	358.67	308.27
116	1-C1-1-C2-CycC5	C8H16	389.15	330.21	284.39
122	Butylcyclpentane	C9H18	425.38	362.07	312.70
155	1,1-Bicyclohexyl	C12H22	505.99	430.30	371.41
158	N-Decylcyclo-C6	C16H32	559.18	482.05	421.08

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Aromatic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
307	1,4-Pentadiene	C5H8	303.73	253.66	215.16
306	1-ts3-Pentadiene	C5H8	306.70	255.73	216.59
414	2-Methyl-1-Butenyne	C5H6	312.25	260.15	220.23
305	Cs1,3-Pentadiene	C5H8	306.70	255.73	216.59
309	Isoprene	C5H8	301.27	251.30	212.92
421	1-Pentene-4-yne	C5H6	314.60	262.42	222.41
303	1,3-Butadiene	C4H6	265.98	221.02	186.47
332	1,4-CyclHexadien	C6H8	360.07	300.05	253.88
501	Benzene	C6H6	352.64	295.74	251.76
315	Cyclopentadiene	C5H6	323.14	268.22	225.94
319	Diisopropenyl	C6H10	333.20	278.83	237.08
615	Ethynylbezene	C8H6	428.62	365.83	316.57
601	Styrene	C8H8	420.24	359.00	310.86
331	1,3-CycHexadiene	C6H8	360.07	300.05	253.88
310	1,5-Hexadiene	C6H10	337.38	282.92	241.00
312	MthCycPentadiene	C6H8	351.21	294.39	250.53
420	1-Pentene-3-yne	C5H6	325.93	274.82	235.20
502	Toluene	C7H8	386.16	325.65	278.75
521	T-Butylbenzene	C10H14	452.90	387.89	336.76
320	Dipropylene	C6H10	343.76	287.50	244.29
520	Sec-Butylbenzene	C10H14	447.41	380.24	327.96
313	1,4-Hexadiene	C6H10	340.49	285.15	242.61
314	Dipropylene	C6H10	343.76	287.50	244.29
316	DiCycPentadiene	C10H12	479.52	397.26	334.42
333	1,5-CycOctadiene	C8H12	423.72	355.24	302.56
701	Naphthalene	C10H8	478.85	415.07	363.96
504	Ethylbenzene	C8H10	409.58	346.72	297.89
820	Indan	C9H10	444.75	377.99	325.86
505	O-Xylene	C8H10	416.07	352.46	303.00
612	P-Methylstyrene	C9H10	446.02	382.15	331.80
330	DIISOCROTYL	C8H14	396.69	335.51	288.14
507	P-Xylene	C8H10	416.07	352.46	303.00
329	DIISOBUTENYL	C8H14	392.36	330.67	283.11
506	M-Xylene	C8H10	416.07	352.46	303.00
603	Methylstyrene	C9H10	446.02	382.15	331.80
613	Alpha-MthStyrene	C9H10	442.25	378.23	327.89
510	Isopropylbenzene	C9H12	423.87	359.38	309.27
724	2-Methylindene	C10H10	474.01	408.19	355.95
285	Vinylcyclohexene	C8H12	409.02	342.10	290.74
803	Indene	C9H8	458.51	397.83	349.11
706	Tetralin	C10H12	469.81	399.84	345.17
511	O-Ethyltoluene	C9H12	437.09	371.49	320.35

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

723	1-Methylindene	C10H10	498.79	414.14	349.38
738	Fluorene	C13H10	539.18	472.58	418.43
619	Tr-1PropenylBz	C9H10	446.28	381.61	330.77
525	O-Diethylbenzene	C10H14	456.49	389.14	336.50
618	Propenyl Bz(cis)	C9H10	446.28	381.61	330.77
602	O-Methylstyrene	C9H10	446.02	382.15	331.80
702	1-MthNaphthalene	C11H10	499.30	433.60	380.86
509	N-Propylbenzene	C9H12	434.38	368.62	317.46
526	M-Diethylbenzene	C10H14	456.49	389.14	336.50
583	Cs-2-PhnButene-2	C10H12	465.18	399.01	346.83
543	M-DiisopropylBz	C12H18	479.65	409.96	355.40
584	Ts-2-PhnButene-2	C10H12	465.18	399.01	346.83
580	1,2-DiC1-3C2-Bz	C10H14	462.12	394.16	340.99
704	1-EthNaphthalene	C12H12	514.07	447.09	393.25
512	M-Ethyltoluene	C9H12	437.09	371.49	320.35
522	1-Mth-2-iC3-Benz	C10H14	449.98	382.98	330.72
513	P-Ethyltoluene	C9H12	437.09	371.49	320.35
514	1,2,3-Mesitylene	C9H12	443.08	376.80	325.09
614	M-Divinylbenzene	C10H10	472.00	407.94	356.86
524	1-Mth-4-iC3-Benz	C10H14	449.98	382.98	330.72
822	Gamma-Terpinene	C10H16	452.14	382.33	328.34
821	Alpha-Terpinene	C10H16	452.14	382.33	328.34
523	1-Mth-3-iC3-Benz	C10H14	449.98	382.98	330.72
703	2-MthNaphthalene	C11H10	499.30	433.60	380.86
557	CycHexylBenzene	C12H16	511.30	434.77	375.18
515	1,2,4-Mesitylene	C9H12	443.08	376.80	325.09
519	Isobutylbenzene	C10H14	455.69	385.74	331.54
424	DiPhnAcetylene	C14H10	562.60	488.58	429.26
544	P-DiisopropylBz	C12H18	479.65	409.96	355.40
518	N-Butylbenzene	C10H14	457.34	389.01	335.74
516	1,3,5-Mesitylene	C9H12	443.08	376.80	325.09
809	Acenaphthalene	C12H8	525.47	463.29	412.26
725	123-TriMthIndene	C12H14	505.82	436.93	382.11
527	1,4-DiEthBenzene	C10H14	456.49	389.14	336.50
558	Diphenyl	C12H10	518.70	449.47	394.09
576	2-Ethyl-m-Xylene	C10H14	462.12	394.16	340.99
620	p-ISOPROPENYLSTY	C11H12	489.99	423.81	371.03
585	o-PropylToluene	C10H14	459.74	391.60	338.38
577	2-Ethyl-p-Xylene	C10H14	462.12	394.16	340.99
579	4-Ethyl-o-Xylene	C10H14	462.12	394.16	340.99
586	m-Propyltoluene	C10H14	459.74	391.60	338.38
587	p-Propyltoluene	C10H14	459.74	391.60	338.38
578	4-Ethyl-m-Xylene	C10H14	462.12	394.16	340.99
575	5-Ethyl-m-Xylene	C10H14	462.12	394.16	340.99
530	Prehnitene	C10H14	467.68	399.11	345.43

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

709	2,6-2Mth-Naphtha	C12H12	518.30	450.91	396.72
715	2,7-2Mth-Naphtha	C12H12	518.30	450.91	396.72
719	2-ETHYLNAPHTHALENE	C12H12	514.07	447.09	393.25
621	p-tert-BUTYLSTY	C12H16	498.45	431.56	378.21
532	1,2,4,5-TetMthBz	C10H14	467.68	399.11	345.43
531	1,2,3,5-TetMthBz	C10H14	467.68	399.11	345.43
533	p-tert-BUTYL ET	C12H18	495.61	430.62	378.53
567	N-Pentylbenzene	C11H16	478.71	408.08	352.91
718	1-n-PROPYLNAPHTH	C13H14	531.53	466.11	412.92
562	1,1-DiPhnEthane	C14H14	547.21	470.60	410.05
616	4-ISOBUTYLSTYRE	C12H16	503.77	436.75	383.17
260	1-Decene	C10H20	441.72	376.98	326.39
735	Cis-Stilbene	C14H12	559.99	484.36	424.09
568	Hexylbenzene	C12H18	498.68	425.98	369.09
563	Diphenylmethane	C13H12	538.11	462.29	402.41
564	1,2-DiPhnEthane	C14H14	564.44	480.03	414.30
804	Anthracene	C14H10	556.98	490.79	436.58
736	Trans-Stilbene	C14H12	559.99	484.36	424.09
805	Phenanthrene	C14H10	556.98	490.79	436.58
713	1-ButNaphthalene	C14H16	545.98	475.78	419.27
807	Pyrene	C16H10	587.07	523.19	469.99
261	1-Undecene	C11H22	462.84	395.81	343.32
581	23-2C1-23-2PhnC4	C18H22	602.93	522.20	457.90
549	N-Heptylbenzene	C13H20	517.41	442.86	384.40
710	1-PhnNaphthalene	C16H12	586.97	517.05	459.85
566	2,4-Diphenyl-4-M	C18H20	612.20	530.27	464.98
561	O-Terphenyl	C18H14	615.61	542.20	482.21
569	N-Octylbenzene	C14H22	535.04	458.82	398.92
565	Triphenylmethane	C19H16	636.44	555.83	490.79
714	N-C6-Naphthalene	C16H20	574.79	501.91	443.12
717	Fluoranthene	C16H10	587.07	523.19	469.99
716	1-Hexyl-Tetralin	C16H24	569.36	497.15	438.92
731	TriPhnEthylene	C20H16	653.18	570.90	504.45
806	Chrysene	C18H12	612.25	545.43	489.83
588	1,1,2TriPhenEth	C20H18	648.23	566.71	500.86
711	1-n-NonylNaphtha	C19H26	613.27	537.14	475.50
570	N-Nonylbenzene	C15H24	551.67	473.95	412.74
712	1-Decyl Naphtha	C20H28	625.03	547.98	485.52
559	P-Terphenyl	C18H14	615.61	542.20	482.21
560	M-Terphenyl	C18H14	615.61	542.20	482.21
589	TetraPhenylMetha	C25H20	710.94	625.15	555.29
554	Decylbenzene	C16H26	567.41	488.32	425.91
732	TetraPhnEthylene	C26H20	722.78	637.08	567.03
574	N-Dodecylbenzene	C18H30	596.51	515.07	450.54
571	N-Undecylbenzene	C17H28	582.33	502.01	438.50

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

572	Tridecylbenzene	C19H32	610.01	527.55	462.08
573	n-TETRADECYLBENZ	C20H34	616.72	538.13	474.92
2575	n-PENTADECYLBENZ	C21H36	628.49	549.05	485.04
2576	n-HEXADECYLBENZ	C22H38	639.78	559.55	494.81
2577	n-HEPTADECYLBENZ	C23H40	650.63	569.68	504.25
2578	n-OCTADECYLBENZE	C24H42	661.06	579.46	513.37

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

Halocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1544	Allyl Chloride	C3H5Cl	317.79	266.57	226.89
1595	2-Chloropropene	C3H5Cl	292.39	246.12	210.22
1531	3-Chloropropyne	C3H3Cl	328.87	275.47	234.23
1561	6Cl-1,3Butadiene	C4Cl6	473.33	408.85	357.47
1535	T-Butyl Chloride	C4H9Cl	318.25	269.52	231.61
1583	Chloroprene	C4H5Cl	322.70	269.86	229.15
1530	Isopropyl Cl	C3H7Cl	303.86	257.21	220.86
1572	O-DiCl-Benzene	C6H4Cl2	451.04	381.57	327.53
1585	Propyl Chloride	C3H7Cl	321.36	271.99	233.49
1684	Isopropyl Iodide	C3H7I	367.20	306.63	260.11
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	398.02	336.97	289.45
1651	2-Bromopropane	C3H7Br	328.23	276.38	236.19
1691	Iodobenzene	C6H5I	473.46	403.78	349.12
1860	Fluorobenzene	C6H5F	352.15	296.41	253.26
1571	Chlorobenzene	C6H5Cl	404.64	340.97	291.60
1680	Bromobenzene	C6H5Br	440.54	377.68	327.98
1526	1,2-DiCl-Propane	C3H6Cl2	373.93	316.77	272.20
1683	Propyl Iodide	C3H7I	371.79	312.81	267.22
1576	Benzotrichloride	C7H5Cl3	466.36	410.30	364.46
1536	2,3-DICHLOROBUT	C4H8Cl2	384.71	326.67	281.39
2638	2-Bromobutane	C4H9Br	359.11	303.26	259.94
1586	1-Chlorobutane	C4H9Cl	351.88	298.48	256.82
1573	M-DiCl-Benzene	C6H4Cl2	451.04	381.57	327.53
2634	Benzotrifluoride	C7H5F3	366.09	321.64	285.35
1574	P-DiCl-Benzene	C6H4Cl2	451.04	381.57	327.53
1650	1-Bromopropane	C3H7Br	336.35	285.06	245.04
1587	2-Chlorobutane	C4H9Cl	335.09	284.27	244.64
2653	8F-2-Butene	C4F8	304.57	273.99	248.12
1678	M-Dibromobenzene	C6H4Br2	504.28	438.06	384.78

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1537	1,2-DiCl-Butane	C4H8Cl2	401.20	340.63	293.37
1597	34-DiCl-1-Butene	C4H6Cl2	404.38	340.86	291.62
1577	O-Chlorotoluene	C7H7Cl	433.23	366.75	315.06
1532	123-3Cl-Propane	C3H5Cl3	440.86	373.78	321.44
1578	P-Chlorotoluene	C7H7Cl	433.23	366.75	315.06
1562	Benzyl Chloride	C7H7Cl	452.28	387.95	337.10
2661	P-Bromotoluene	C7H7Br	464.96	399.65	347.89
1508	1,4-DiCl-Butane	C4H8Cl2	417.80	354.69	305.43
1655	1-Bromobutane	C4H9Br	365.61	310.52	267.51
1599	BenzylDichloride	C7H6Cl2	476.00	409.17	356.24
2652	Perfluoropropane	C3F8	261.73	234.32	211.28
1505	2-Butylene DiCl	C4H6Cl2	426.70	357.59	304.14
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	427.43	359.81	307.41
1588	1-Chloropentane	C5H11Cl	379.80	322.86	278.39
1592	1,2,4-TriCl-Bz	C6H3Cl3	492.96	418.45	360.32
1579	2,4-2Cl-Toluene	C7H6Cl2	475.78	404.12	348.23
2593	1,3,5-TriCl-BZ	C6H3Cl3	492.96	418.45	360.32
1697	1-Br-Naphthalene	C10H7Br	532.70	466.40	412.55
1622	Perfluorobutane	C4F10	268.49	241.35	218.42
1857	P-Cl-Benzo-TriF	C7H4ClF3	397.78	349.77	310.55
1509	1,5-DiCl-Pentane	C5H10Cl2	442.17	376.19	324.62
1589	1-Cl-Naphthalene	C10H7Cl	511.23	443.81	389.69
1582	6ClCycPentadiene	C5Cl6	513.03	439.57	381.65
1864	Perfluorobenzene	C6F6	355.81	303.48	262.52
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	427.79	376.49	334.55
1667	1-Bromoheptane	C7H15Br	440.27	376.19	325.95
1575	HexaCl-Benzene	C6Cl6	598.88	512.57	444.67
2640	Freon 123B1	C2HBrClF3	331.94	289.99	255.98
1504	Vinyl Chloride	C2H3Cl	275.48	232.85	199.43
1672	1,1-DiBr-Ethane	C2H4Br2	386.77	325.64	278.18
1580	Acetylene DiCl	C2H2Cl2	333.34	281.87	241.59
1692	Diiodomethane	CH2I2	456.49	379.21	319.85
1698	Bromoform	CHBr3	447.03	376.29	321.28
2687	Freon 13B1	CBrF3	270.72	236.74	209.07
2690	Br-3F-Ethylene	C2BrF3	281.86	246.00	216.90
1649	Tetrabromoethane	C2H2Br4	557.47	469.06	400.57
2686	Freon 12B1	CBrClF2	284.95	245.39	213.90
1503	Ethyl Chloride	C2H5Cl	287.77	243.01	208.07
2641	Br-TriCl-Methane	CBrCl3	389.80	341.03	301.35
1641	Methyl Bromide	CH3Br	268.76	226.79	193.96
2688	Freon 12B2	CBr2F2	314.23	270.11	235.09
2545	2,3-DiCl-Propene	C3H4Cl2	365.69	309.29	265.27
1673	1,2-DiBr-Ethane	C2H4Br2	390.22	330.66	284.14
2637	Dibromomethane	CH2Br2	361.04	305.23	261.62
1542	TetraCl-Ethylene	C2Cl4	406.31	347.02	300.36

Table C.3 Boiling Temperatures Calculated by the GC-PC-SAFT method (Continued)

1541	TriCl-Ethylene	C2HCl3	364.72	309.63	266.53
1527	111-TriCl-Ethane	C2H3Cl3	354.03	309.84	273.87
1612	Cl-2F-Ethylene	C2HClF2	245.01	210.93	183.76
2639	Br-Cl-Methane	CH2BrCl	346.06	292.12	249.98
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	333.34	281.87	241.59
1682	Ethyl Iodide	C2H5I	340.95	285.85	243.29
1522	1,1-DiCl-Ethane	C2H4Cl2	325.26	275.63	236.86
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	256.52	213.45	180.36
1525	Hexachloroethane	C2Cl6	431.05	383.53	344.01
1528	1112-4Cl-Ethane	C2H2Cl4	400.71	350.54	309.77
1590	Penta-Cl-Ethane	C2HCl5	422.79	370.20	327.43
1529	1122-4Cl-Ethane	C2H2Cl4	423.79	360.47	310.89
2693	Perfluoroethane	C2F6	253.58	226.01	202.94
2692	Cl-PentaF-Ethane	C2ClF5	261.98	227.75	200.18
2655	122-3Cl-112-3FC2	C2Cl3F3	337.46	281.34	238.38
1609	12-2Cl-1122-4FC2	C2Cl2F4	314.67	257.68	214.45
2526	1,1-DiCl-Propane	C3H6Cl2	355.48	301.86	259.96
1645	Ethyl Bromide	C2H5Br	304.25	257.29	220.64
2658	1112-4Cl-22-2FC2	C2Cl4F2	385.69	335.70	295.41
1619	111-3F-Ethane	C2H3F3	236.20	206.96	183.06
1524	1,1,2-3Cl-Ethane	C2H3Cl3	394.58	334.60	287.71
2691	Genetron 1113	C2ClF3	258.20	225.81	199.42
1591	Vinylidene DiCl	C2H2Cl2	303.28	259.56	224.95
1614	Difluoromethane	CH2F2	201.37	176.28	155.45
2694	Vinyl Bromide	C2H3Br	299.25	250.59	212.85
1694	Refrigerant 123	C2HCl2F3	310.05	271.12	239.51
1523	1,2-DiCl-Ethane	C2H4Cl2	362.38	306.21	262.38
2656	1122-4Cl-12-2FC2	C2Cl4F2	358.25	302.10	258.72
2527	1,3-DiCl-Propane	C3H6Cl2	391.34	331.48	284.78

Table C. 4 Boiling Temperatures Calculated by the GC-SAFT method.

Alcohols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1181	Phenol	C6H6O	427.65	373.32	330.84
1182	O-Cresol	C7H8O	451.59	393.46	348.13
1183	M-Cresol	C7H8O	451.58	393.45	348.11
1176	2,6-Xylenol	C8H10O	474.29	412.76	364.79
1111	2-Mth-2-Butanol	C5H12O	373.35	324.56	286.32
1178	3,5-Xylenol	C8H10O	474.27	412.73	364.76
1133	2-Octanol	C8H18O	453.76	390.68	342.59
2885	4-HYDROXYSTYREN	C8H8O	485.74	421.81	372.02
1197	P-t-Butylphenol	C10H14O	504.90	439.96	389.19
1172	2,4-Xylenol	C8H10O	474.28	412.74	364.77
1184	P-Cresol	C7H8O	451.48	393.32	347.97
1151	Cyclohexanol	C6H12O	418.60	361.77	317.76
1170	2,3-Xylenol	C8H10O	478.97	415.76	366.66
1187	P-Ethyl Phenol	C8H10O	478.97	415.76	366.65
2859	P-Methoxyphenol	C7H8O2	477.98	419.14	372.62
1121	2-Ethylhexanol	C8H18O	453.75	390.66	342.58
1179	PropargylAlcohol	C3H4O	345.18	301.13	265.78
1123	3-Mth-1-Butanol	C5H12O	382.72	332.45	293.19
2196	P-t-Amylphenol	C11H16O	522.78	455.23	402.44
1174	2,5-Xylenol	C8H10O	474.27	412.73	364.75
1115	2-Hexanol	C6H14O	407.02	352.33	310.09
1152	1-MthCycHexanol	C7H14O	436.25	375.73	329.25
4854	Guaiacol	C7H8O2	478.00	419.17	372.65
1107	Sec-Butanol	C4H10O	358.02	312.19	275.85
1167	Allyl Alcohol	C3H6O	339.52	296.47	261.70
1130	4-Mth-2-Pentanol	C6H14O	396.84	343.66	302.50
1177	3,4-Xylenol	C8H10O	474.27	412.72	364.74
1114	1-Hexanol	C6H14O	417.00	360.84	317.55
1106	Isobutanol	C4H10O	357.98	312.16	275.82
1125	1-Heptanol	C7H16O	440.45	380.07	333.83
1105	N-Butanol	C4H10O	368.31	321.01	283.66
1109	1-Pentanol	C5H12O	392.93	341.16	300.84
1132	1-Octanol	C8H18O	463.21	398.84	349.73
1113	T-Butylcarbinol	C5H12O	373.30	324.51	286.28
1137	1-Undecanol	C11H24O	526.99	452.27	395.29
1108	Tert-Butanol	C4H10O	348.55	304.16	268.81
1103	N-Propanol	C3H8O	343.17	300.31	265.89
1134	1-Nonanol	C9H20O	485.23	417.14	365.26
2195	P-t-Octylphenol	C14H22O	559.98	486.70	429.65
1102	Ethanol	C2H6O	317.42	278.90	247.39
1124	3-Mth-2-Butanol	C5H12O	372.42	323.69	285.48
1136	1-Decanol	C10H22O	506.48	434.94	380.43
1140	Dodecanol	C12H26O	546.70	469.03	409.73
1104	Isopropanol	C3H8O	332.75	291.28	257.83
1110	2-Pentanol	C5H12O	382.79	332.52	293.24

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1120	3-Pentanol	C5H12O	382.78	332.50	293.22
1112	2-Mth-1-Butanol	C5H12O	382.73	332.46	293.19
1154	Ts-2-Mth-CycC6OH	C7H14O	436.22	375.70	329.23
1153	Cs-2-Mth-CycC6OH	C7H14O	436.23	375.70	329.23
1156	Ts-3-Mth-CycC6OH	C7H14O	436.20	375.68	329.21
1157	Cs-4-Mth-CycC6OH	C7H14O	436.21	375.69	329.22
2197	P-Cumylphenol	C15H16O	595.80	520.16	460.73
1180	Benzyl Alcohol	C7H8O	453.25	392.86	346.09
1158	Ts-4-Mth-CycC6OH	C7H14O	436.21	375.69	329.22
1155	Cs-3-Mth-CycC6OH	C7H14O	436.20	375.68	329.21
1168	2-Phn-2-Propanol	C9H12O	480.22	414.55	364.07
1141	1-Tridecanol	C13H28O	565.69	485.28	423.80
1147	2-Eth-1-Butanol	C6H14O	407.00	352.30	310.06
1117	2-Mth-1-Pentanol	C6H14O	406.99	352.29	310.06
2115	2-Phenylethanol	C8H10O	475.97	408.40	356.74
1142	1-Tetradecanol	C14H30O	583.97	501.01	437.51
2118	1-PHN-1-PROPANOL	C9H12O	488.52	421.72	370.30
2119	1-PHN-2-PROPANOL	C9H12O	488.52	421.72	370.30
1126	2-Heptanol	C7H16O	430.72	371.71	326.52
1143	1-Pentadecanol	C15H32O	601.57	516.22	450.83
1129	Isoheptanol	C7H16O	430.68	371.67	326.49
2117	2,6-DiMth-4-C7OH	C9H20O	457.20	392.80	343.95
1144	1-Hexadecanol	C16H34O	618.56	530.98	463.82
1145	Heptadecanol	C17H36O	634.95	545.26	476.45
1199	Nonylphenol	C15H24O	607.61	525.65	462.02
1146	1-Octadecanol	C18H38O	650.76	559.08	488.72
1135	2-Nonanol	C9H20O	476.10	409.16	358.24
1149	1-Nonadecanol	C19H40O	666.04	572.47	500.64
1139	Isodecanol	C10H22O	497.68	427.17	373.57
1148	1-Eicosanol	C20H42O	680.83	585.47	512.25
2198	Dinonylphenol	C24H42O	743.04	643.73	567.02
1159	Menthol	C10H20O	495.55	420.38	362.44

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Amines

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1742	Ethyleneimine	C2H5N	279.43	236.86	203.90
1745	Piperidine	C5H11N	378.55	319.93	274.72
1766	Pyrrolidine	C4H9N	347.75	293.89	252.33
1719	Isopropylamine	C3H9N	298.17	250.54	214.25
1711	N-Propylamine	C3H9N	314.19	265.34	227.76

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1726	Sec-Butylamine	C4H11N	332.63	279.30	238.68
1704	Ethylamine	C2H7N	279.84	236.67	203.44
1702	Dimethylamine	C2H7N	275.44	233.67	201.34
1710	Diethylamine	C4H11N	335.03	284.05	244.60
1740	Allylamine	C3H7N	306.13	257.34	220.09
1712	N-Butylamine	C4H11N	346.42	292.47	250.98
1794	HexMthyleneimine	C6H13N	407.39	344.48	295.96
1729	Cyclohexylamine	C6H13N	411.99	344.96	293.99
1714	Isobutylamine	C4H11N	332.84	280.50	240.39
2853	Acetamide	C2H5NO	434.74	371.93	322.27
2731	N-C1-CycC6-Amine	C7H15N	429.88	362.68	311.05
1743	Diisopropylamine	C6H15N	348.16	298.81	260.18
1796	N,N-DiMthAniline	C8H11N	495.01	424.92	369.84
1792	Aniline	C6H7N	445.33	381.22	330.81
1713	N-Pentylamine	C5H13N	376.65	318.11	273.06
1733	Benzylamine	C7H9N	446.38	380.74	329.48
1737	M-Toluidine	C7H9N	471.12	403.85	350.97
3796	N-Ethylaniline	C8H11N	457.01	391.16	339.63
1878	2-Methacrylamide	C4H7NO	488.74	415.87	358.86
1736	O-Toluidine	C7H9N	471.12	403.85	350.97
2739	Diallylamine	C6H11N	386.99	325.02	277.74
2706	Hexylamine	C6H15N	405.05	342.34	294.06
2724	O-Ethylaniline	C8H11N	503.52	430.48	373.32
1707	Dipropylamine	C6H15N	392.09	332.66	286.70
1738	P-Toluidine	C7H9N	471.12	403.85	350.97
1795	N-Methylaniline	C7H9N	438.61	375.00	325.19
1718	Diisobutylamine	C8H19N	421.87	357.35	307.70
1879	Acrylamide	C3H5NO	463.38	394.49	340.46
2707	1-Aminoheptane	C7H17N	431.81	365.28	314.05
2730	DiCycHexylAmine	C12H23N	507.31	434.70	378.26
2787	P-Aminodiphenyl	C12H11N	580.41	504.20	443.87
1744	Dibutylamine	C8H19N	443.06	376.47	324.99
2708	1-Octylamine	C8H19N	457.08	387.04	333.09
2791	2,6-DiEthAniline	C10H15N	557.79	476.59	413.28
2709	1-Nonylamine	C9H21N	481.01	407.72	351.26
2710	1-Decylamine	C10H23N	503.72	427.41	368.63
3722	Diamylamine	C10H23N	489.00	416.21	359.98
3724	Undecylamine	C11H25N	525.32	446.20	385.25
2712	Dodecylamine	C12H27N	545.92	464.17	401.20
1720	Tetradecylamine	C14H31N	584.41	497.87	431.23
2752	Piperazine	C4H10N2	397.97	338.38	292.18
1752	Propylenediamine	C3H10N2	365.86	308.55	264.85
1741	Ethylenediamine	C2H8N2	347.25	294.49	253.89
2725	O-Aminoaniline	C6H8N2	522.84	453.42	398.09
2750	P-Aminoaniline	C6H8N2	522.83	453.41	398.08
2727	M-Aminoaniline	C6H8N2	522.83	453.41	398.08

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1750	AEP	C6H15N3	471.47	399.89	344.67
1732	Toluene Diamine	C7H10N2	543.46	471.56	414.35
1731	hexamethyleneDiamine	C6H16N2	463.33	392.39	337.76
3750	P-Benzidine	C12H12N2	631.64	552.88	490.18

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Nitrilies

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1773	Propionitrile	C3H5N	347.35	292.53	250.39
1782	Butyronitrile	C4H7N	380.87	320.57	274.27
2720	Allyl Cyanide	C4H5N	376.61	315.47	268.76
1783	Valeronitrile	C5H9N	412.01	346.84	296.81
3874	Benzyl Cyanide	C8H7N	504.78	429.63	371.05
1786	Hexanenitrile	C6H11N	441.04	371.52	318.14
1776	Succinonitrile	C4H4N2	481.73	405.71	347.26
1781	Glutaronitrile	C5H6N2	511.44	430.44	368.33
2735	14-2Cyano-2-C4H8	C6H6N2	546.16	457.73	390.21
1777	Adiponitrile	C6H8N2	539.12	453.76	388.34

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Silanes

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
3985	Dimethyl Silane	C2H8Si	241.15	201.31	171.09
3984	Methyl Silane	CH6Si	208.20	173.32	146.86
3986	Trimethyl Silane	C3H10Si	270.57	226.71	193.34
1984	TetraMth Silane	C4H12Si	296.78	249.58	213.58
2994	TETRAETHYL Si	C8H20Si	407.07	344.16	296.09
1965	HexMthDisiloxane	C6H18OSi2	364.74	311.32	270.25
1966	6C1Cyc3Siloxane	C6H18O3Si3	383.45	331.79	291.70
1988	8C1Cyc4Siloxane	C8H24O4Si4	425.28	369.82	327.00
3991	DecaMethcyclpenS	C10H30O5Si5	459.05	400.65	355.83
3992	DodecaMethCyHexS	C12H36O6Si6	487.30	426.47	380.12

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Imines

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1767	N-MthPyrrolidine	C5H11N	339.28	284.62	242.80
2797	3-Methylpyridine	C6H7N	403.78	340.08	291.05
1797	2-Methylpyridine	C6H7N	403.78	340.08	291.05
2799	4-Methylpyridine	C6H7N	403.78	340.08	291.05
1753	N,N-DiEthAniline	C10H15N	465.41	397.60	344.91
1754	N-Methylpyrrole	C5H7N	329.10	276.82	236.66
3740	Acridine	C13H9N	568.14	494.93	436.88

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Tert-N

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1703	Trimethylamine	C3H9N	266.18	224.86	192.92
2856	DiMth Acetamide	C4H9NO	356.69	303.14	261.48
1706	Triethylamine	C6H15N	347.97	294.03	252.55
2716	Tributylamine	C12H27N	494.64	420.68	363.82
2719	Tripropylamine	C9H21N	426.95	361.96	311.97
3723	Triamylamine	C15H33N	553.68	472.27	409.70

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Nitrate

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1761	Nitroethane	C2H5NO2	373.07	318.00	274.80
1763	2-Nitropropane	C3H7NO2	384.64	325.69	279.97
1762	1-Nitropropane	C3H7NO2	401.01	341.81	295.47
1779	P-Nitrotoluene	C7H7NO2	487.98	409.01	348.64
1886	Nitrobenzene	C6H5NO2	458.44	383.04	325.54
1778	O-Nitrotoluene	C7H7NO2	487.98	409.01	348.64
1780	M-Nitrotoluene	C7H7NO2	487.98	409.01	348.64
1891	O-Nitroanisole	C7H7NO3	503.89	431.18	374.18
2740	M-Dinitrobenzene	C6H4N2O4	586.62	488.59	413.92
2742	P-Dinitrobenzene	C6H4N2O4	586.62	488.59	413.92
2741	O-Dinitrobenzene	C6H4N2O4	586.62	488.59	413.92
2749	3,5-DiNitToluene	C7H6N2O4	613.50	512.72	435.90

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

2743	DNT	C7H6N2O4	613.50	512.72	435.90
2745	3,4-DiNitToluene	C7H6N2O4	613.50	512.72	435.90
2744	2,6-DiNitToluene	C7H6N2O4	613.50	512.72	435.90
2748	2,5-DiNitToluene	C7H6N2O4	613.50	512.72	435.90
2746	1,3,5-TrinitroBz	C6H3N3O6	606.00	511.54	437.01
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	782.08	675.79	592.74
2747	Trinitrotoluene	C7H5N3O6	749.90	634.88	544.50

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Thiols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1802	Ethyl Mercaptan	C2H6S	295.31	246.74	209.66
1820	Dimethyl Sulfide	C2H6S	298.67	251.83	215.61
1843	Thiacyclopentane	C4H8S	366.25	309.45	265.47
1803	1-Propanethiol	C3H8S	330.82	276.61	235.29
1805	Isobut Mercaptan	C4H10S	349.82	292.14	248.32
6860	Ethylenedithiol	C2H6S2	392.99	326.39	275.90
1811	Cyclohexanethiol	C6H12S	432.74	362.52	308.99
1828	DiMth Disulfide	C2H6S2	392.99	326.39	275.90
1841	Butanethiol	C4H10S	363.81	304.55	259.36
1814	Methylproylsulf	C4H10S	363.81	304.55	259.36
2816	ETHYLtBUTYL SUL	C6H14S	385.18	326.13	280.55
1818	Diethyl Sulfide	C4H10S	352.07	298.50	256.93
1812	Benzyl Mercaptan	C7H8S	464.83	394.21	339.47
1838	T-OctylMercaptan	C8H18S	454.62	381.65	326.06
1827	1-Pentanethiol	C5H12S	394.56	330.74	282.04
2815	METHnBUTYL SULFD	C5H12S	392.34	331.37	284.34
1824	DiethylDisulfide	C4H10S2	417.02	355.53	307.55
1807	N-Hexylmercaptan	C6H14S	423.32	355.37	303.47
6857	Dimercaptoethyl	C4H10OS2	477.47	397.60	337.18
1839	1-Heptanethiol	C7H16S	450.31	378.60	323.78
1829	DiProp Disulfide	C6H14S2	465.15	396.99	343.93
1809	1-Octanethiol	C8H18S	475.73	400.57	343.07
1808	N-Nonanethiol	C9H20S	499.74	421.40	361.42
1826	1-Decanethiol	C10H22S	522.49	441.20	378.94
2838	tertDodecanThiol	C12H26S	547.45	462.43	397.45
1825	1-Undecanethiol	C11H24S	544.09	460.07	395.68
1837	Dodecylthiol	C12H26S	564.65	478.07	411.71

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Aldehydes

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1037	Methacrolein	C4H6O	325.21	273.20	233.50
1002	Acetaldehyde	C2H4O	265.87	225.23	193.87
1003	Propionaldehyde	C3H6O	301.35	254.68	218.74
1041	Benzaldehyde	C7H6O	437.30	373.01	322.73
1034	Acrolein	C3H4O	292.15	245.88	210.47
1005	N-Butyraldehyde	C4H8O	334.63	282.58	242.52
1036	Trans-2-Butenal	C4H6O	328.97	276.42	236.29
1007	Valeraldehyde	C5H10O	365.80	308.92	265.13
1006	Isobutyraldehyde	C4H8O	320.69	270.33	231.72
1009	1-Hexanal	C6H12O	395.04	333.80	286.63
1040	P-Tolualdehyde	C8H8O	463.81	396.28	343.46
1016	2-Methylhexanal	C7H14O	411.10	347.02	297.80
1017	3-Methylhexanal	C7H14O	411.10	347.02	297.80
1008	1-Heptanal	C7H14O	422.55	357.32	307.08
1013	2-Ethylhexanal	C8H16O	437.72	369.87	317.72
1010	1-Octanal	C8H16O	448.48	379.60	326.54
1011	1-Nonanal	C9H18O	473.00	400.76	345.09
1020	1-Decanal	C10H20O	496.24	420.88	362.81
1021	1-Undecanal	C11H22O	518.32	440.06	379.75
1025	Dodecanal	C12H24O	539.35	458.38	395.99
1026	1-Tridecanal	C13H26O	559.41	475.91	411.57
1014	1,2-Ethanedione	C2H2O2	320.86	273.07	236.05
1044	1,4BenzDicarboxAldehy	C8H6O2	512.17	441.84	386.25

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Epoxides

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1440	ISOBUTYLENE OXID	C4H8O	279.90	233.70	198.48
1479	Tetrahydrofuran	C4H8O	330.36	278.26	238.12
1477	2,5-Dihydrofuran	C4H6O	302.47	251.93	213.34
1408	1-Methoxypropane	C4H10O	310.26	263.90	227.74
1411	2-Methoxypropane	C4H10O	297.01	252.19	217.31
1421	1,4-Dioxane	C4H8O2	332.43	278.43	237.11
2422	1,3-DIOXANE	C4H8O2	332.43	278.43	237.11
1426	2-Methoxybutane	C5H12O	326.93	277.66	239.39
1413	1-Methoxybutane	C5H12O	339.43	288.76	249.32
1461	Methoxybenzene	C7H8O	408.90	350.91	305.28
1448	1-Ethoxybutane	C6H14O	359.47	303.10	259.77
1429	1-MethoxyPentane	C6H14O	359.47	303.10	259.77
6885	Ethyl-3-Ethoxypr	C7H14O3	436.78	369.81	318.15

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Ether

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1401	Dimethyl Ether	C2H6O	246.77	210.14	181.38
1407	MethylEthylEther	C3H8O	262.44	220.82	188.78
1470	VinylMethylEther	C3H6O	270.32	228.79	196.52
1405	MTBE	C5H12O	315.43	267.63	230.56
1445	VinylEthyl Ether	C4H8O	288.68	241.46	205.44
1402	Diethyl Ether	C4H10O	296.87	249.87	213.73
1431	Methylal	C3H8O2	311.94	267.47	232.38
1428	T-But EthylEther	C6H14O	334.18	280.87	240.08
1427	TAME	C6H14O	344.23	292.22	251.93
1410	Mth Isobut Ether	C5H12O	326.93	277.66	239.39
1430	Eth-t-Pent-Ether	C7H16O	364.15	306.45	262.29
1403	DiisopropylEther	C6H14O	333.54	280.08	239.23
1415	Eth Propyl Ether	C5H12O	329.17	277.27	237.38
1455	Dimethyl Acetal	C4H10O2	318.33	267.74	228.90
1446	Dipropyl Ether	C6H14O	359.47	303.10	259.77
1447	Butyl VinylEther	C6H12O	355.64	298.13	254.24
1462	EthylPhenylEther	C8H10O	430.95	367.18	317.50
1406	Di-sec-But Ether	C8H18O	392.13	330.19	282.81
1432	Acetal	C6H14O2	366.73	308.47	263.86
1460	BenzylEthylEther	C9H12O	456.72	383.22	327.10
1050	Paraldehyde	C6H12O3	380.75	317.26	269.21
1404	Di-n-Butyl Ether	C8H18O	414.81	350.57	301.17
1420	Anethole	C10H12O	486.93	420.53	368.23
1456	DimethylCarbitol	C6H14O3	407.19	348.86	303.23
1463	Dibenzyl Ether	C14H14O	582.34	495.45	428.21
1425	Di-n-PentylEther	C10H22O	464.24	393.27	338.69
1458	Diethyl Carbitol	C8H18O3	451.73	381.56	327.68
1412	Dihexyl Ether	C12H26O	508.84	432.02	372.94
1454	Triglyme	C8H18O4	468.16	401.27	349.13
1459	Dibutyl Carbitol	C12H26O3	541.42	459.54	396.62
1424	Di-n-Octyl Ether	C16H34O	586.60	500.08	433.57
1457	Tetraglyme	C10H22O5	532.95	451.13	388.33
1418	Dinonyl Ether	C18H38O	620.90	530.28	460.66
2432	ETHYLAL	C5H12O2	349.83	294.52	252.05
2405	DIISOBUTYL ETHER	C8H18O	391.44	329.60	282.30
2456	Ethyl Glyme	C6H14O2	379.37	319.75	273.96
2417	ETHYLHEXYL ETHER	C8H18O	414.81	350.57	301.17
2415	ETHYLISOPROPETH	C5H12O	315.93	265.55	226.95

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Formate

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1301	Methyl Formate	C2H4O2	286.23	240.29	205.01
1311	Vinyl Formate	C3H4O2	313.97	262.06	222.52
1302	Ethyl Formate	C3H6O2	320.80	269.44	230.04
2306	t-Butyl Formate	C5H10O2	358.31	300.55	256.45
1303	Propyl Formate	C4H8O2	353.04	296.79	253.65
2305	sec-ButylFormate	C5H10O2	370.43	311.11	265.73
2311	CYCLOHEXL FORMAT	C7H12O2	443.16	372.06	317.73
1304	N-Butyl Formate	C5H10O2	383.20	322.51	275.94
1305	Isobutyl Formate	C5H10O2	370.43	311.11	265.73
2350	Benzyl Formate	C8H8O2	476.89	406.00	350.88
2307	n-Hexyl Formate	C7H14O2	438.12	369.65	317.08
1306	N-Pentyl Formate	C6H12O2	411.49	346.74	297.05
2308	n-Heptyl Formate	C8H16O2	463.25	391.35	336.13
1308	N-Octyl Formate	C9H18O2	487.04	411.97	354.29
1309	n-Nonyl Formate	C10H20O2	509.61	431.59	371.64
1310	n-Decyl Formate	C11H22O2	531.09	450.31	388.24

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Ester

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1351	Mth Methacrylate	C5H8O2	364.13	310.49	268.55
1312	Methyl Acetate	C3H6O2	314.78	269.73	234.14
1331	Vinyl Propionate	C5H8O2	363.27	304.51	259.58
1321	Vinyl Acetate	C4H6O2	338.08	288.36	249.38
1352	Eth MthAcrylate	C6H10O2	391.78	328.66	280.41
1322	MethylPropionate	C4H8O2	343.10	293.85	255.08
1341	Methyl Acrylate	C4H6O2	327.69	275.27	235.03
1313	Ethyl Acetate	C4H8O2	335.68	282.83	242.09
1319	IsopropylAcetate	C5H10O2	358.74	306.76	266.02
1332	Methyl Butyrate	C5H10O2	366.73	309.22	264.91
1342	Ethyl Acrylate	C5H8O2	359.78	302.49	258.52
1318	Allyl Acetate	C5H8O2	366.32	312.45	270.30
1314	N-Propyl Acetate	C5H10O2	369.88	316.74	275.02
1323	Ethyl Propionate	C5H10O2	366.73	309.22	264.91
1360	I-But I-Butyrate	C8H16O2	422.90	361.49	313.67
1320	Sec-ButylAcetate	C6H12O2	384.68	329.00	285.44
1336	PropylI-Butyrate	C7H14O2	407.16	344.25	295.79
1353	N-C3-Mthacrylate	C7H12O2	419.00	351.42	299.80
1333	Ethyl Butyrate	C6H12O2	395.82	334.06	286.49

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1347	EthylIsovalerate	C7H14O2	411.75	347.23	297.66
1315	N-Butyl Acetate	C6H12O2	395.25	338.51	294.04
1390	Methyl Benzoate	C8H8O2	454.90	392.38	343.01
1388	ISOBUTYL MTHACR	C8H14O2	431.17	363.01	310.82
1343	1-PropylAcrylate	C6H10O2	394.19	330.82	282.34
1316	Isobutyl Acetate	C6H12O2	384.68	329.00	285.44
1344	N-Butyl Acrylate	C7H12O2	430.31	361.36	308.58
1357	Pentyl Acetate	C7H14O2	419.36	359.25	312.23
1327	N-PropN-Butyrate	C7H14O2	423.16	357.52	306.95
1324	N-PropPropionate	C6H12O2	395.82	334.06	286.49
1291	Acetic Anhydride	C4H6O3	392.53	337.63	294.17
1389	N-ButMthacrylate	C8H14O2	442.30	373.08	319.93
1359	Benzyl Acetate	C9H10O2	478.03	407.70	352.90
1326	N-But Propionate	C7H14O2	423.16	357.52	306.95
1391	Ethyl Benzoate	C9H10O2	480.55	410.73	356.24
1897	CH3OC3H600CH3	C6H12O3	406.23	349.61	305.05
1392	DiethylCarbonate	C5H10O3	387.10	326.22	279.37
1385	N-But N-Butyrate	C8H16O2	448.93	379.72	326.40
1317	IsopentylAcetate	C7H14O2	409.31	350.18	304.00
1363	N-Hexyl Acetate	C8H16O2	443.61	376.10	323.99
1387	Ethylene Acetate	C6H10O4	438.32	379.36	332.68
1393	Diethyl Oxalate	C6H10O4	450.72	380.58	326.50
1365	Butyl Benzoate	C11H14O2	523.17	447.67	388.86
1361	I-C5 I-Valerate	C10H20O2	477.01	403.10	346.38
1367	Heptyl Acetate	C9H18O2	467.52	396.77	342.18
1346	N-Butyl Valerate	C9H18O2	473.31	400.79	344.92
1358	2-C2-C6 Acetate	C10H20O2	476.44	408.20	355.11
1394	Diethyl Malonate	C7H12O4	470.15	398.38	342.91
1292	Propionyl Oxide	C6H10O3	442.49	376.69	325.42
1364	Benzyl Benzoate	C14H12O2	603.44	514.67	445.79
1381	2Mth p-Phthalate	C10H10O4	530.57	464.06	411.14
1368	n-Octyl Acetate	C10H20O2	490.23	416.47	359.56
1377	DiMthI-Phthalate	C10H10O4	542.75	468.99	410.93
1896	Ethylene DiAcr	C8H10O4	493.96	415.97	356.18
1386	2-Ethylhexyl Acr	C11H20O2	506.21	428.06	368.11
1395	Methyl Decanoate	C11H22O2	518.38	439.93	379.50
1369	n-Nonyl Acetate	C11H22O2	511.86	435.27	376.20
1370	n-Decyl Acetate	C12H24O2	532.49	453.26	392.16
1345	N-ButylNonanoate	C13H26O2	559.27	475.64	411.23
1375	DiProp Phthalate	C14H18O4	610.69	528.18	463.64
1376	Diisobutyl Phtha	C16H22O4	629.32	543.78	477.14
1396	IsopropMyristate	C17H34O2	616.54	526.61	457.44
1383	Butyl Stearate	C22H44O2	706.74	605.79	528.25
1362	Methyl Oleate	C19H36O2	671.98	572.97	496.96
1355	Diisooctyl Phtha	C24H38O4	736.42	638.21	562.27
1382	DioctylTerephtha	C24H38O4	745.62	646.94	570.58

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1384	DIBUTYL SEBACATE	C18H34O4	687.30	587.48	510.62
1371	Diisodecyl Phtha	C28H46O4	781.59	678.27	598.68
1354	DioctylPhthalate	C24H38O4	736.42	638.21	562.27
2375	DiethylPhthalate	C12H14O4	590.05	508.84	445.16
2388	Dipropyl Maleate	C10H16O4	536.15	454.75	392.01
2381	Diallyl Maleate	C10H12O4	568.37	474.74	403.72
2370	Glyceryl Triacet	C9H14O6	519.85	452.77	399.73
2382	Dibutyl Maleate	C12H20O4	576.69	490.19	423.53
2376	DibutylPhthalate	C16H22O4	641.15	554.86	487.52
2353	CetylMthacrylate	C20H38O2	676.59	578.21	502.67
2379	Dihexyl Adipate	C18H34O4	687.30	587.48	510.62
2321	T-Butyl Acetate	C6H12O2	368.41	310.81	266.52
2332	Methl.I-butyrate	C5H10O2	350.64	295.86	253.66
2354	AllylMthacrylate	C7H10O2	415.30	347.85	296.45
2364	CYCLOHEXL ACETAT	C8H14O2	448.37	378.50	324.75
2337	EthylIsobutyrate	C6H12O2	379.75	320.74	275.28
2384	IsobutylAcrylate	C7H12O2	406.12	341.56	292.14
2380	1,1-Diacetoxy C2	C6H10O4	429.22	363.59	312.86
2392	n-PropylBenzoate	C10H12O2	502.37	429.61	372.89
2377	DiMth Phthalate	C10H10O4	530.57	464.06	411.14
2386	Diethyl Maleate	C8H12O4	491.39	415.85	357.63
2385	Mth Dodecanoate	C13H26O2	559.27	475.64	411.23
3379	Dioctyl Adipate	C22H42O4	710.40	609.09	531.35
5886	Mth Acetoacetate	C5H8O3	421.40	357.47	307.79
5884	Ethoxy Acetate	C6H12O3	412.13	352.78	306.33
5887	EthAcetoAcetate	C6H10O3	447.68	380.01	327.46
5885	Carbitol Acetate	C8H16O4	474.08	405.98	352.88

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Ketone

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1096	Methyl Isopropen	C5H8O	361.59	304.94	261.24
1079	Cyclopentanone	C5H8O	378.39	320.91	276.16
1051	Acetone	C3H6O	305.99	259.43	223.14
1052	MEK	C4H8O	337.71	286.30	246.32
1065	Mesityl Oxide	C6H10O	383.06	325.34	280.49
1066	T-But Mth Ketone	C6H12O	372.72	315.38	271.07
1060	2-Pentanone	C5H10O	367.43	311.60	268.25
1061	Mth iC3 Ketone	C5H10O	355.08	300.57	258.34
1053	Diethyl Ketone	C5H10O	364.41	310.01	267.60
1059	3-Hexanone	C6H12O	391.68	333.34	287.93

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1099	Diketene	C4H4O2	342.26	285.46	241.92
1055	Sec-ButMthKetone	C6H12O	383.76	325.07	279.64
1054	MIBK	C6H12O	383.76	325.07	279.64
1095	EthIsopropKetone	C6H12O	380.32	323.15	278.73
1063	2-Heptanone	C7H14O	421.71	358.10	308.79
1064	5-Mth-2-Hexanone	C7H14O	410.77	348.24	299.86
1058	4-Heptanone	C7H14O	417.45	355.48	307.28
1057	3-Heptanone	C7H14O	417.45	355.48	307.28
1076	2,4-Pentanedione	C5H8O2	419.57	357.74	309.35
1068	DiisobutylKetone	C9H18O	445.53	378.82	327.21
1097	2-CycC6 CycC6one	C12H20O	544.62	462.30	398.74
1083	2-Octanone	C8H16O	446.62	379.56	327.60
1073	Dibutyl Ketone	C9H18O	465.07	396.57	343.38
1062	2-Hexanone	C6H12O	395.36	335.49	289.03
1077	Isophorone	C9H14O	452.11	383.64	330.66
1090	Acetophenone	C8H8O	459.76	393.70	341.87
1080	Cyclohexanone	C6H10O	406.76	345.11	297.18
1074	2-Nonanone	C9H18O	470.24	399.97	345.56

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Alcohol-Ethers

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
2862	2-Butoxyethanol	C6H14O2	433.46	374.23	328.75
4857	butyl carbitol	C8H18O3	495.15	425.06	371.68
2898	2-Chloroethanol	C2H5ClO	373.07	325.10	286.91
2864	Carbitol	C6H14O3	449.95	387.66	339.98
3854	Methyl propasol	C4H10O2	380.79	332.20	294.13
2860	2-Methoxyethanol	C3H8O2	366.52	320.88	284.74
2854	DiacetoneAlcohol	C6H12O2	439.65	380.54	335.01
2861	2-Ethoxyethanol	C4H10O2	385.02	334.63	295.14
2889	HydroxyAcetone	C3H6O2	386.58	337.76	299.21
3856	1tButoxy2Propnol	C7H16O2	427.98	368.81	323.58
3858	PROPGLYC2tBUTYL	C7H16O2	428.55	369.27	323.98
4855	2-Propoxyethanol	C5H12O2	409.55	354.67	312.18
4849	Acetovanillone	C9H10O3	550.95	484.99	432.41
5883	Ethyl Lactate	C5H10O3	429.86	371.32	326.12
6883	2-HydroxyEth Acr	C5H8O3	435.03	375.48	329.53
2863	Methyl Carbitol	C5H12O3	426.22	368.21	323.52
3855	Dowanol DPM	C7H16O3	473.94	409.26	359.61
3857	TriPropGlymEthlE	C10H22O4	549.08	472.59	413.80

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
404	DiMth-Acetylene	C4H6	278.42	237.38	205.23
202	Propylene	C3H6	227.76	190.72	162.31
412	2-Pentyne	C5H8	363.13	309.70	268.11
207	2-Methylpropene	C4H8	262.50	219.67	186.95
204	1-Butene	C4H8	265.59	222.35	189.30
205	Cis-2-Butene	C4H8	266.60	223.17	189.98
402	Propyne	C3H4	237.05	198.46	168.94
406	3-Hexyne	C6H10	336.36	286.76	248.09
206	Trans-2-Butene	C4H8	266.60	223.17	189.98
407	2-Hexyne	C6H10	336.36	286.76	248.09
231	33-2Mth-1-Butene	C6H12	326.57	275.76	236.60
230	23-2Mth-1-Butene	C6H12	326.57	275.76	236.60
229	2-Ethyl-1-Butene	C6H12	331.62	278.01	237.08
8	I-Pentane	C5H12	293.92	247.21	211.37
14	2,2-DiMth-Butane	C6H14	313.43	263.55	225.36
232	23-2Mth-2-Butene	C6H12	333.70	281.27	240.95
213	3-Mth-1-Butene	C5H10	285.57	238.67	202.97
212	2-Mth-1-Butene	C5H10	298.23	249.74	212.73
211	Trans-2-Pentene	C5H10	302.12	253.08	215.63
210	Cis-2-Pentene	C5H10	302.12	253.08	215.63
223	4-Mth-1-Pentene	C6H12	319.88	267.66	227.90
221	2-Mth-1-Pentene	C6H12	331.62	278.01	237.08
248	2-t-Butylpropene	C7H14	336.63	281.60	239.77
227	Cs-4-Mth-2-C5H10	C6H12	320.89	268.49	228.60
224	2-Mth-2-Pentene	C6H12	326.57	275.76	236.60
403	1-Butyne	C4H6	273.92	229.38	195.36
15	2,3-DiMth-Butane	C6H14	311.86	261.99	223.86
214	2-Mth-2-Butene	C5H10	295.21	249.11	213.56
228	Ts-4-Mth-2-C5H10	C6H12	320.89	268.49	228.60
225	Cs-3-Mth-2-C5H10	C6H12	326.57	275.76	236.60
218	Trans-2-Hexene	C6H12	335.30	281.19	239.86
2226	3-METH-Tr-2Pente	C6H12	326.57	275.76	236.60
222	3-Mth-1-Pentene	C6H12	319.88	267.66	227.90
257	2-Diisobutylene	C8H16	360.56	304.17	260.91
256	1-Diisobutylene	C8H16	367.52	307.93	262.60
217	Cis-2-Hexene	C6H12	335.30	281.19	239.86
2414	1-Heptyne	C7H12	371.21	311.93	266.62
13	3-Methylpentane	C6H14	325.92	274.38	234.85
219	Cis-3-Hexene	C6H12	326.57	275.76	236.60
12	2-Methylpentane	C6H14	325.92	274.38	234.85
220	Trans-3-Hexene	C6H12	326.57	275.76	236.60
405	1-Pentyne	C5H8	308.53	258.59	220.46
209	1-Pentene	C5H10	301.12	252.26	214.95
11	N-Hexane	C6H14	339.41	286.32	245.48

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

235	Cis-2-Heptene	C7H14	366.32	307.61	262.73
249	Cis-3-Heptene	C7H14	366.32	307.61	262.73
216	1-Hexene	C6H12	334.30	280.37	239.17
239	3-Eth-1-Pentene	C7H14	351.93	294.90	251.45
226	4-Mth-1-Hexene	C7H14	351.93	294.90	251.45
240	3-Mth-1-Hexene	C7H14	351.93	294.90	251.45
419	3-Mth-1-Butyne	C5H8	293.33	245.27	208.71
233	2-Eth-1-Pentene	C7H14	362.83	304.58	260.08
238	2-Mth-1-Hexene	C7H14	362.83	304.58	260.08
416	1-Octyne	C8H14	399.68	336.33	287.87
289	2,3Dimeth Hexene	C8H16	379.50	318.37	271.77
234	1-Heptene	C7H14	365.34	306.80	262.06
413	1-Hexyne	C6H10	340.90	286.07	244.18
237	Trans-3-Heptene	C7H14	366.32	307.61	262.73
236	Trans-2-Heptene	C7H14	366.32	307.61	262.73
251	Trans-2-Octene	C8H16	395.40	332.49	284.38
279	Trans-4-Octene	C8H16	395.40	332.49	284.38
277	Trans-3-Octene	C8H16	395.40	332.49	284.38
2252	2Methl-1-Heptene	C8H16	392.09	329.61	281.84
250	1-Octene	C8H16	394.43	331.69	283.71
258	2-Ethyl-1-Hexene	C8H16	392.09	329.61	281.84
280	3-Octene	C8H16	395.40	332.49	284.38
278	4-Octene	C8H16	395.40	332.49	284.38
276	2-Octene	C8H16	395.40	332.49	284.38
259	1-Nonene	C9H18	421.79	355.21	304.25
262	1-Dodecene	C12H24	495.12	418.69	360.10
263	1-Tridecene	C13H26	517.11	437.84	377.07
264	1-Tetradecene	C14H28	538.06	456.14	393.32
265	1-Pentadecene	C15H30	558.06	473.65	408.91
266	1-Hexadecene	C16H32	577.18	490.43	423.90
267	1-Octadecene	C18H36	613.08	522.04	452.21
281	1-Heptadecene	C17H34	595.50	506.55	438.32
284	1-Eicosene	C20H40	646.23	551.33	478.57
283	1-Nonadecene	C19H38	629.97	536.96	465.62
3	Propane	C3H8	240.26	202.44	173.23
4	I-Butane	C4H10	259.90	218.48	186.67
9	Neopentane	C5H12	280.75	235.85	201.46
5	N-Butane	C4H10	275.31	231.93	198.51
7	pentane	C5H12	308.36	259.91	222.61
44	Hexamethylethane	C8H18	348.51	292.87	250.42
25	223-TriMthButane	C7H16	330.61	277.76	237.40
24	3,3-DiMthPentane	C7H16	344.14	289.72	248.04
51	2,2,3,3-4Mth-C5	C9H20	377.16	317.42	271.80
21	2,2-DiMthPentane	C7H16	344.14	289.72	248.04
42	2,3,3-TriMth-C5	C8H18	360.39	303.20	259.50
22	2,3-DiMthPentane	C7H16	342.85	288.39	246.72

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

40	2,2,3-TriMth-C5	C8H18	360.39	303.20	259.50
23	2,4-DiMthPentane	C7H16	342.85	288.39	246.72
41	2,2,4-TriMth-C5	C8H18	360.39	303.20	259.50
39	3-Mth-3-Eth-C5	C8H18	373.05	314.46	269.56
20	3-Ethylpentane	C7H16	355.99	300.04	257.11
52	2,2,3,4-4Mth-C5	C9H20	376.12	316.29	270.65
54	2334TetrMethPent	C9H20	376.12	316.29	270.65
53	2,2,4,4-4Mth-C5	C9H20	377.16	317.42	271.80
43	2,3,4-TriMth-C5	C8H18	359.22	301.97	258.26
36	3,3-DiMth-Hexane	C8H18	373.05	314.46	269.56
19	3-Methylhexane	C7H16	355.99	300.04	257.11
18	2-Methylhexane	C7H16	355.99	300.04	257.11
38	2-Mth-3-Eth-C5	C8H18	372.00	313.32	268.40
190	2,2-2C1-3-C2-C5	C9H20	388.43	327.26	280.48
32	2,2-DiMth-Hexane	C8H18	373.05	314.46	269.56
37	3,4-DiMth-Hexane	C8H18	372.00	313.32	268.40
50	3,3-DiEthPentane	C9H20	400.30	337.87	290.01
34	2,4-DiMth-Hexane	C8H18	372.00	313.32	268.40
33	2,3-DiMth-Hexane	C8H18	372.00	313.32	268.40
17	N-Heptane	C7H16	368.62	311.28	267.16
49	244TriMethHexane	C9H20	388.43	327.26	280.48
192	2,4-2C1-3-C2-C5	C9H20	387.49	326.21	279.39
47	2,2,5-TriMth-C6	C9H20	388.43	327.26	280.48
35	2,5-DiMth-Hexane	C8H18	372.00	313.32	268.40
31	3-Ethylhexane	C8H18	384.29	324.28	278.23
30	4-Methylheptane	C8H18	384.29	324.28	278.23
29	3-Methylheptane	C8H18	384.29	324.28	278.23
28	2-Methylheptane	C8H18	384.29	324.28	278.23
96	2,2-DiMthHeptane	C9H20	400.30	337.87	290.01
176	2,6-DiMthHeptane	C9H20	399.46	336.90	289.00
27	N-Octane	C8H18	396.14	334.89	287.76
94	3-Ethylheptane	C9H20	411.00	347.25	298.32
92	3-Methyloctane	C9H20	411.00	347.25	298.32
93	4-Methyloctane	C9H20	411.00	347.25	298.32
91	2-Methyloctane	C9H20	411.00	347.25	298.32
72	2,2-DiMthOctane	C10H22	426.05	360.07	309.48
2095	2,3Dimethloctane	C10H22	425.40	359.26	308.59
2096	2,4Dimethloctane	C10H22	425.40	359.26	308.59
2098	2,6DimethlOctane	C10H22	425.40	359.26	308.59
2097	2,5Dimethloctane	C10H22	425.40	359.26	308.59
2099	2,7DimethlOctane	C10H22	425.40	359.26	308.59
46	N-Nonane	C9H20	422.14	357.27	307.37
88	5-Methylnonane	C10H22	436.26	369.05	317.45
85	3-Methylnonane	C10H22	436.26	369.05	317.45
87	4-Methylnonane	C10H22	436.26	369.05	317.45
86	2-Methylnonane	C10H22	436.26	369.05	317.45

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

56	N-Decane	C10H22	446.76	378.54	326.05
63	N-Undecane	C11H24	470.14	398.80	343.90
64	N-Dodecane	C12H26	492.38	418.12	360.99
65	N-Tridecane	C13H28	513.59	436.59	377.36
66	N-Tetradecane	C14H30	533.86	454.28	393.08
67	N-Pentadecane	C15H32	553.25	471.25	408.19
68	N-Hexadecane	C16H34	571.83	487.54	422.74
69	N-Heptadecane	C17H36	589.68	503.22	436.76
70	N-Octadecane	C18H38	606.84	518.32	450.30
71	N-Nonadecane	C19H40	623.36	532.88	463.37
73	N-Eicosane	C20H42	639.28	546.94	476.02
74	n-HENEICOSANE	C21H44	654.65	560.53	488.27
75	n-DOCOSANE	C22H46	669.49	573.68	500.14
76	n-TRICOSANE	C23H48	683.85	586.41	511.65
77	n-Tetracosane	C24H50	697.75	598.75	522.82
78	n-PENTACOSANE	C25H52	711.22	610.72	533.68
79	n-HEXACOSANE	C26H54	724.28	622.34	544.23
81	n-Octacosane	C28H58	749.27	644.61	564.49
2081	n-TRICONTANE	C30H62	772.88	665.69	583.72
2082	n-Dotriacontane	C32H66	795.24	685.69	602.00
2086	Hexatriacontane	C36H74	836.71	722.86	636.08

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Cyclic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
269	Cyclopentene	C5H8	315.64	263.29	223.40
270	Cyclohexene	C6H10	350.66	292.78	248.74
287	3MthCyclopentene	C6H10	333.96	278.48	236.35
286	1-MthCyclPentene	C6H10	340.39	286.28	244.73
288	4MthCyclopenten	C6H10	333.96	278.48	236.35
273	Cycloheptene	C7H12	383.11	320.29	272.49
274	Cyclooctene	C8H14	413.31	346.06	294.83
101	Cyclopropane	C3H6	248.95	208.97	178.15
810	ADAMANTANE	C10H16	450.40	375.54	318.86
102	Cyclobutane	C4H8	286.49	240.39	204.99
104	Cyclopentane	C5H10	321.41	269.81	230.24
137	Cyclohexane	C6H12	353.91	297.37	254.01
105	MthCyclopentane	C6H12	338.29	283.93	242.32
146	Cs-1,4-2C1-CycC6	C8H16	383.89	322.69	275.87
142	Cs-1,2-2C1-CycC6	C8H16	383.89	322.69	275.87
141	1,1-2C1-CycC6	C8H16	389.89	327.22	279.38

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

145	Ts-1,3-2C1-CycC6	C8H16	383.89	322.69	275.87
144	Cs-1,3-2C1-CycC6	C8H16	383.89	322.69	275.87
147	Ts-1,4-2C1-CycC6	C8H16	383.89	322.69	275.87
143	Ts-1,2-2C1-CycC6	C8H16	383.89	322.69	275.87
138	MthCyclohexane	C7H14	369.36	310.37	265.21
159	Cycloheptane	C7H14	384.26	323.23	276.43
140	Ethylcyclohexane	C8H16	398.44	335.25	286.85
154	Trans-Decalin	C10H18	457.79	384.30	328.21
149	N-PropylCyc-C6	C9H18	425.75	358.73	307.35
109	Cs-1,2-2C1-CycC5	C7H14	354.12	297.25	253.78
110	Ts-1,2-2C1-CycC5	C7H14	354.12	297.25	253.78
112	Ts-1,3-2C1-CycC5	C7H14	354.12	297.25	253.78
107	Eth-Cyclopentane	C7H14	369.36	310.37	265.21
114	N-PropCycPentane	C8H16	398.44	335.25	286.85
108	1,1-DiMthCycC5	C7H14	359.88	301.59	257.13
111	Cs-1,3-2C1-CycC5	C7H14	354.12	297.25	253.78
152	N-ButylCycHexane	C10H20	451.48	380.93	326.83
160	Cyclooctane	C8H16	412.69	347.58	297.63
153	Cis-Decalin	C10H18	457.79	384.30	328.21
115	Isopropylcyclopentane	C8H16	383.89	322.69	275.87
150	Isopropyl-CycC6	C9H18	411.83	346.67	296.80
116	1-C1-1-C2-CycC5	C8H16	383.89	322.69	275.87
122	Butylcyclpentane	C9H18	425.75	358.73	307.35
155	1,1-Bicyclohexyl	C12H22	507.37	427.26	366.01
158	N-Decylcyclo-C6	C16H32	580.43	493.39	426.55

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Aromatic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
307	1,4-Pentadiene	C5H8	292.83	243.70	206.47
306	1-ts3-Pentadiene	C5H8	293.89	244.57	207.19
414	2-Methyl-1-Butenyne	C5H6	297.91	247.93	210.11
305	Cs1,3-Pentadiene	C5H8	293.89	244.57	207.19
309	Isoprene	C5H8	289.70	240.99	204.09
421	1-Pentene-4-yne	C5H6	300.96	250.58	212.44
303	1,3-Butadiene	C4H6	254.31	211.48	178.92
332	1,4-CyclHexadien	C6H8	346.90	287.77	242.92
501	Benzene	C6H6	333.45	279.55	238.29
315	Cyclopentadiene	C5H6	309.09	255.97	215.46
319	Diisopropenyl	C6H10	322.80	268.74	227.83
615	Ethynylbezene	C8H6	417.32	354.29	305.37

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

601	Styrene	C8H8	412.19	349.82	301.40
331	1,3-CycHexadiene	C6H8	346.90	287.77	242.92
310	1,5-Hexadiene	C6H10	328.60	273.81	232.30
312	MthCycPentadiene	C6H8	336.32	281.07	238.98
420	1-Pentene-3-yne	C5H6	301.06	255.42	219.95
502	Toluene	C7H8	369.30	310.54	265.45
521	T-Butylbenzene	C10H14	442.36	376.66	325.68
320	Dipropylene	C6H10	330.71	275.54	233.74
520	Sec-Butylbenzene	C10H14	436.46	368.78	316.73
313	1,4-Hexadiene	C6H10	329.65	274.67	233.02
314	Dipropylene	C6H10	330.71	275.54	233.74
316	DiCycPentadiene	C10H12	451.97	371.43	310.81
333	1,5-CycOctadiene	C8H12	414.22	344.61	292.00
701	Naphthalene	C10H8	477.70	410.61	357.83
504	Ethylbenzene	C8H10	408.06	342.00	291.57
820	Indan	C9H10	472.55	393.90	334.21
505	O-Xylene	C8H10	401.67	338.78	290.38
612	P-Methylstyrene	C9H10	440.09	374.34	323.24
330	DIISOCROTYL	C8H14	371.78	314.79	270.84
507	P-Xylene	C8H10	401.67	338.78	290.38
329	DIISOBUTENYL	C8H14	387.79	323.91	275.47
506	M-Xylene	C8H10	401.67	338.78	290.38
603	Methylstyrene	C9H10	440.09	374.34	323.24
613	Alpha-MthStyrene	C9H10	436.11	370.28	319.23
510	Isopropylbenzene	C9H12	410.13	346.12	296.90
724	2-Methylindene	C10H10	487.29	414.30	357.55
285	Vinylcyclohexene	C8H12	396.84	329.77	279.16
803	Indene	C9H8	459.74	395.25	344.42
706	Tetralin	C10H12	500.27	417.64	354.90
511	O-Ethyltoluene	C9H12	438.74	368.96	315.50
723	1-Methylindene	C10H10	452.41	376.07	318.43
738	Fluorene	C13H10	563.52	487.08	426.78
619	Tr-1PropenylBz	C9H10	439.01	372.83	321.49
525	O-Diethylbenzene	C10H14	476.45	399.56	340.92
618	Propenyl Bz(cis)	C9H10	439.01	372.83	321.49
602	O-Methylstyrene	C9H10	440.09	374.34	323.24
702	1-MthNaphthalene	C11H10	500.18	430.48	375.68
509	N-Propylbenzene	C9H12	436.65	366.49	312.88
526	M-Diethylbenzene	C10H14	476.45	399.56	340.92
583	Cs-2-PhnButene-2	C10H12	450.29	384.54	333.31
543	M-DiisopropylBz	C12H18	470.81	399.74	344.94
584	Ts-2-PhnButene-2	C10H12	450.29	384.54	333.31
580	1,2-DiC1-3C2-Bz	C10H14	466.67	393.68	337.61
704	1-EthNaphthalene	C12H12	529.69	454.92	396.34
512	M-Ethyltoluene	C9H12	438.74	368.96	315.50
522	1-Mth-2-iC3-Benz	C10H14	438.55	371.15	319.22

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

513	P-Ethyltoluene	C9H12	438.74	368.96	315.50
514	1,2,3-Mesitylene	C9H12	431.16	364.69	313.41
614	M-Divinylbenzene	C10H10	472.87	404.95	351.80
524	1-Mth-4-iC3-Benz	C10H14	438.55	371.15	319.22
822	Gamma-Terpinene	C10H16	427.32	361.00	310.04
821	Alpha-Terpinene	C10H16	427.32	361.00	310.04
523	1-Mth-3-iC3-Benz	C10H14	438.55	371.15	319.22
703	2-MthNaphthalene	C11H10	500.18	430.48	375.68
557	CycHexylBenzene	C12H16	504.98	426.18	365.68
515	1,2,4-Mesitylene	C9H12	431.16	364.69	313.41
519	Isobutylbenzene	C10H14	452.42	379.52	323.94
424	DiPhnAcetylene	C14H10	539.01	466.31	409.18
544	P-DiisopropylBz	C12H18	470.81	399.74	344.94
518	N-Butylbenzene	C10H14	463.46	389.56	333.06
516	1,3,5-Mesitylene	C9H12	431.16	364.69	313.41
809	Acenaphthalene	C12H8	537.27	467.29	411.59
725	123-TriMthIndene	C12H14	507.66	434.45	377.36
527	1,4-DiEthBenzene	C10H14	476.45	399.56	340.92
558	Diphenyl	C12H10	515.69	443.34	386.59
576	2-Ethyl-m-Xylene	C10H14	466.67	393.68	337.61
620	p-ISOPROPENYLSTY	C11H12	492.95	422.23	366.99
585	o-PropylToluene	C10H14	465.08	391.65	335.36
577	2-Ethyl-p-Xylene	C10H14	466.67	393.68	337.61
579	4-Ethyl-o-Xylene	C10H14	466.67	393.68	337.61
586	m-Propyltoluene	C10H14	465.08	391.65	335.36
587	p-Propyltoluene	C10H14	465.08	391.65	335.36
578	4-Ethyl-m-Xylene	C10H14	466.67	393.68	337.61
575	5-Ethyl-m-Xylene	C10H14	466.67	393.68	337.61
530	Prehnitene	C10H14	458.22	388.60	334.79
709	2,6-2Mth-Naphtha	C12H12	521.23	449.16	392.52
715	2,7-2Mth-Naphtha	C12H12	521.23	449.16	392.52
719	2-ETHYLNAPHTHALENE	C12H12	521.23	449.16	392.52
621	p-tert-BUTYLSTY	C12H16	523.78	453.98	398.85
532	1,2,4,5-TetMthBz	C10H14	458.22	388.60	334.79
531	1,2,3,5-TetMthBz	C10H14	458.22	388.60	334.79
533	p-tert-BUTYL ET	C12H18	495.12	426.16	372.25
567	N-Pentylbenzene	C11H16	488.69	411.38	352.21
718	1-n-PROPYLNAPHTH	C13H14	541.77	469.58	412.67
562	1,1-DiPhnEthane	C14H14	539.52	460.83	399.71
616	4-ISOBUTYLSTYRE	C12H16	504.74	433.47	377.81
260	1-Decene	C10H20	447.59	377.47	323.77
735	Cis-Stilbene	C14H12	559.18	479.65	417.56
568	Hexylbenzene	C12H18	512.51	432.06	370.45
563	Diphenylmethane	C13H12	545.51	463.81	400.51
564	1,2-DiPhnEthane	C14H14	586.01	491.26	419.12
804	Anthracene	C14H10	569.24	495.74	437.47

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

736	Trans-Stilbene	C14H12	559.18	479.65	417.56
805	Phenanthrene	C14H10	569.24	495.74	437.47
713	1-ButNaphthalene	C14H16	567.89	488.13	425.80
807	Pyrene	C16H10	611.29	537.00	477.81
261	1-Undecene	C11H22	471.99	398.59	342.36
581	23-2C1-23-2PhnC4	C18H22	596.00	512.17	447.09
549	N-Heptylbenzene	C13H20	535.06	451.71	387.84
710	1-PhnNaphthalene	C16H12	598.42	521.01	459.88
566	2,4-Diphenyl-4-M	C18H20	613.85	526.81	459.24
561	O-Terphenyl	C18H14	625.99	544.96	481.17
569	N-Octylbenzene	C14H22	556.46	470.42	404.46
565	Triphenylmethane	C19H16	638.40	552.24	484.85
714	N-C6-Naphthalene	C16H20	603.03	518.81	453.15
717	Fluoranthene	C16H10	611.29	537.00	477.81
716	1-Hexyl-Tetralin	C16H24	588.69	507.14	443.58
731	TriPhnEthylene	C20H16	650.34	563.38	495.35
806	Chrysene	C18H12	636.39	558.75	497.14
588	1,1,2TriPhenEth	C20H18	653.32	565.33	496.57
711	1-n-NonylNaphtha	C19H26	650.97	560.87	490.82
570	N-Nonylbenzene	C15H24	576.84	488.28	420.37
712	1-Decyl Naphtha	C20H28	665.84	573.96	502.60
559	P-Terphenyl	C18H14	625.99	544.96	481.17
560	M-Terphenyl	C18H14	625.99	544.96	481.17
589	TetraPhenylMetha	C25H20	719.84	625.68	552.17
554	Decylbenzene	C16H26	596.26	505.36	435.63
732	TetraPhnEthylene	C26H20	740.95	644.63	569.44
574	N-Dodecylbenzene	C18H30	632.60	537.42	464.38
571	N-Undecylbenzene	C17H28	614.83	521.72	450.28
572	Tridecylbenzene	C19H32	649.65	552.50	477.96
573	n-TETRADECYLBENZ	C20H34	646.72	555.61	485.22
2575	n-PENTADECYLBENZ	C21H36	661.64	568.78	497.08
2576	n-HEXADECYLBENZ	C22H38	676.07	581.53	508.58
2577	n-HEPTADECYLBENZ	C23H40	690.04	593.89	519.75
2578	n-OCTADECYLBENZE	C24H42	703.57	605.88	530.59

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

Halocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1544	Allyl Chloride	C3H5Cl	305.91	255.74	217.39
1595	2-Chloropropene	C3H5Cl	280.35	235.52	201.09
1531	3-Chloropropyne	C3H3Cl	314.02	262.56	223.29

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1561	6Cl-1,3Butadiene	C4Cl6	466.22	399.96	348.03
1535	T-Butyl Chloride	C4H9Cl	305.81	258.22	221.50
1583	Chloroprene	C4H5Cl	346.77	291.04	248.24
1530	Isopropyl Cl	C3H7Cl	292.62	246.88	211.54
1572	O-DiCl-Benzene	C6H4Cl2	447.77	375.23	319.79
1585	Propyl Chloride	C3H7Cl	313.29	263.51	225.21
1684	Isopropyl Iodide	C3H7I	351.16	292.30	247.72
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	376.57	318.58	273.70
1651	2-Bromopropane	C3H7Br	312.85	263.09	224.84
1691	Iodobenzene	C6H5I	469.25	396.97	341.08
1860	Fluorobenzene	C6H5F	335.92	282.20	240.99
1571	Chlorobenzene	C6H5Cl	391.51	328.12	279.65
1680	Bromobenzene	C6H5Br	430.53	367.01	317.35
1526	1,2-DiCl-Propane	C3H6Cl2	362.28	305.38	261.51
1683	Propyl Iodide	C3H7I	365.64	305.09	259.09
1576	Benzotrichloride	C7H5Cl3	462.31	403.14	356.11
1536	2,3-DICHLOROBUT	C4H8Cl2	392.15	330.83	283.56
2638	2-Bromobutane	C4H9Br	345.15	290.48	248.48
1586	1-Chlorobutane	C4H9Cl	345.97	291.19	249.06
1573	M-DiCl-Benzene	C6H4Cl2	447.77	375.23	319.79
2634	Benzotrifluoride	C7H5F3	368.71	320.11	281.55
1574	P-DiCl-Benzene	C6H4Cl2	447.77	375.23	319.79
1650	1-Bromopropane	C3H7Br	327.01	275.60	235.96
1587	2-Chlorobutane	C4H9Cl	324.98	274.31	235.21
2653	8F-2-Butene	C4F8	388.88	329.59	283.64
1678	M-Dibromobenzene	C6H4Br2	501.71	432.48	377.77
1537	1,2-DiCl-Butane	C4H8Cl2	370.89	313.71	269.51
1597	34-DiCl-1-Butene	C4H6Cl2	390.28	327.37	279.23
1577	O-Chlorotoluene	C7H7Cl	423.90	356.40	304.63
1532	123-3Cl-Propane	C3H5Cl3	429.85	362.16	310.03
1578	P-Chlorotoluene	C7H7Cl	423.90	356.40	304.63
1562	Benzyl Chloride	C7H7Cl	446.75	380.44	328.72
2661	P-Bromotoluene	C7H7Br	457.12	390.39	338.20
1508	1,4-DiCl-Butane	C4H8Cl2	414.52	348.75	298.22
1655	1-Bromobutane	C4H9Br	358.35	302.23	258.97
1599	BenzylDichloride	C7H6Cl2	463.77	396.62	344.08
2652	Perfluoropropane	C3F8	256.28	226.57	202.50
1505	2-Butylene DiCl	C4H6Cl2	408.68	340.91	289.29
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	415.19	347.25	295.43
1588	1-Chloropentane	C5H11Cl	376.51	317.19	271.58
1592	1,2,4-TriCl-Bz	C6H3Cl3	502.57	421.16	358.97
1579	2,4-2Cl-Toluene	C7H6Cl2	476.87	400.92	342.69
2593	1,3,5-TriCl-BZ	C6H3Cl3	502.57	421.16	358.97
1697	1-Br-Naphthalene	C10H7Br	537.98	466.39	409.70
1622	Perfluorobutane	C4F10	262.78	233.30	209.46
1857	P-Cl-Benzo-TriF	C7H4ClF3	406.24	352.39	309.76

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

1509	1,5-DiCl-Pentane	C5H10Cl2	442.59	372.78	319.13
1589	1-Cl-Naphthalene	C10H7Cl	518.94	445.83	388.40
1582	6ClCycPentadiene	C5Cl6	503.92	429.08	370.84
1864	Perfluorobenzene	C6F6	346.51	293.84	253.08
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	443.27	384.24	337.62
1667	1-Bromoheptane	C7H15Br	441.34	373.35	320.96
1575	HexaCl-Benzene	C6Cl6	660.01	553.32	471.84
2640	Freon 123B1	C2HBrClF3	319.80	276.47	242.11
1504	Vinyl Chloride	C2H3Cl	267.71	225.12	192.18
1672	1,1-DiBr-Ethane	C2H4Br2	364.50	306.74	262.29
1580	Acetylene DiCl	C2H2Cl2	322.00	271.12	231.81
1692	Diiodomethane	CH2I2	436.82	360.74	302.99
1698	Bromoform	CHBr3	414.70	349.24	298.78
2687	Freon 13B1	CBrF3	267.24	231.30	202.59
2690	Br-3F-Ethylene	C2BrF3	324.30	270.19	228.84
1649	Tetrabromoethane	C2H2Br4	506.91	427.13	365.73
2686	Freon 12B1	CBrClF2	272.49	234.54	204.48
1503	Ethyl Chloride	C2H5Cl	278.23	234.00	199.90
2641	Br-TriCl-Methane	CBrCl3	381.56	331.67	291.81
1641	Methyl Bromide	CH3Br	257.48	217.05	185.73
2688	Freon 12B2	CBr2F2	300.36	257.83	224.26
2545	2,3-DiCl-Propene	C3H4Cl2	357.59	300.35	256.35
1673	1,2-DiBr-Ethane	C2H4Br2	377.38	318.26	272.61
2637	Dibromomethane	CH2Br2	345.59	291.35	249.41
1542	TetraCl-Ethylene	C2Cl4	386.14	329.37	284.95
1541	TriCl-Ethylene	C2HCl3	338.76	288.55	249.29
1527	111-TriCl-Ethane	C2H3Cl3	346.70	301.40	265.19
1612	Cl-2F-Ethylene	C2HClF2	236.39	202.94	176.41
2639	Br-Cl-Methane	CH2BrCl	331.97	279.36	238.75
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	322.00	271.12	231.81
1682	Ethyl Iodide	C2H5I	331.33	276.15	234.20
1522	1,1-DiCl-Ethane	C2H4Cl2	310.90	262.98	225.81
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	236.70	200.07	171.69
1525	Hexachloroethane	C2Cl6	427.16	376.40	335.67
1528	1112-4Cl-Ethane	C2H2Cl4	394.97	342.91	301.44
1590	Penta-Cl-Ethane	C2HCl5	413.16	359.41	316.62
1529	1122-4Cl-Ethane	C2H2Cl4	401.83	341.40	294.35
2693	Perfluoroethane	C2F6	248.58	218.57	194.24
2692	Cl-PentaF-Ethane	C2ClF5	253.66	219.78	192.80
2655	122-3Cl-112-3FC2	C2Cl3F3	308.74	259.42	221.66
1609	12-2Cl-1122-4FC2	C2Cl2F4	265.30	224.85	193.51
2526	1,1-DiCl-Propane	C3H6Cl2	342.27	289.61	248.82
1645	Ethyl Bromide	C2H5Br	293.45	247.26	211.58
2658	1112-4Cl-22-2FC2	C2Cl4F2	364.60	317.01	279.16
1619	111-3F-Ethane	C2H3F3	229.75	199.20	174.70
1524	1,1,2-3Cl-Ethane	C2H3Cl3	378.86	320.17	274.73

Table C.4 Boiling Temperatures Calculated by the GC-SAFT method.(Continued)

2691	Genetron 1113	C2ClF3	284.30	237.60	201.87
1591	Vinylidene DiCl	C2H2Cl2	297.07	252.40	217.48
1614	Difluoromethane	CH2F2	184.95	161.20	141.65
2694	Vinyl Bromide	C2H3Br	284.70	238.45	202.96
1694	Refrigerant 123	C2HCl2F3	307.51	266.27	233.47
1523	1,2-DiCl-Ethane	C2H4Cl2	352.25	295.91	252.58
2656	1122-4Cl-12-2FC2	C2Cl4F2	359.64	299.58	254.12
2527	1,3-DiCl-Propane	C3H6Cl2	384.50	323.19	276.09

Table C. 5 Boiling Temperatures Calculated by the GC-ESD method.

Alcohols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1181	Phenol	C6H6O	435.12	383.20	341.28
1182	O-Cresol	C7H8O	455.83	401.36	357.51
1183	M-Cresol	C7H8O	455.83	401.36	357.51
1176	2,6-Xylenol	C8H10O	475.09	418.43	372.84
1111	2-Mth-2-Butanol	C5H12O	385.86	336.47	296.78
1178	3,5-Xylenol	C8H10O	475.09	418.43	372.84
1133	2-Octanol	C8H18O	458.65	399.07	352.10
2885	4-HYDROXYSTYREN	C8H8O	483.09	425.03	378.30
1197	P-t-Butylphenol	C10H14O	499.95	441.66	394.63
1172	2,4-Xylenol	C8H10O	475.09	418.43	372.84
1184	P-Cresol	C7H8O	455.83	401.36	357.51
1151	Cyclohexanol	C6H12O	430.94	374.57	329.73
1170	2,3-Xylenol	C8H10O	475.26	418.06	372.11
1187	P-Ethyl Phenol	C8H10O	475.26	418.06	372.11
2859	P-Methoxyphenol	C7H8O2	475.46	422.15	378.69
1121	2-Ethylhexanol	C8H18O	458.65	399.07	352.10
1179	PropargylAlcohol	C3H4O	360.31	314.06	276.37
1123	3-Mth-1-Butanol	C5H12O	394.19	343.87	303.50
2196	P-t-Amylphenol	C11H16O	515.23	455.20	406.77
1174	2,5-Xylenol	C8H10O	475.09	418.43	372.84
1115	2-Hexanol	C6H14O	416.70	363.09	320.42
1152	1-MthCycHexanol	C7H14O	445.33	386.54	340.05
4854	Guaiacol	C7H8O2	475.46	422.15	378.69
1107	Sec-Butanol	C4H10O	370.60	323.72	285.73
1167	Allyl Alcohol	C3H6O	352.39	307.58	270.87
1130	4-Mth-2-Pentanol	C6H14O	410.11	356.79	314.37
1177	3,4-Xylenol	C8H10O	475.09	418.43	372.84
1114	1-Hexanol	C6H14O	423.11	369.21	326.29
1106	Isobutanol	C4H10O	370.60	323.72	285.73
1125	1-Heptanol	C7H16O	444.09	387.19	342.11
1105	N-Butanol	C4H10O	378.03	330.74	292.45
1109	1-Pentanol	C5H12O	401.10	350.42	309.77
1132	1-Octanol	C8H18O	464.07	404.41	357.29
1113	T-Butylcarbinol	C5H12O	385.86	336.47	296.78
1137	1-Undecanol	C11H24O	518.26	451.85	399.41
1108	Tert-Butanol	C4H10O	361.94	316.01	278.70
1103	N-Propanol	C3H8O	353.82	310.06	274.20
1134	1-Nonanol	C9H20O	483.07	420.92	371.87
2195	P-t-Octylphenol	C14H22O	549.25	484.89	433.09
1102	Ethanol	C2H6O	328.30	288.15	254.82
1124	3-Mth-2-Butanol	C5H12O	387.07	337.12	297.02
1136	1-Decanol	C10H22O	501.12	436.72	385.90
1140	Dodecanol	C12H26O	534.53	466.34	412.41
1104	Isopropanol	C3H8O	345.83	302.50	266.95
1110	2-Pentanol	C5H12O	394.19	343.87	303.50

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1120	3-Pentanol	C5H12O	394.19	343.87	303.50
1112	2-Mth-1-Butanol	C5H12O	394.19	343.87	303.50
1154	Ts-2-Mth-CycC6OH	C7H14O	445.33	386.54	340.05
1153	Cs-2-Mth-CycC6OH	C7H14O	445.33	386.54	340.05
1156	Ts-3-Mth-CycC6OH	C7H14O	445.33	386.54	340.05
1157	Cs-4-Mth-CycC6OH	C7H14O	445.33	386.54	340.05
2197	P-Cumylphenol	C15H16O	579.33	514.23	461.26
1180	Benzyl Alcohol	C7H8O	459.51	402.25	356.46
1158	Ts-4-Mth-CycC6OH	C7H14O	445.33	386.54	340.05
1155	Cs-3-Mth-CycC6OH	C7H14O	445.33	386.54	340.05
1168	2-Phn-2-Propanol	C9H12O	486.75	424.82	375.66
1141	1-Tridecanol	C13H28O	549.99	480.20	424.92
1147	2-Eth-1-Butanol	C6H14O	416.70	363.09	320.42
1117	2-Mth-1-Pentanol	C6H14O	416.70	363.09	320.42
2115	2-Phenylethanol	C8H10O	481.69	417.59	367.00
1142	1-Tetradecanol	C14H30O	564.69	493.47	436.97
2118	1-PHN-1-PROPANOL	C9H12O	493.22	430.76	381.11
2119	1-PHN-2-PROPANOL	C9H12O	493.22	430.76	381.11
1126	2-Heptanol	C7H16O	438.19	381.47	336.59
1143	1-Pentadecanol	C15H32O	578.68	506.18	448.57
1129	Isoheptanol	C7H16O	438.19	381.47	336.59
2117	2,6-DiMth-4-C7OH	C9H20O	467.76	405.58	356.85
1144	1-Hexadecanol	C16H34O	592.01	518.35	459.74
1145	Heptadecanol	C17H36O	604.72	530.01	470.51
1199	Nonylphenol	C15H24O	581.62	512.76	457.35
1146	1-Octadecanol	C18H38O	616.85	541.20	480.88
1135	2-Nonanol	C9H20O	478.12	415.94	366.99
1149	1-Nonadecanol	C19H40O	628.44	551.95	490.88
1139	Isodecanol	C10H22O	496.61	432.09	381.31
1148	1-Eicosanol	C20H42O	639.54	562.26	500.53
2198	Dinonylphenol	C24H42O	677.21	601.35	540.14
1159	Menthol	C10H20O	504.77	433.38	376.65

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Amines

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1742	Ethyleneimine	C2H5N	286.27	243.65	209.76
1745	Piperidine	C5H11N	382.84	326.93	282.45
1766	Pyrrolidine	C4H9N	353.18	301.09	259.69
1719	Isopropylamine	C3H9N	308.10	259.69	221.83
1711	N-Propylamine	C3H9N	328.31	277.78	238.00

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1726	Sec-Butylamine	C4H11N	341.02	288.25	246.85
1704	Ethylamine	C2H7N	293.95	248.14	212.19
1702	Dimethylamine	C2H7N	287.74	243.96	209.42
1710	Diethylamine	C4H11N	344.48	293.80	253.60
1740	Allylamine	C3H7N	323.96	271.92	231.33
1712	N-Butylamine	C4H11N	359.56	305.03	262.01
1794	HexMthyleneimine	C6H13N	410.36	351.06	303.87
1729	Cyclohexylamine	C6H13N	412.80	350.35	301.08
1714	Isobutylamine	C4H11N	349.27	294.97	252.39
2853	Acetamide	C2H5NO	481.13	411.65	355.67
2731	N-C1-CycC6-Amine	C7H15N	428.59	366.63	317.40
1743	Diisopropylamine	C6H15N	359.78	310.42	270.90
1796	N,N-DiMthAniline	C8H11N	495.25	430.82	378.59
1792	Aniline	C6H7N	453.68	392.38	342.80
1713	N-Pentylamine	C5H13N	388.08	330.15	284.35
1733	Benzylamine	C7H9N	456.21	393.06	342.34
1737	M-Toluidine	C7H9N	475.49	412.47	361.45
3796	N-Ethylaniline	C8H11N	460.81	399.07	349.32
1878	2-Methacrylamide	C4H7NO	535.26	457.23	394.71
1736	O-Toluidine	C7H9N	475.49	412.47	361.45
2739	Diallylamine	C6H11N	397.86	336.96	289.08
2706	Hexylamine	C6H15N	414.23	353.36	305.15
2724	O-Ethylaniline	C8H11N	496.40	431.02	378.12
1707	Dipropylamine	C6H15N	397.94	340.95	295.62
1738	P-Toluidine	C7H9N	475.49	412.47	361.45
1795	N-Methylaniline	C7H9N	447.20	386.18	337.06
1718	Diisobutylamine	C8H19N	430.62	368.35	319.06
1879	Acrylamide	C3H5NO	515.63	439.45	378.40
2707	1-Aminoheptane	C7H17N	438.32	374.90	324.58
2730	DiCycHexylAmine	C12H23N	504.54	438.59	385.62
2787	P-Aminodiphenyl	C12H11N	565.94	499.89	445.71
1744	Dibutylamine	C8H19N	443.78	381.91	332.60
2708	1-Octylamine	C8H19N	460.61	394.95	342.79
2791	2,6-DiEthAniline	C10H15N	532.98	464.49	409.06
2709	1-Nonylamine	C9H21N	481.31	413.68	359.88
2710	1-Decylamine	C10H23N	500.62	431.24	375.99
3722	Diamylamine	C10H23N	483.62	417.90	365.43
3724	Undecylamine	C11H25N	518.68	447.74	391.19
2712	Dodecylamine	C12H27N	535.63	463.30	405.58
1720	Tetradecylamine	C14H31N	566.62	491.91	432.20
2752	Piperazine	C4H10N2	400.26	343.32	297.79
1752	Propylenediamine	C3H10N2	379.74	320.31	273.70
1741	Ethylenediamine	C2H8N2	366.39	309.32	264.42
2725	O-Aminoaniline	C6H8N2	520.78	457.54	405.56
2750	P-Aminoaniline	C6H8N2	520.78	457.54	405.56
2727	M-Aminoaniline	C6H8N2	520.78	457.54	405.56

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1750	AEP	C6H15N3	478.66	410.23	355.82
1732	Toluene Diamine	C7H10N2	537.38	472.94	419.99
1731	hexamethyleneDiamine	C6H16N2	475.71	406.37	351.38
3750	P-Benzidine	C12H12N2	607.53	541.37	486.67

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Nitrilies

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1773	Propionitrile	C3H5N	372.43	313.51	267.18
1782	Butyronitrile	C4H7N	403.69	340.97	291.52
2720	Allyl Cyanide	C4H5N	407.59	341.41	289.66
1783	Valeronitrile	C5H9N	431.89	365.98	313.92
3874	Benzyl Cyanide	C8H7N	517.34	445.47	387.73
1786	Hexanenitrile	C6H11N	457.53	388.92	334.62
1776	Succinonitrile	C4H4N2	530.36	446.42	380.24
1781	Glutaronitrile	C5H6N2	553.38	467.62	399.86
2735	14-2Cyano-2-C4H8	C6H6N2	603.78	507.30	431.55
1777	Adiponitrile	C6H8N2	574.40	487.11	418.01

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Silanes

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
3985	Dimethyl Silane	C2H8Si	248.18	207.98	176.66
3984	Methyl Silane	CH6Si	215.10	179.79	152.23
3986	Trimethyl Silane	C3H10Si	279.11	234.69	200.08
1984	TetraMth Silane	C4H12Si	307.40	259.38	221.91
2994	TETRAETHYL Si	C8H20Si	411.88	352.07	305.00
1965	HexMthDisiloxane	C6H18OSi2	376.35	323.33	281.49
1966	6C1Cyc3Siloxane	C6H18O3Si3	391.06	341.45	301.73
1988	8C1Cyc4Siloxane	C8H24O4Si4	431.25	379.33	337.73
3991	DecaMethcyclpenS	C10H30O5Si5	462.70	409.38	366.66
3992	DodecaMethCyHexS	C12H36O6Si6	488.22	434.01	390.64

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Imines

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1767	N-MthPyrrolidine	C5H11N	346.17	292.80	250.73
2797	3-Methylpyridine	C6H7N	413.24	351.46	302.44
1797	2-Methylpyridine	C6H7N	413.24	351.46	302.44
2799	4-Methylpyridine	C6H7N	413.24	351.46	302.44
1753	N,N-DiEthAniline	C10H15N	472.55	408.31	356.89
1754	N-Methylpyrrole	C5H7N	374.10	310.96	262.01
3740	Acridine	C13H9N	562.42	497.39	444.01

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Tert-N

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1703	Trimethylamine	C3H9N	294.15	244.57	206.14
2856	DiMth Acetamide	C4H9NO	401.44	338.59	289.15
1706	Triethylamine	C6H15N	360.51	306.27	263.53
2716	Tributylamine	C12H27N	492.90	425.34	371.64
2719	Tripropylamine	C9H21N	433.77	371.70	322.55
3723	Triamylamine	C15H33N	541.98	470.41	413.37

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Nitrates

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1761	Nitroethane	C2H5NO2	383.56	329.35	285.71
1763	2-Nitropropane	C3H7NO2	394.12	336.58	290.69
1762	1-Nitropropane	C3H7NO2	409.36	352.15	306.13
1779	P-Nitrotoluene	C7H7NO2	499.77	424.32	364.57
1886	Nitrobenzene	C6H5NO2	477.34	402.77	344.00
1778	O-Nitrotoluene	C7H7NO2	499.77	424.32	364.57
1780	M-Nitrotoluene	C7H7NO2	499.77	424.32	364.57
1891	O-Nitroanisole	C7H7NO3	505.83	438.72	384.43
2740	M-Dinitrobenzene	C6H4N2O4	601.72	509.25	436.08
2742	P-Dinitrobenzene	C6H4N2O4	601.72	509.25	436.08
2741	O-Dinitrobenzene	C6H4N2O4	601.72	509.25	436.08
2749	3,5-DiNitToluene	C7H6N2O4	614.29	522.87	450.23

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

2743	DNT	C7H6N2O4	614.29	522.87	450.23
2745	3,4-DiNitToluene	C7H6N2O4	614.29	522.87	450.23
2744	2,6-DiNitToluene	C7H6N2O4	614.29	522.87	450.23
2748	2,5-DiNitToluene	C7H6N2O4	614.29	522.87	450.23
2746	1,3,5-TrinitroBz	C6H3N3O6	721.65	612.37	525.62
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	775.98	683.26	607.93
2747	Trinitrotoluene	C7H5N3O6	725.11	618.60	533.75

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Thiols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1802	Ethyl Mercaptan	C2H6S	305.23	255.99	217.39
1820	Dimethyl Sulfide	C2H6S	310.03	262.18	224.27
1843	Thiacyclopentane	C4H8S	370.33	316.13	272.86
1803	1-Propanethiol	C3H8S	339.17	285.63	243.57
1805	Isobut Mercaptan	C4H10S	359.95	302.81	258.08
6860	Ethylenedithiol	C2H6S2	402.50	337.54	286.73
1811	Cyclohexanethiol	C6H12S	435.19	369.53	317.70
1828	DiMth Disulfide	C2H6S2	402.50	337.54	286.73
1841	Butanethiol	C4H10S	369.87	312.67	267.65
1814	Methylproylsulf	C4H10S	369.87	312.67	267.65
2816	ETHYLtBUTYL SUL	C6H14S	395.45	337.55	291.65
1818	Diethyl Sulfide	C4H10S	361.20	308.45	266.43
1812	Benzyl Mercaptan	C7H8S	465.23	400.01	347.80
1838	T-OctylMercaptan	C8H18S	455.06	387.51	334.26
1827	1-Pentanethiol	C5H12S	397.82	337.49	289.90
2815	METHnBUTYL SULFD	C5H12S	398.69	340.16	293.66
1824	DiethylDisulfide	C4H10S2	426.83	367.25	319.48
1807	N-Hexylmercaptan	C6H14S	423.42	360.37	310.55
6857	Dimercaptoethyl	C4H10OS2	486.92	410.95	351.33
1839	1-Heptanethiol	C7H16S	446.99	381.57	329.79
1829	DiProp Disulfide	C6H14S2	469.62	405.68	354.38
1809	1-Octanethiol	C8H18S	468.81	401.30	347.79
1808	N-Nonanethiol	C9H20S	489.08	419.73	364.69
1826	1-Decanethiol	C10H22S	507.98	437.01	380.59
2838	tertDodecanThiol	C12H26S	532.87	458.65	399.77
1825	1-Undecanethiol	C11H24S	525.68	453.24	395.61
1837	Dodecylthiol	C12H26S	542.30	468.55	409.82

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Aldehydes

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1037	Methacrolein	C4H6O	339.54	286.00	244.06
1002	Acetaldehyde	C2H4O	278.28	235.21	201.33
1003	Propionaldehyde	C3H6O	313.89	265.73	227.77
1041	Benzaldehyde	C7H6O	445.63	384.01	334.46
1034	Acrolein	C3H4O	308.23	258.86	220.31
1005	N-Butyraldehyde	C4H8O	346.24	293.81	252.39
1036	Trans-2-Butenal	C4H6O	348.24	292.71	249.29
1007	Valeraldehyde	C5H10O	375.73	319.67	275.30
1006	Isobutyraldehyde	C4H8O	335.39	283.31	242.43
1009	1-Hexanal	C6H12O	402.73	343.55	296.62
1040	P-Tolualdehyde	C8H8O	468.13	404.78	353.73
1016	2-Methylhexanal	C7H14O	420.42	358.30	309.17
1017	3-Methylhexanal	C7H14O	420.42	358.30	309.17
1008	1-Heptanal	C7H14O	427.57	365.67	316.53
1013	2-Ethylhexanal	C8H16O	444.26	379.66	328.48
1010	1-Octanal	C8H16O	450.52	386.25	335.16
1011	1-Nonanal	C9H18O	471.81	405.46	352.64
1020	1-Decanal	C10H20O	491.64	423.44	369.09
1021	1-Undecanal	C11H22O	510.17	440.33	384.62
1025	Dodecanal	C12H24O	527.55	456.23	399.30
1026	1-Tridecanal	C13H26O	543.88	471.25	413.22
1014	1,2-Ethanedione	C2H2O2	335.56	283.64	242.61
1044	1,4BenzDicarboxAldehy	C8H6O2	509.82	445.63	393.28

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Epoxides

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1440	ISOBUTYLENE OXID	C4H8O	289.15	242.17	205.41
1479	Tetrahydrofuran	C4H8O	349.63	294.77	251.58
1477	2,5-Dihydrofuran	C4H6O	314.32	262.62	222.21
1408	1-Methoxypropane	C4H10O	319.00	272.78	235.87
1411	2-Methoxypropane	C4H10O	307.77	262.14	225.87
1421	1,4-Dioxane	C4H8O2	343.48	289.33	246.71
2422	1,3-DIOXANE	C4H8O2	343.48	289.33	246.71
1426	2-Methoxybutane	C5H12O	336.99	287.76	248.60
1413	1-Methoxybutane	C5H12O	346.97	297.34	257.71
1461	Methoxybenzene	C7H8O	415.35	359.92	315.10
1448	1-Ethoxybutane	C6H14O	369.42	313.78	269.85
1429	1-MethoxyPentane	C6H14O	369.42	313.78	269.85
6885	Ethyl-3-Ethoxypr	C7H14O3	441.20	378.03	327.78

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Ether

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1401	Dimethyl Ether	C2H6O	255.99	218.07	187.73
1407	MethylEthylEther	C3H8O	274.33	230.57	196.20
1470	VinylMethylEther	C3H6O	280.62	237.85	203.91
1405	MTBE	C5H12O	326.35	278.08	239.78
1445	VinylEthyl Ether	C4H8O	302.89	253.32	214.64
1402	Diethyl Ether	C4H10O	308.99	260.66	222.64
1431	Methylal	C3H8O2	322.38	277.57	241.44
1428	T-But EthylEther	C6H14O	348.58	294.06	251.35
1427	TAME	C6H14O	354.15	302.56	261.60
1410	Mth Isobut Ether	C5H12O	336.99	287.76	248.60
1430	Eth-t-Pent-Ether	C7H16O	377.28	319.46	274.06
1403	DiisopropylEther	C6H14O	344.73	291.07	248.99
1415	Eth Propyl Ether	C5H12O	340.56	288.31	247.13
1455	Dimethyl Acetal	C4H10O2	336.77	283.30	241.38
1446	Dipropyl Ether	C6H14O	369.42	313.78	269.85
1447	Butyl VinylEther	C6H12O	367.96	310.42	265.29
1462	EthylPhenylEther	C8H10O	439.67	378.39	329.29
1406	Di-sec-But Ether	C8H18O	399.68	339.83	292.70
1432	Acetal	C6H14O2	387.03	326.62	279.27
1460	BenzylEthylEther	C9H12O	462.57	393.22	338.45
1050	Paraldehyde	C6H12O3	387.16	326.06	278.23
1404	Di-n-Butyl Ether	C8H18O	420.34	359.17	310.71
1420	Anethole	C10H12O	483.98	423.75	374.77
1456	DimethylCarbitol	C6H14O3	418.36	361.38	315.62
1463	Dibenzyl Ether	C14H14O	572.14	495.50	434.02
1425	Di-n-PentylEther	C10H22O	464.01	398.54	346.54
1458	Diethyl Carbitol	C8H18O3	470.97	401.13	346.00
1412	Dihexyl Ether	C12H26O	502.03	433.14	378.31
1454	Triglyme	C8H18O4	480.29	415.82	364.11
1459	Dibutyl Carbitol	C12H26O3	547.00	470.86	410.41
1424	Di-n-Octyl Ether	C16H34O	565.41	491.52	432.52
1457	Tetraglyme	C10H22O5	563.01	480.98	416.18
1418	Dinonyl Ether	C18H38O	592.25	516.49	455.95
2432	ETHYLAL	C5H12O2	367.62	310.48	265.58
2405	DIISOBUTYL ETHER	C8H18O	405.03	343.57	295.27
2456	Ethyl Glyme	C6H14O2	395.71	335.42	287.93
2417	ETHYLHEXYL ETHER	C8H18O	420.34	359.17	310.71
2415	ETHYLISOPROPETH	C5H12O	325.42	275.03	235.40

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Formate

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1301	Methyl Formate	C2H4O2	290.73	245.94	210.49
1311	Vinyl Formate	C3H4O2	318.22	267.99	228.49
1302	Ethyl Formate	C3H6O2	323.26	274.28	235.48
2306	t-Butyl Formate	C5H10O2	360.94	306.12	262.92
1303	Propyl Formate	C4H8O2	353.01	300.40	258.69
2305	sec-ButylFormate	C5H10O2	371.32	315.66	271.67
2311	CYCLOHEXL FORMAT	C7H12O2	437.66	373.37	322.43
1304	N-Butyl Formate	C5H10O2	380.31	324.54	280.28
1305	Isobutyl Formate	C5H10O2	371.32	315.66	271.67
2350	Benzyl Formate	C8H8O2	467.55	404.52	353.81
2307	n-Hexyl Formate	C7H14O2	428.77	367.80	319.30
1306	N-Pentyl Formate	C6H12O2	405.48	346.95	300.44
2308	n-Heptyl Formate	C8H16O2	450.43	387.29	337.02
1308	N-Octyl Formate	C9H18O2	470.62	405.56	353.70
1309	n-Nonyl Formate	C10H20O2	489.51	422.72	369.45
1310	n-Decyl Formate	C11H22O2	507.25	438.91	384.35

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Ester

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1351	Mth Methacrylate	C5H8O2	373.57	320.88	278.62
1312	Methyl Acetate	C3H6O2	325.64	280.17	243.48
1331	Vinyl Propionate	C5H8O2	365.46	309.90	265.97
1321	Vinyl Acetate	C4H6O2	349.56	299.69	259.68
1352	Eth MthAcrylate	C6H10O2	390.16	331.86	285.70
1322	MethylPropionate	C4H8O2	353.04	304.19	264.82
1341	Methyl Acrylate	C4H6O2	335.60	283.91	243.08
1313	Ethyl Acetate	C4H8O2	338.72	288.26	248.15
1319	IsopropylAcetate	C5H10O2	370.05	318.39	276.93
1332	Methyl Butyrate	C5H10O2	367.30	313.42	270.56
1342	Ethyl Acrylate	C5H8O2	365.66	310.36	266.61
1318	Allyl Acetate	C5H8O2	376.43	323.36	280.80
1314	N-Propyl Acetate	C5H10O2	378.38	326.55	284.81
1323	Ethyl Propionate	C5H10O2	367.30	313.42	270.56
1360	I-But I-Butyrate	C8H16O2	432.03	372.81	325.41
1320	Sec-ButylAcetate	C6H12O2	394.45	340.02	296.35
1336	PropylI-Butyrate	C7H14O2	410.15	350.84	303.76
1353	N-C3-Mthacrylate	C7H12O2	407.74	348.14	300.80

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1333	Ethyl Butyrate	C6H12O2	393.56	336.70	291.43
1347	EthylIsovalerate	C7H14O2	410.49	350.88	303.55
1315	N-Butyl Acetate	C6H12O2	401.90	347.43	303.58
1390	Methyl Benzoate	C8H8O2	459.60	400.90	353.18
1388	ISOBUTYL MTHACR	C8H14O2	432.14	368.70	318.50
1343	1-PropylAcrylate	C6H10O2	393.33	334.59	288.07
1316	Isobutyl Acetate	C6H12O2	394.45	340.02	296.35
1344	N-Butyl Acrylate	C7H12O2	416.66	356.47	308.55
1357	Pentyl Acetate	C7H14O2	423.81	366.99	321.24
1327	N-PropN-Butyrate	C7H14O2	417.81	358.32	310.92
1324	N-PropPropionate	C6H12O2	393.56	336.70	291.43
1291	Acetic Anhydride	C4H6O3	406.57	351.99	307.73
1389	N-ButMthacrylate	C8H14O2	438.79	375.64	325.48
1359	Benzyl Acetate	C9H10O2	478.79	413.86	361.65
1326	N-But Propionate	C7H14O2	417.81	358.32	310.92
1391	Ethyl Benzoate	C9H10O2	476.73	413.38	362.32
1897	CH3OC3H600CH3	C6H12O3	416.45	361.40	316.93
1392	DiethylCarbonate	C5H10O3	392.82	334.50	288.23
1385	N-But N-Butyrate	C8H16O2	440.29	378.49	329.20
1317	IsopentylAcetate	C7H14O2	417.14	360.25	314.60
1363	N-Hexyl Acetate	C8H16O2	439.70	378.22	329.18
1387	Ethylene Acetate	C6H10O4	445.96	389.83	344.11
1393	Diethyl Oxalate	C6H10O4	438.48	376.83	327.50
1365	Butyl Benzoate	C11H14O2	512.68	445.97	392.19
1361	I-C5 I-Valerate	C10H20O2	470.39	403.91	351.11
1367	Heptyl Acetate	C9H18O2	460.43	396.90	346.20
1346	N-Butyl Valerate	C9H18O2	461.21	397.35	346.38
1358	2-C2-C6 Acetate	C10H20O2	476.73	413.89	363.42
1394	Diethyl Malonate	C7H12O4	459.50	395.97	345.11
1292	Propionyl Oxide	C6H10O3	443.53	382.41	333.29
1364	Benzyl Benzoate	C14H12O2	580.61	505.17	444.39
1381	2Mth p-Phthalate	C10H10O4	524.32	465.33	416.74
1368	n-Octyl Acetate	C10H20O2	479.80	414.46	362.26
1377	DiMthI-Phthalate	C10H10O4	525.13	461.70	409.97
1896	Ethylene DiAcr	C8H10O4	487.22	417.28	361.68
1386	2-Ethylhexyl Acr	C11H20O2	497.74	428.03	372.65
1395	Methyl Decanoate	C11H22O2	499.07	431.72	377.88
1369	n-Nonyl Acetate	C11H22O2	497.97	430.99	377.45
1370	n-Decyl Acetate	C12H24O2	515.06	446.60	391.85
1345	N-ButylNonanoate	C13H26O2	532.49	462.31	406.14
1375	DiProp Phthalate	C14H18O4	579.41	511.31	455.91
1376	Diisobutyl Phtha	C16H22O4	599.10	528.24	470.80
1396	IsopropMyristate	C17H34O2	585.26	510.64	450.93
1383	Butyl Stearate	C22H44O2	645.97	567.96	505.36
1362	Methyl Oleate	C19H36O2	625.22	546.04	482.67
1355	Diisooctyl Phtha	C24H38O4	678.27	602.23	540.73

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1382	DioctylTerephtha	C24H38O4	679.72	604.69	543.91
1384	DIBUTYL SEBACATE	C18H34O4	627.89	550.55	488.39
1371	Diisodecyl Phtha	C28H46O4	709.82	632.09	569.30
1354	DioctylPhthalate	C24H38O4	678.27	602.23	540.73
2375	DiethylPhthalate	C12H14O4	555.63	489.18	435.03
2388	Dipropyl Maleate	C10H16O4	524.89	453.10	395.76
2381	Diallyl Maleate	C10H12O4	543.74	464.66	401.96
2370	Glyceryl Triacet	C9H14O6	523.77	462.05	411.60
2382	Dibutyl Maleate	C12H20O4	557.61	483.22	423.72
2376	DibutylPhthalate	C16H22O4	602.90	532.98	476.17
2353	CetylMthacrylate	C20H38O2	627.96	549.71	487.04
2379	Dihexyl Adipate	C18H34O4	627.89	550.55	488.39
2321	T-Butyl Acetate	C6H12O2	375.45	319.61	275.44
2332	Methl.I-butyrate	C5H10O2	358.18	304.68	262.30
2354	AllylMthacrylate	C7H10O2	416.88	353.85	304.12
2364	CYCLOHEXL ACETAT	C8H14O2	448.74	384.05	332.62
2337	EthylIsobutyrate	C6H12O2	385.22	328.62	283.74
2384	IsobutylAcrylate	C7H12O2	410.90	349.56	301.09
2380	1,1-Diacetoxy C2	C6H10O4	430.97	369.68	320.81
2392	n-PropylBenzoate	C10H12O2	495.28	430.15	377.66
2377	DiMth Phthalate	C10H10O4	524.32	465.33	416.74
2386	Diethyl Maleate	C8H12O4	487.66	419.12	364.47
2385	Mth Dodecanoate	C13H26O2	532.49	462.31	406.14
3379	Dioctyl Adipate	C22H42O4	662.97	582.06	517.25
5886	Mth Acetoacetate	C5H8O3	425.10	364.87	316.60
5884	Ethoxy Acetate	C6H12O3	423.72	365.71	319.11
5887	EthAcetoAcetate	C6H10O3	448.31	385.61	335.34
5885	Carbitol Acetate	C8H16O4	486.66	421.01	368.33

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Ketone

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1096	Methyl Isopropen	C5H8O	373.78	317.30	272.53
1079	Cyclopentanone	C5H8O	383.78	328.71	284.57
1051	Acetone	C3H6O	318.94	271.05	232.90
1052	MEK	C4H8O	349.85	298.08	256.83
1065	Mesityl Oxide	C6H10O	403.35	344.00	296.82
1066	T-But Mth Ketone	C6H12O	386.56	329.12	283.59
1060	2-Pentanone	C5H10O	378.07	322.94	279.00
1061	Mth iC3 Ketone	C5H10O	369.11	314.05	270.36
1053	Diethyl Ketone	C5H10O	374.84	321.12	278.17

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1059	3-Hexanone	C6H12O	400.23	343.64	298.37
1099	Diketene	C4H4O2	337.25	285.45	244.37
1055	Sec-ButMthKetone	C6H12O	396.13	338.00	291.81
1054	MIBK	C6H12O	396.13	338.00	291.81
1095	EthIsopropKetone	C6H12O	392.37	335.75	290.64
1063	2-Heptanone	C7H14O	427.87	367.26	318.88
1064	5-Mth-2-Hexanone	C7H14O	420.98	360.16	311.79
1058	4-Heptanone	C7H14O	423.72	364.59	317.27
1057	3-Heptanone	C7H14O	423.72	364.59	317.27
1076	2,4-Pentanedione	C5H8O2	435.12	373.83	324.61
1068	DiisobutylKetone	C9H18O	454.69	390.67	339.70
1097	2-CycC6 CycC6one	C12H20O	541.50	467.07	407.59
1083	2-Octanone	C8H16O	450.02	387.15	336.92
1073	Dibutyl Ketone	C9H18O	465.89	402.50	351.73
1062	2-Hexanone	C6H12O	403.97	345.93	299.62
1077	Isophorone	C9H14O	464.11	397.81	345.01
1090	Acetophenone	C8H8O	466.41	403.90	353.40
1080	Cyclohexanone	C6H10O	410.99	352.60	305.82
1074	2-Nonanone	C9H18O	470.63	405.74	353.88

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Alcohol-Ethers

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
2862	2-Butoxyethanol	C6H14O2	445.60	387.53	341.56
4857	butyl carbitol	C8H18O3	508.67	441.02	387.83
2898	2-Chloroethanol	C2H5ClO	386.82	337.77	297.95
2864	Carbitol	C6H14O3	469.36	406.87	357.62
3854	Methyl propasol	C4H10O2	393.21	344.52	305.25
2860	2-Methoxyethanol	C3H8O2	377.41	331.69	294.46
2854	DiacetoneAlcohol	C6H12O2	454.47	396.17	349.86
2861	2-Ethoxyethanol	C4H10O2	400.99	349.42	308.03
2889	HydroxyAcetone	C3H6O2	401.99	352.42	312.24
3856	1tButoxy2Propnol	C7H16O2	447.92	387.77	340.49
3858	PROPGLYC2tBUTYL	C7H16O2	442.02	383.42	337.26
4855	2-Propoxyethanol	C5H12O2	423.85	368.93	325.20
4849	Acetovanillone	C9H10O3	539.25	481.73	434.36
5883	Ethyl Lactate	C5H10O3	436.10	379.91	335.19
6883	2-HydroxyEth Acr	C5H8O3	443.73	386.04	340.18
2863	Methyl Carbitol	C5H12O3	448.05	388.56	341.49
3855	Dowanol DPM	C7H16O3	482.33	420.86	372.14
3857	TriPropGlymEthlE	C10H22O4	554.57	483.56	427.25

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
404	DiMth-Acetylene	C4H6	289.23	246.98	213.25
202	Propylene	C3H6	236.34	197.59	167.25
412	2-Pentyne	C5H8	371.68	319.43	277.70
207	2-Methylpropene	C4H8	270.77	227.22	193.09
204	1-Butene	C4H8	274.39	230.27	195.70
205	Cis-2-Butene	C4H8	277.72	232.50	197.16
402	Propyne	C3H4	246.86	206.22	174.48
406	3-Hexyne	C6H10	346.23	296.91	257.55
206	Trans-2-Butene	C4H8	277.72	232.50	197.16
407	2-Hexyne	C6H10	346.23	296.91	257.55
231	33-2Mth-1-Butene	C6H12	340.66	288.59	247.55
230	23-2Mth-1-Butene	C6H12	340.66	288.59	247.55
229	2-Ethyl-1-Butene	C6H12	337.41	285.29	244.30
8	I-Pentane	C5H12	302.93	255.93	218.95
14	2,2-DiMth-Butane	C6H14	322.40	272.63	233.52
232	23-2Mth-2-Butene	C6H12	352.87	297.76	254.49
213	3-Mth-1-Butene	C5H10	296.05	248.07	210.63
212	2-Mth-1-Butene	C5H10	305.63	257.47	219.66
211	Trans-2-Pentene	C5H10	313.00	263.15	224.10
210	Cis-2-Pentene	C5H10	313.00	263.15	224.10
223	4-Mth-1-Pentene	C6H12	329.47	277.27	236.42
221	2-Mth-1-Pentene	C6H12	337.41	285.29	244.30
248	2-t-Butylpropene	C7H14	345.25	290.90	248.41
227	Cs-4-Mth-2-C5H10	C6H12	333.77	280.32	238.58
224	2-Mth-2-Pentene	C6H12	340.66	288.59	247.55
403	1-Butyne	C4H6	284.21	238.41	202.58
15	2,3-DiMth-Butane	C6H14	322.42	272.09	232.63
214	2-Mth-2-Butene	C5H10	309.53	261.31	223.37
228	Ts-4-Mth-2-C5H10	C6H12	333.77	280.32	238.58
225	Cs-3-Mth-2-C5H10	C6H12	340.66	288.59	247.55
218	Trans-2-Hexene	C6H12	345.00	291.20	248.96
2226	3-METH-Tr-2Pente	C6H12	340.66	288.59	247.55
222	3-Mth-1-Pentene	C6H12	329.47	277.27	236.42
257	2-Diisobutylene	C8H16	376.80	319.28	274.11
256	1-Diisobutylene	C8H16	374.17	316.49	271.28
217	Cis-2-Hexene	C6H12	345.00	291.20	248.96
2414	1-Heptyne	C7H12	377.53	320.31	275.26
13	3-Methylpentane	C6H14	333.83	282.99	242.93
219	Cis-3-Hexene	C6H12	340.66	288.59	247.55
12	2-Methylpentane	C6H14	333.83	282.99	242.93
220	Trans-3-Hexene	C6H12	340.66	288.59	247.55
405	1-Pentyne	C5H8	318.23	268.03	228.68
209	1-Pentene	C5H10	309.12	260.44	222.21
11	N-Hexane	C6H14	344.44	293.19	252.62

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

235	Cis-2-Heptene	C7H14	374.16	316.97	271.97
249	Cis-3-Heptene	C7H14	374.16	316.97	271.97
216	1-Hexene	C6H12	340.76	288.15	246.77
239	3-Eth-1-Pentene	C7H14	359.87	304.05	260.27
226	4-Mth-1-Hexene	C7H14	359.87	304.05	260.27
240	3-Mth-1-Hexene	C7H14	359.87	304.05	260.27
419	3-Mth-1-Butyne	C5H8	305.56	255.98	217.35
233	2-Eth-1-Pentene	C7H14	366.46	310.93	267.16
238	2-Mth-1-Hexene	C7H14	366.46	310.93	267.16
416	1-Octyne	C8H14	403.55	343.49	296.12
289	2,3Dimeth Hexene	C8H16	384.46	325.97	279.99
234	1-Heptene	C7H14	369.67	313.68	269.55
413	1-Hexyne	C6H10	349.21	295.24	252.84
237	Trans-3-Heptene	C7H14	374.16	316.97	271.97
236	Trans-2-Heptene	C7H14	374.16	316.97	271.97
251	Trans-2-Octene	C8H16	400.86	340.74	293.33
279	Trans-4-Octene	C8H16	400.86	340.74	293.33
277	Trans-3-Octene	C8H16	400.86	340.74	293.33
2252	2Methl-1-Heptene	C8H16	393.13	334.62	288.43
250	1-Octene	C8H16	396.20	337.27	290.73
258	2-Ethyl-1-Hexene	C8H16	393.13	334.62	288.43
280	3-Octene	C8H16	400.86	340.74	293.33
278	4-Octene	C8H16	400.86	340.74	293.33
276	2-Octene	C8H16	400.86	340.74	293.33
259	1-Nonene	C9H18	420.66	359.15	310.50
262	1-Dodecene	C12H24	484.03	416.44	362.76
263	1-Tridecene	C13H26	502.42	433.23	378.22
264	1-Tetradecene	C14H28	519.69	449.07	392.86
265	1-Pentadecene	C15H30	535.96	464.03	406.74
266	1-Hexadecene	C16H32	551.31	478.21	419.94
267	1-Octadecene	C18H36	579.59	504.46	444.50
281	1-Heptadecene	C17H34	565.83	491.66	432.50
284	1-Eicosene	C20H40	605.12	528.30	466.92
283	1-Nonadecene	C19H38	592.67	516.66	455.96
3	Propane	C3H8	248.35	209.55	178.89
4	I-Butane	C4H10	269.25	226.69	193.25
9	Neopentane	C5H12	290.45	244.72	208.86
5	N-Butane	C4H10	283.04	239.50	205.09
7	pentane	C5H12	315.03	267.36	229.67
44	Hexamethylethane	C8H18	358.89	303.61	260.31
25	223-TriMthButane	C7H16	341.15	288.24	246.78
24	3,3-DiMthPentane	C7H16	351.73	298.45	256.50
51	2,2,3,3-4Mth-C5	C9H20	385.80	327.52	281.76
21	2,2-DiMthPentane	C7H16	351.73	298.45	256.50
42	2,3,3-TriMth-C5	C8H18	369.45	313.27	269.15
22	2,3-DiMthPentane	C7H16	352.23	298.33	255.97

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

40	2,2,3-TriMth-C5	C8H18	369.45	313.27	269.15
23	2,4-DiMthPentane	C7H16	352.23	298.33	255.97
41	2,2,4-TriMth-C5	C8H18	369.45	313.27	269.15
39	3-Mth-3-Eth-C5	C8H18	378.71	322.37	277.93
20	3-Ethylpentane	C7H16	362.21	308.03	265.26
52	2,2,3,4-4Mth-C5	C9H20	386.83	327.84	281.61
54	2334TetrMethPent	C9H20	386.83	327.84	281.61
53	2,2,4,4-4Mth-C5	C9H20	385.80	327.52	281.76
43	2,3,4-TriMth-C5	C8H18	370.27	313.40	268.82
36	3,3-DiMth-Hexane	C8H18	378.71	322.37	277.93
19	3-Methylhexane	C7H16	362.21	308.03	265.26
18	2-Methylhexane	C7H16	362.21	308.03	265.26
38	2-Mth-3-Eth-C5	C8H18	379.60	322.59	277.70
190	2,2-2C1-3-C2-C5	C9H20	395.49	336.46	290.00
32	2,2-DiMth-Hexane	C8H18	378.71	322.37	277.93
37	3,4-DiMth-Hexane	C8H18	379.60	322.59	277.70
50	3,3-DiEthPentane	C9H20	403.64	344.60	297.96
34	2,4-DiMth-Hexane	C8H18	379.60	322.59	277.70
33	2,3-DiMth-Hexane	C8H18	379.60	322.59	277.70
17	N-Heptane	C7H16	371.55	317.15	274.04
49	244TriMethHexane	C9H20	395.49	336.46	290.00
192	2,4-2C1-3-C2-C5	C9H20	396.65	336.90	289.95
47	2,2,5-TriMth-C6	C9H20	395.49	336.46	290.00
35	2,5-DiMth-Hexane	C8H18	379.60	322.59	277.70
31	3-Ethylhexane	C8H18	388.36	331.25	286.11
30	4-Methylheptane	C8H18	388.36	331.25	286.11
29	3-Methylheptane	C8H18	388.36	331.25	286.11
28	2-Methylheptane	C8H18	388.36	331.25	286.11
96	2,2-DiMthHeptane	C9H20	403.64	344.60	297.96
176	2,6-DiMthHeptane	C9H20	404.83	345.10	297.99
27	N-Octane	C8H18	396.60	339.44	294.08
94	3-Ethylheptane	C9H20	412.55	352.87	305.62
92	3-Methyloctane	C9H20	412.55	352.87	305.62
93	4-Methyloctane	C9H20	412.55	352.87	305.62
91	2-Methyloctane	C9H20	412.55	352.87	305.62
72	2,2-DiMthOctane	C10H22	426.74	365.33	316.73
2095	2,3Dimethloctane	C10H22	428.19	366.06	316.97
2096	2,4Dimethloctane	C10H22	428.19	366.06	316.97
2098	2,6DimethlOctane	C10H22	428.19	366.06	316.97
2097	2,5Dimethloctane	C10H22	428.19	366.06	316.97
2099	2,7DimethlOctane	C10H22	428.19	366.06	316.97
46	N-Nonane	C9H20	419.84	360.24	312.88
88	5-Methylnonane	C10H22	435.00	373.05	323.92
85	3-Methylnonane	C10H22	435.00	373.05	323.92
87	4-Methylnonane	C10H22	435.00	373.05	323.92
86	2-Methylnonane	C10H22	435.00	373.05	323.92

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

56	N-Decane	C10H22	441.48	379.70	330.56
63	N-Undecane	C11H24	461.69	397.97	347.23
64	N-Dodecane	C12H26	480.63	415.16	362.98
65	N-Tridecane	C13H28	498.42	431.37	377.90
66	N-Tetradecane	C14H30	515.19	446.71	392.07
67	N-Pentadecane	C15H32	531.01	461.25	405.53
68	N-Hexadecane	C16H34	545.99	475.05	418.37
69	N-Heptadecane	C17H36	560.20	488.18	430.61
70	N-Octadecane	C18H38	573.69	500.70	442.32
71	N-Nonadecane	C19H40	586.54	512.65	453.53
73	N-Eicosane	C20H42	598.79	524.07	464.27
74	n-HENEICOSANE	C21H44	610.48	535.00	474.58
75	n-DOCOSANE	C22H46	621.66	545.49	484.49
76	n-TRICOSANE	C23H48	632.37	555.55	494.02
77	n-Tetracosane	C24H50	642.63	565.22	503.20
78	n-PENTACOSANE	C25H52	652.49	574.52	512.05
79	n-HEXACOSANE	C26H54	661.96	583.48	520.60
81	n-Octacosane	C28H58	679.84	600.45	536.82
2081	n-TRICONTANE	C30H62	696.45	616.27	552.01
2082	n-Dotriacontane	C32H66	711.93	631.08	566.27
2086	Hexatriacontane	C36H74	740.01	658.04	592.37

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Cyclic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
269	Cyclopentene	C5H8	323.22	271.45	230.83
270	Cyclohexene	C6H10	357.24	301.02	256.85
287	3MthCyclopentene	C6H10	345.42	289.69	246.13
286	1-MthCyclPentene	C6H10	350.63	296.79	254.30
288	4MthCyclopenten	C6H10	345.42	289.69	246.13
273	Cycloheptene	C7H12	388.40	328.32	281.04
274	Cyclooctene	C8H14	417.10	353.62	303.60
101	Cyclopropane	C3H6	254.80	214.84	183.20
810	ADAMANTANE	C10H16	454.74	384.47	329.28
102	Cyclobutane	C4H8	291.77	246.52	210.73
104	Cyclopentane	C5H10	325.88	276.01	236.56
137	Cyclohexane	C6H12	357.35	303.42	260.74
105	MthCyclopentane	C6H12	346.14	292.74	250.67
146	Cs-1,4-2C1-CycC6	C8H16	395.24	334.91	287.45
142	Cs-1,2-2C1-CycC6	C8H16	395.24	334.91	287.45
141	1,1-2C1-CycC6	C8H16	393.65	334.18	287.31

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

145	Ts-1,3-2C1-CycC6	C8H16	395.24	334.91	287.45
144	Cs-1,3-2C1-CycC6	C8H16	395.24	334.91	287.45
147	Ts-1,4-2C1-CycC6	C8H16	395.24	334.91	287.45
143	Ts-1,2-2C1-CycC6	C8H16	395.24	334.91	287.45
138	MthCyclohexane	C7H14	376.51	319.32	274.21
159	Cycloheptane	C7H14	386.46	328.95	283.40
140	Ethylcyclohexane	C8H16	404.62	344.08	296.28
154	Trans-Decalin	C10H18	458.17	390.24	336.56
149	N-PropylCyc-C6	C9H18	430.73	367.22	317.00
109	Cs-1,2-2C1-CycC5	C7H14	365.92	309.13	264.53
110	Ts-1,2-2C1-CycC5	C7H14	365.92	309.13	264.53
112	Ts-1,3-2C1-CycC5	C7H14	365.92	309.13	264.53
107	Eth-Cyclopentane	C7H14	376.51	319.32	274.21
114	N-PropCycPentane	C8H16	404.62	344.08	296.28
108	1,1-DiMthCycC5	C7H14	364.77	308.79	264.73
111	Cs-1,3-2C1-CycC5	C7H14	365.92	309.13	264.53
152	N-ButylCycHexane	C10H20	455.07	388.90	336.52
160	Cyclooctane	C8H16	413.48	352.79	304.67
153	Cis-Decalin	C10H18	458.17	390.24	336.56
115	ISOPROPYLCYCLOPENTANE	C8H16	395.24	334.91	287.45
150	Isopropyl-CycC6	C9H18	422.39	358.94	308.94
116	1-C1-1-C2-CycC5	C8H16	395.24	334.91	287.45
122	Butylcyclpentane	C9H18	430.73	367.22	317.00
155	1,1-Bicyclohexyl	C12H22	503.86	431.23	373.70
158	N-Decylcyclo-C6	C16H32	573.04	495.57	433.90

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Aromatic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
307	1,4-Pentadiene	C5H8	303.04	253.06	214.16
306	1-ts3-Pentadiene	C5H8	307.45	256.10	216.23
414	2-Methyl-1-Butenyne	C5H6	309.13	258.07	218.39
305	Cs1,3-Pentadiene	C5H8	307.45	256.10	216.23
309	Isoprene	C5H8	299.19	249.82	211.39
421	1-Pentene-4-yne	C5H6	312.96	261.31	221.15
303	1,3-Butadiene	C4H6	264.92	220.08	185.28
332	1,4-CyclHexadien	C6H8	358.54	299.34	253.22
501	Benzene	C6H6	348.99	293.55	250.02
315	Cyclopentadiene	C5H6	321.54	267.23	225.03
319	Diisopropenyl	C6H10	329.98	276.80	235.31
615	Ethynylbezene	C8H6	424.42	364.06	315.85

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

601	Styrene	C8H8	417.16	357.94	310.57
331	1,3-CycHexadiene	C6H8	358.54	299.34	253.22
310	1,5-Hexadiene	C6H10	337.29	283.01	240.64
312	MthCycPentadiene	C6H8	348.91	293.12	249.39
420	1-Pentene-3-yne	C5H6	313.02	266.25	229.14
502	Toluene	C7H8	381.84	323.33	277.16
521	T-Butylbenzene	C10H14	446.06	384.34	335.00
320	Dipropylene	C6H10	347.26	290.10	245.65
520	Sec-Butylbenzene	C10H14	445.49	380.43	328.89
313	1,4-Hexadiene	C6H10	342.11	286.44	243.06
314	Dipropylene	C6H10	347.26	290.10	245.65
316	DiCycPentadiene	C10H12	478.63	397.82	335.30
333	1,5-CycOctadiene	C8H12	422.52	355.57	303.16
701	Naphthalene	C10H8	471.86	411.50	362.46
504	Ethylbenzene	C8H10	410.41	348.40	299.42
820	Indan	C9H10	446.19	380.66	328.59
505	O-Xylene	C8H10	410.66	349.71	301.40
612	P-Methylstyrene	C9H10	441.31	380.16	331.14
330	DIISOCROTYL	C8H14	394.39	334.74	287.76
507	P-Xylene	C8H10	410.66	349.71	301.40
329	DIISOBUTENYL	C8H14	389.81	329.69	282.52
506	M-Xylene	C8H10	410.66	349.71	301.40
603	Methylstyrene	C9H10	441.31	380.16	331.14
613	Alpha-MthStyrene	C9H10	437.50	376.19	327.14
510	Isopropylbenzene	C9H12	421.83	359.17	309.61
724	2-Methylindene	C10H10	469.74	406.83	356.11
285	Vinylcyclohexene	C8H12	408.91	342.98	291.57
803	Indene	C9H8	451.95	394.32	347.40
706	Tetralin	C10H12	470.79	402.55	348.30
511	O-Ethyltoluene	C9H12	436.51	372.53	321.79
723	1-Methylindene	C10H10	480.20	402.11	341.27
738	Fluorene	C13H10	529.43	467.04	415.91
619	Tr-1PropenylBz	C9H10	445.07	382.28	332.09
525	O-Diethylbenzene	C10H14	460.66	393.97	341.03
618	Propenyl Bz(cis)	C9H10	445.07	382.28	332.09
602	O-Methylstyrene	C9H10	441.31	380.16	331.14
702	1-MthNaphthalene	C11H10	490.43	428.71	378.54
509	N-Propylbenzene	C9H12	435.53	370.90	319.76
526	M-Diethylbenzene	C10H14	460.66	393.97	341.03
583	Cs-2-PhnButene-2	C10H12	460.25	397.06	346.42
543	M-DiisopropylBz	C12H18	477.33	410.16	356.78
584	Ts-2-PhnButene-2	C10H12	460.25	397.06	346.42
580	1,2-DiC1-3C2-Bz	C10H14	459.87	394.28	342.09
704	1-EthNaphthalene	C12H12	508.43	444.79	393.11
512	M-Ethyltoluene	C9H12	436.51	372.53	321.79
522	1-Mth-2-iC3-Benz	C10H14	446.38	381.94	330.79

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

513	P-Ethyltoluene	C9H12	436.51	372.53	321.79
514	1,2,3-Mesitylene	C9H12	436.26	373.33	323.27
614	M-Divinylbenzene	C10H10	466.85	405.71	356.31
524	1-Mth-4-iC3-Benz	C10H14	446.38	381.94	330.79
822	Gamma-Terpinene	C10H16	448.81	381.59	328.61
821	Alpha-Terpinene	C10H16	448.81	381.59	328.61
523	1-Mth-3-iC3-Benz	C10H14	446.38	381.94	330.79
703	2-MthNaphthalene	C11H10	490.43	428.71	378.54
557	CycHexylBenzene	C12H16	503.07	431.22	374.14
515	1,2,4-Mesitylene	C9H12	436.26	373.33	323.27
519	Isobutylbenzene	C10H14	452.75	385.33	332.10
424	DiPhnAcetylene	C14H10	535.26	469.92	416.81
544	P-DiisopropylBz	C12H18	477.33	410.16	356.78
518	N-Butylbenzene	C10H14	458.66	391.75	338.71
516	1,3,5-Mesitylene	C9H12	436.26	373.33	323.27
809	Acenaphthalene	C12H8	509.69	451.64	403.71
725	123-TriMthIndene	C12H14	496.66	432.05	379.92
527	1,4-DiEthBenzene	C10H14	460.66	393.97	341.03
558	Diphenyl	C12H10	510.30	445.30	392.61
576	2-Ethyl-m-Xylene	C10H14	459.87	394.28	342.09
620	p-ISOPROPENYLSTY	C11H12	483.05	420.38	369.75
585	o-PropylToluene	C10H14	459.25	393.01	340.41
577	2-Ethyl-p-Xylene	C10H14	459.87	394.28	342.09
579	4-Ethyl-o-Xylene	C10H14	459.87	394.28	342.09
586	m-Propyltoluene	C10H14	459.25	393.01	340.41
587	p-Propyltoluene	C10H14	459.25	393.01	340.41
578	4-Ethyl-m-Xylene	C10H14	459.87	394.28	342.09
575	5-Ethyl-m-Xylene	C10H14	459.87	394.28	342.09
530	Prehnitene	C10H14	459.23	394.67	343.18
709	2,6-2Mth-Naphtha	C12H12	507.52	444.65	393.51
715	2,7-2Mth-Naphtha	C12H12	507.52	444.65	393.51
719	2-ETHYLNAPHTHALENE	C12H12	506.80	446.75	397.61
621	p-tert-BUTYLSTY	C12H16	489.35	426.44	375.67
532	1,2,4,5-TetMthBz	C10H14	459.23	394.67	343.18
531	1,2,3,5-TetMthBz	C10H14	459.23	394.67	343.18
533	p-tert-BUTYL ET	C12H18	486.87	425.53	375.92
567	N-Pentylbenzene	C11H16	480.07	411.14	356.44
718	1-n-PROPYLNAPHTH	C13H14	521.58	460.14	409.92
562	1,1-DiPhnEthane	C14H14	538.86	467.15	409.58
616	4-ISOBUTYLSTYRE	C12H16	495.44	432.24	381.17
260	1-Decene	C10H20	443.31	379.53	329.01
735	Cis-Stilbene	C14H12	552.06	481.23	424.00
568	Hexylbenzene	C12H18	499.95	429.26	373.08
563	Diphenylmethane	C13H12	533.18	461.44	403.85
564	1,2-DiPhnEthane	C14H14	562.66	482.29	418.46
804	Anthracene	C14H10	542.86	481.60	431.19

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

736	Trans-Stilbene	C14H12	552.06	481.23	424.00
805	Phenanthrene	C14H10	542.86	481.60	431.19
713	1-ButNaphthalene	C14H16	539.46	473.02	419.11
807	Pyrene	C16H10	567.87	509.30	460.68
261	1-Undecene	C11H22	464.37	398.58	346.39
581	23-2C1-23-2PhnC4	C18H22	583.22	510.06	451.15
549	N-Heptylbenzene	C13H20	518.50	446.24	388.74
710	1-PhnNaphthalene	C16H12	571.24	506.83	453.97
566	2,4-Diphenyl-4-M	C18H20	594.21	519.69	459.62
561	O-Terphenyl	C18H14	598.21	530.88	475.75
569	N-Octylbenzene	C14H22	535.86	462.20	403.53
565	Triphenylmethane	C19H16	616.17	543.20	483.88
714	N-C6-Naphthalene	C16H20	567.34	498.56	442.80
717	Fluoranthene	C16H10	567.87	509.30	460.68
716	1-Hexyl-Tetralin	C16H24	561.57	493.38	438.17
731	TriPhnEthylene	C20H16	633.19	558.66	498.06
806	Chrysene	C18H12	720.01	530.36	479.79
588	1,1,2TriPhenEth	C20H18	627.47	553.69	493.74
711	1-n-NonylNaphtha	C19H26	604.33	532.73	474.72
570	N-Nonylbenzene	C15H24	552.17	477.25	417.53
712	1-Decyl Naphtha	C20H28	615.58	543.17	484.52
559	P-Terphenyl	C18H14	598.21	530.88	475.75
560	M-Terphenyl	C18H14	598.21	530.88	475.75
589	TetraPhenylMetha	C25H20	681.47	605.14	542.99
554	Decylbenzene	C16H26	567.52	491.48	430.81
732	TetraPhnEthylene	C26H20	708.97	629.79	565.31
574	N-Dodecylbenzene	C18H30	595.72	517.75	455.47
571	N-Undecylbenzene	C17H28	582.01	504.96	443.44
572	Tridecylbenzene	C19H32	608.72	529.93	466.94
573	n-TETRADECYLBENZ	C20H34	609.74	535.38	475.55
2575	n-PENTADECYLBENZ	C21H36	621.01	545.91	485.48
2576	n-HEXADECYLBENZ	C22H38	631.79	556.01	495.03
2577	n-HEPTADECYLBENZ	C23H40	642.13	565.72	504.23
2578	n-OCTADECYLBENZE	C24H42	652.05	575.05	513.09

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

Halocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1544	Allyl Chloride	C3H5Cl	317.53	266.37	226.24
1595	2-Chloropropene	C3H5Cl	288.39	243.32	207.77
1531	3-Chloropropyne	C3H3Cl	327.58	274.69	233.28

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1561	6Cl-1,3Butadiene	C4Cl6	470.84	408.72	358.55
1535	T-Butyl Chloride	C4H9Cl	317.77	269.14	230.76
1583	Chloroprene	C4H5Cl	356.75	301.55	257.89
1530	Isopropyl Cl	C3H7Cl	303.12	256.54	219.70
1572	O-DiCl-Benzene	C6H4Cl2	448.80	381.59	328.31
1585	Propyl Chloride	C3H7Cl	322.32	272.62	233.33
1684	Isopropyl Iodide	C3H7I	364.95	305.53	259.21
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	392.71	334.08	287.56
1651	2-Bromopropane	C3H7Br	323.85	273.51	233.82
1691	Iodobenzene	C6H5I	472.08	404.81	351.05
1860	Fluorobenzene	C6H5F	349.80	295.12	252.09
1571	Chlorobenzene	C6H5Cl	401.62	339.77	290.95
1680	Bromobenzene	C6H5Br	434.99	375.04	326.77
1526	1,2-DiCl-Propane	C3H6Cl2	373.63	317.17	272.41
1683	Propyl Iodide	C3H7I	374.76	315.45	268.93
1576	Benzotrichloride	C7H5Cl3	473.38	416.84	370.55
1536	2,3-DICHLOROBUT	C4H8Cl2	401.27	341.65	294.34
2638	2-Bromobutane	C4H9Br	354.82	300.69	257.94
1586	1-Chlorobutane	C4H9Cl	353.36	299.83	257.47
1573	M-DiCl-Benzene	C6H4Cl2	448.80	381.59	328.31
2634	Benzotrifluoride	C7H5F3	376.93	329.76	291.33
1574	P-DiCl-Benzene	C6H4Cl2	448.80	381.59	328.31
1650	1-Bromopropane	C3H7Br	335.08	284.34	244.12
1587	2-Chlorobutane	C4H9Cl	334.64	284.08	244.06
2653	8F-2-Butene	C4F8	316.78	281.79	252.75
1678	M-Dibromobenzene	C6H4Br2	494.19	432.41	381.98
1537	1,2-DiCl-Butane	C4H8Cl2	382.74	326.00	280.97
1597	34-DiCl-1-Butene	C4H6Cl2	402.52	340.50	291.58
1577	O-Chlorotoluene	C7H7Cl	429.36	365.35	314.61
1532	123-3Cl-Propane	C3H5Cl3	440.31	374.91	322.93
1578	P-Chlorotoluene	C7H7Cl	429.36	365.35	314.61
1562	Benzyl Chloride	C7H7Cl	449.75	387.72	337.84
2661	P-Bromotoluene	C7H7Br	457.69	395.96	346.18
1508	1,4-DiCl-Butane	C4H8Cl2	420.22	357.66	308.01
1655	1-Bromobutane	C4H9Br	364.57	310.27	267.19
1599	BenzylDichloride	C7H6Cl2	470.92	407.29	356.04
2652	Perfluoropropane	C3F8	263.57	233.14	207.97
1505	2-Butylene DiCl	C4H6Cl2	412.45	348.39	297.86
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	429.64	362.65	309.88
1588	1-Chloropentane	C5H11Cl	381.69	324.86	279.82
1592	1,2,4-TriCl-Bz	C6H3Cl3	491.43	419.68	362.58
1579	2,4-2Cl-Toluene	C7H6Cl2	472.40	403.70	349.05
2593	1,3,5-TriCl-BZ	C6H3Cl3	491.43	419.68	362.58
1697	1-Br-Naphthalene	C10H7Br	520.67	459.10	408.60
1622	Perfluorobutane	C4F10	270.16	239.94	214.94
1857	P-Cl-Benzo-TriF	C7H4ClF3	410.55	359.76	318.38

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

1509	1,5-DiCl-Pentane	C5H10Cl2	444.92	379.78	328.01
1589	1-Cl-Naphthalene	C10H7Cl	504.05	440.47	388.76
1582	6ClCycPentadiene	C5Cl6	502.27	434.00	379.11
1864	Perfluorobenzene	C6F6	355.13	303.31	262.18
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	442.23	388.17	344.10
1667	1-Bromoheptane	C7H15Br	439.47	377.01	327.29
1575	HexaCl-Benzene	C6Cl6	598.45	516.52	450.77
2640	Freon 123B1	C2HBrClF3	330.63	287.02	251.68
1504	Vinyl Chloride	C2H3Cl	273.36	231.12	197.56
1672	1,1-DiBr-Ethane	C2H4Br2	376.72	319.22	273.69
1580	Acetylene DiCl	C2H2Cl2	329.00	279.02	239.26
1692	Diiodomethane	CH2I2	451.24	376.43	318.20
1698	Bromoform	CHBr3	427.39	363.31	312.36
2687	Freon 13B1	CBrF3	276.77	239.86	209.84
2690	Br-3F-Ethylene	C2BrF3	287.93	249.44	218.17
1649	Tetrabromoethane	C2H2Br4	516.55	441.18	381.15
2686	Freon 12B1	CBrClF2	286.46	245.98	213.44
1503	Ethyl Chloride	C2H5Cl	288.12	242.89	207.17
2641	Br-TriCl-Methane	CBrCl3	398.41	348.01	306.80
1641	Methyl Bromide	CH3Br	267.09	225.31	192.21
2688	Freon 12B2	CBr2F2	317.84	272.43	236.04
2545	2,3-DiCl-Propene	C3H4Cl2	363.35	308.13	264.32
1673	1,2-DiBr-Ethane	C2H4Br2	385.46	328.06	282.39
2637	Dibromomethane	CH2Br2	355.90	302.05	259.23
1542	TetraCl-Ethylene	C2Cl4	402.97	345.61	299.66
1541	TriCl-Ethylene	C2HCl3	352.59	301.55	260.74
1527	111-TriCl-Ethane	C2H3Cl3	362.07	315.85	278.12
1612	Cl-2F-Ethylene	C2HClF2	246.34	210.83	182.30
2639	Br-Cl-Methane	CH2BrCl	343.67	290.72	248.72
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	329.00	279.02	239.26
1682	Ethyl Iodide	C2H5I	342.95	287.40	243.96
1522	1,1-DiCl-Ethane	C2H4Cl2	324.50	275.14	236.00
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	248.44	208.85	177.76
1525	Hexachloroethane	C2Cl6	445.14	395.00	353.59
1528	1112-4Cl-Ethane	C2H2Cl4	411.64	359.39	316.77
1590	Penta-Cl-Ethane	C2HCl5	432.50	378.39	334.24
1529	1122-4Cl-Ethane	C2H2Cl4	421.09	359.79	310.90
2693	Perfluoroethane	C2F6	255.60	225.05	199.79
2692	Cl-PentaF-Ethane	C2ClF5	263.88	228.17	199.31
2655	122-3Cl-112-3FC2	C2Cl3F3	324.20	272.68	232.39
1609	12-2Cl-1122-4FC2	C2Cl2F4	283.71	238.55	203.23
2526	1,1-DiCl-Propane	C3H6Cl2	355.03	301.91	259.75
1645	Ethyl Bromide	C2H5Br	302.74	256.12	219.19
2658	1112-4Cl-22-2FC2	C2Cl4F2	385.54	336.02	295.80
1619	111-3F-Ethane	C2H3F3	237.36	205.72	179.93
1524	1,1,2-3Cl-Ethane	C2H3Cl3	393.99	335.05	288.19

Table C.5 Boiling Temperatures Calculated by the GC-ESD method (Continued)

2691	Genetron 1113	C2ClF3	261.20	226.78	198.70
1591	Vinylidene DiCl	C2H2Cl2	303.51	259.50	224.20
1614	Difluoromethane	CH2F2	241.04	187.24	144.16
2694	Vinyl Bromide	C2H3Br	296.11	248.41	210.93
1694	Refrigerant 123	C2HCl2F3	319.80	277.56	243.31
1523	1,2-DiCl-Ethane	C2H4Cl2	363.53	307.46	263.07
2656	1122-4Cl-12-2FC2	C2Cl4F2	364.83	307.06	261.86
2527	1,3-DiCl-Propane	C3H6Cl2	393.23	333.66	286.45

Table C. 6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs.

Nitrates

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1761	Nitroethane	C2H5NO2	380.47	324.85	280.87
1763	2-Nitropropane	C3H7NO2	410.35	350.99	304.15
1762	1-Nitropropane	C3H7NO2	409.98	350.37	303.31
1779	P-Nitrotoluene	C7H7NO2	505.62	436.03	380.56
1886	Nitrobenzene	C6H5NO2	478.13	411.61	358.64
1778	O-Nitrotoluene	C7H7NO2	505.62	436.03	380.56
1780	M-Nitrotoluene	C7H7NO2	505.62	436.03	380.56
1891	O-Nitroanisole	C7H7NO3	533.72	462.56	405.43
2740	M-Dinitrobenzene	C6H4N2O4	578.62	504.47	444.39
2742	P-Dinitrobenzene	C6H4N2O4	578.62	504.47	444.39
2741	O-Dinitrobenzene	C6H4N2O4	578.62	504.47	444.39
2749	3,5-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2743	DNT	C7H6N2O4	599.81	523.50	461.65
2745	3,4-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2744	2,6-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2748	2,5-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2746	1,3,5-TrinitroBz	C6H3N3O6	656.09	577.20	512.49
2747	Trinitrotoluene	C7H5N3O6	673.23	592.72	526.69

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Thiols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1802	Ethyl Mercaptan	C2H6S	275.49	230.81	196.16
1820	Dimethyl Sulfide	C2H6S	299.07	251.97	215.34
1843	Thiacyclopentane	C4H8S	345.95	291.10	248.62
1803	1-Propanethiol	C3H8S	312.53	262.67	224.06
1805	Isobut Mercaptan	C4H10S	347.47	292.64	250.20
6860	Ethylenedithiol	C2H6S2	367.60	310.20	265.35
1811	Cyclohexanethiol	C6H12S	406.88	344.23	295.63
1828	DiMth Disulfide	C2H6S2	367.60	310.20	265.35
1841	Butanethiol	C4H10S	346.45	292.02	249.87
1814	Methylproylsulf	C4H10S	346.45	292.02	249.87
2816	ETHYLtBUTYL SUL	C6H14S	399.38	337.65	289.90
1818	Diethyl Sulfide	C4H10S	347.42	293.30	251.38
1812	Benzyl Mercaptan	C7H8S	456.69	387.55	333.54
1838	T-OctylMercaptan	C8H18S	452.94	384.34	331.08
1827	1-Pentanethiol	C5H12S	377.62	319.15	273.82

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

2815	METHnBUTYL SULFD	C5H12S	395.20	335.32	288.72
1824	DiethylDisulfide	C4H10S2	425.13	361.32	311.50
1807	N-Hexylmercaptan	C6H14S	406.39	344.33	296.15
6857	Dimercaptoethyl	C4H10OS2	452.60	386.94	335.19
1839	1-Heptanethiol	C7H16S	433.06	367.79	317.03
1829	DiProp Disulfide	C6H14S2	475.04	405.34	350.78
1809	1-Octanethiol	C8H18S	457.87	389.74	336.65
1808	N-Nonanethiol	C9H20S	481.06	410.36	355.14
1826	1-Decanethiol	C10H22S	502.79	429.77	372.62
2838	tertDodecanThiol	C12H26S	539.84	462.09	401.19
1825	1-Undecanethiol	C11H24S	523.22	448.11	389.20
1837	Dodecylthiol	C12H26S	542.49	465.48	404.95

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Epoxides

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1440	ISOBUTYLENE OXID	C4H8O	284.97	239.59	204.45
1479	Tetrahydrofuran	C4H8O	296.38	250.41	214.64
1477	2,5-Dihydrofuran	C4H6O	311.63	264.45	227.48
1408	1-Methoxypropane	C4H10O	312.01	264.59	227.65
1411	2-Methoxypropane	C4H10O	312.29	264.64	227.54
1421	1,4-Dioxane	C4H8O2	335.63	286.52	247.84
2422	1,3-DIOXANE	C4H8O2	335.63	286.52	247.84
1426	2-Methoxybutane	C5H12O	344.24	292.32	251.86
1413	1-Methoxybutane	C5H12O	343.78	292.12	251.83
1461	Methoxybenzene	C7H8O	417.38	356.05	307.86
1448	1-Ethoxybutane	C6H14O	364.57	310.13	267.69
1429	1-MethoxyPentane	C6H14O	364.57	310.13	267.69
6885	Ethyl-3-Ethoxypr	C7H14O3	438.17	376.95	328.51

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Formate

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1301	Methyl Formate	C2H4O2	275.67	233.89	201.11
1311	Vinyl Formate	C3H4O2	313.28	266.50	229.77
1302	Ethyl Formate	C3H6O2	311.34	264.48	227.78

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

2306	t-Butyl Formate	C5H10O2	365.48	310.41	267.47
1303	Propyl Formate	C4H8O2	343.83	292.53	252.38
2305	sec-ButylFormate	C5H10O2	374.36	318.85	275.41
2311	CYCLOHEXL FORMAT	C7H12O2	428.06	365.07	315.73
1304	N-Butyl Formate	C5H10O2	373.68	318.46	275.22
1305	Isobutyl Formate	C5H10O2	374.36	318.85	275.41
2350	Benzyl Formate	C8H8O2	469.71	402.25	349.05
2307	n-Hexyl Formate	C7H14O2	426.92	365.11	316.59
1306	N-Pentyl Formate	C6H12O2	401.27	342.58	296.56
2308	n-Heptyl Formate	C8H16O2	450.87	386.26	335.47
1308	N-Octyl Formate	C9H18O2	473.30	406.17	353.31
1309	n-Nonyl Formate	C10H20O2	494.38	424.97	370.22
1310	n-Decyl Formate	C11H22O2	514.26	442.78	386.30

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

	Ester				
Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1351	Mth Methacrylate	C5H8O2	370.32	316.52	274.19
1312	Methyl Acetate	C3H6O2	305.00	259.70	224.14
1331	Vinyl Propionate	C5H8O2	356.25	303.94	262.91
1321	Vinyl Acetate	C4H6O2	339.15	289.49	250.43
1352	Eth MthAcrylate	C6H10O2	385.99	329.83	285.75
1322	MethylPropionate	C4H8O2	337.23	287.52	248.51
1341	Methyl Acrylate	C4H6O2	327.79	278.84	240.52
1313	Ethyl Acetate	C4H8O2	323.69	275.41	237.65
1319	IsopropylAcetate	C5H10O2	367.43	313.55	271.29
1332	Methyl Butyrate	C5H10O2	354.21	301.90	260.95
1342	Ethyl Acrylate	C5H8O2	358.50	305.46	263.93
1318	Allyl Acetate	C5H8O2	368.81	315.23	273.08
1314	N-Propyl Acetate	C5H10O2	366.88	313.27	271.19
1323	Ethyl Propionate	C5H10O2	354.21	301.90	260.95
1360	I-But I-Butyrate	C8H16O2	437.57	374.14	324.42
1320	Sec-ButylAcetate	C6H12O2	395.00	337.63	292.59
1336	PropylI-Butyrate	C7H14O2	411.95	351.77	304.64
1353	N-C3-Mthacrylate	C7H12O2	400.71	340.91	294.24
1333	Ethyl Butyrate	C6H12O2	382.44	326.53	282.71
1347	EthylIsovalerate	C7H14O2	409.41	349.98	303.37
1315	N-Butyl Acetate	C6H12O2	394.32	337.23	292.39
1390	Methyl Benzoate	C8H8O2	461.07	395.52	343.71

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

1388	ISOBUTYL MTHACR	C8H14O2	440.26	376.87	327.08
1343	1-PropylAcrylate	C6H10O2	384.45	328.52	284.62
1316	Isobutyl Acetate	C6H12O2	395.00	337.63	292.59
1344	N-Butyl Acrylate	C7H12O2	408.48	348.42	301.38
1357	Pentyl Acetate	C7H14O2	419.84	359.65	312.30
1327	N-PropN-Butyrate	C7H14O2	408.66	349.53	303.13
1324	N-PropPropionate	C6H12O2	382.44	326.53	282.71
1291	Acetic Anhydride	C4H6O3	406.16	349.49	304.41
1389	N-ButMthacrylate	C8H14O2	439.31	376.25	326.69
1359	Benzyl Acetate	C9H10O2	477.75	410.28	356.94
1326	N-But Propionate	C7H14O2	408.66	349.53	303.13
1391	Ethyl Benzoate	C9H10O2	477.57	409.23	355.38
1897	CH3OC3H600CH3	C6H12O3	430.45	370.76	323.38
1392	DiethylCarbonate	C5H10O3	386.43	331.92	288.79
1385	N-But N-Butyrate	C8H16O2	433.13	371.11	322.35
1317	IsopentylAcetate	C7H14O2	420.65	360.15	312.60
1363	N-Hexyl Acetate	C8H16O2	435.73	372.95	323.68
1387	Ethylene Acetate	C6H10O4	446.80	386.28	337.99
1393	Diethyl Oxalate	C6H10O4	426.76	368.03	321.34
1365	Butyl Benzoate	C11H14O2	520.53	447.43	389.68
1361	I-C5 I-Valerate	C10H20O2	479.67	412.00	358.69
1367	Heptyl Acetate	C9H18O2	458.74	393.35	341.93
1346	N-Butyl Valerate	C9H18O2	456.07	391.42	340.53
1358	2-C2-C6 Acetate	C10H20O2	488.16	420.02	366.20
1394	Diethyl Malonate	C7H12O4	452.11	389.98	340.62
1292	Propionyl Oxide	C6H10O3	436.51	375.67	327.42
1364	Benzyl Benzoate	C14H12O2	593.02	511.44	446.67
1381	2Mth p-Phthalate	C10H10O4	550.73	477.81	419.36
1368	n-Octyl Acetate	C10H20O2	480.36	412.60	359.23
1377	DiMthI-Phthalate	C10H10O4	540.96	467.58	409.09
1896	Ethylene DiAcr	C8H10O4	479.61	414.33	362.37
1386	2-Ethylhexyl Acr	C11H20O2	503.74	433.43	377.93
1395	Methyl Decanoate	C11H22O2	497.93	428.76	374.12
1369	n-Nonyl Acetate	C11H22O2	500.73	430.82	375.65
1370	n-Decyl Acetate	C12H24O2	519.98	448.11	391.29
1345	N-ButylNonanoate	C13H26O2	535.31	462.40	404.58
1375	DiProp Phthalate	C14H18O4	609.34	529.21	465.07
1376	Diisobutyl Phtha	C16H22O4	641.78	558.33	491.43
1396	IsopropMyristate	C17H34O2	603.89	524.13	460.51
1383	Butyl Stearate	C22H44O2	665.25	581.62	514.19
1362	Methyl Oleate	C19H36O2	634.94	553.66	488.37
1355	Diisooctyl Phtha	C24H38O4	736.52	646.49	573.41
1382	DioctylTerephtha	C24H38O4	733.35	644.04	571.48
1384	DIBUTYL SEBACATE	C18H34O4	633.74	554.33	490.23
1371	Diisodecyl Phtha	C28H46O4	774.07	682.19	607.07

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

1354	DioctylPhthalate	C24H38O4	736.52	646.49	573.41
2375	DiethylPhthalate	C12H14O4	570.26	494.81	434.43
2388	Dipropyl Maleate	C10H16O4	524.99	454.93	399.00
2381	Diallyl Maleate	C10H12O4	522.48	453.85	398.84
2370	Glyceryl Triacet	C9H14O6	545.58	476.49	420.67
2382	Dibutyl Maleate	C12H20O4	559.86	486.31	427.45
2376	DibutylPhthalate	C16H22O4	638.63	555.96	489.62
2353	CetylMthacrylate	C20H38O2	646.63	563.75	497.21
2379	Dihexyl Adipate	C18H34O4	633.74	554.33	490.23
2321	T-Butyl Acetate	C6H12O2	376.91	320.39	276.35
2332	Methl.I-butyrate	C5H10O2	356.95	303.65	262.02
2354	AllylMthacrylate	C7H10O2	416.73	356.58	309.29
2364	CYCLOHEXL ACETAT	C8H14O2	437.05	373.05	322.94
2337	EthylIsobutyrate	C6H12O2	385.48	328.54	284.02
2384	IsobutylAcrylate	C7H12O2	413.99	353.78	306.56
2380	1,1-Diacetoxy C2	C6H10O4	432.46	372.05	324.19
2392	n-PropylBenzoate	C10H12O2	499.73	428.89	373.00
2377	DiMth Phthalate	C10H10O4	550.73	477.81	419.36
2386	Diethyl Maleate	C8H12O4	486.12	420.25	367.77
2385	Mth Dodecanoate	C13H26O2	535.31	462.40	404.58
3379	Dioctyl Adipate	C22H42O4	691.06	606.03	537.11
5886	Mth Acetoacetate	C5H8O3	421.20	362.20	315.39
5884	Ethoxy Acetate	C6H12O3	422.55	363.89	317.35
5887	EthAcetoAcetate	C6H10O3	445.69	383.68	334.46
5885	Carbitol Acetate	C8H16O4	489.07	424.44	372.68

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Ketone

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1096	Methyl Isopropen	C5H8O	378.72	322.37	278.23
1079	Cyclopentanone	C5H8O	361.70	306.69	263.74
1051	Acetone	C3H6O	310.94	263.47	226.35
1052	MEK	C4H8O	344.35	292.28	251.59
1065	Mesityl Oxide	C6H10O	413.14	352.53	304.97
1066	T-But Mth Ketone	C6H12O	396.26	336.46	289.87
1060	2-Pentanone	C5H10O	374.95	318.84	274.98
1061	Mth iC3 Ketone	C5H10O	375.79	319.35	275.25
1053	Diethyl Ketone	C5H10O	364.03	309.42	266.77
1059	3-Hexanone	C6H12O	392.68	334.41	288.87

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

1099	Diketene	C4H4O2	321.76	273.61	235.79
1055	Sec-ButMthKetone	C6H12O	404.14	344.09	297.15
1054	MIBK	C6H12O	404.14	344.09	297.15
1095	EthIsopropKetone	C6H12O	393.53	334.93	289.16
1063	2-Heptanone	C7H14O	429.37	366.48	317.21
1064	5-Mth-2-Hexanone	C7H14O	430.43	367.17	317.65
1058	4-Heptanone	C7H14O	419.25	357.72	309.56
1057	3-Heptanone	C7H14O	419.25	357.72	309.56
1076	2,4-Pentanedione	C5H8O2	442.09	379.43	329.78
1068	DiisobutylKetone	C9H18O	469.41	401.60	348.41
1097	2-CycC6 CycC6one	C12H20O	539.93	462.39	401.49
1083	2-Octanone	C8H16O	453.77	388.01	336.42
1073	Dibutyl Ketone	C9H18O	467.13	400.04	347.36
1062	2-Hexanone	C6H12O	403.19	343.49	296.79
1077	Isophorone	C9H14O	474.26	404.60	350.06
1090	Acetophenone	C8H8O	474.14	405.24	351.01
1080	Cyclohexanone	C6H10O	391.68	332.75	286.74
1074	2-Nonanone	C9H18O	476.59	408.25	354.55

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
404	DiMth-Acetylene	C4H6	291.60	245.13	209.13
202	Propylene	C3H6	219.25	182.91	155.00
412	2-Pentyne	C5H8	388.79	329.44	283.36
207	2-Methylpropene	C4H8	261.75	219.24	186.56
204	1-Butene	C4H8	259.96	217.75	185.31
205	Cis-2-Butene	C4H8	274.88	231.04	197.20
402	Propyne	C3H4	234.40	196.81	167.67
406	3-Hexyne	C6H10	359.10	303.52	260.44
206	Trans-2-Butene	C4H8	274.88	231.04	197.20
407	2-Hexyne	C6H10	359.10	303.52	260.44
231	33-2Mth-1-Butene	C6H12	320.14	268.74	229.30
230	23-2Mth-1-Butene	C6H12	332.80	280.38	239.98
229	2-Ethyl-1-Butene	C6H12	332.24	280.13	239.94
8	I-Pentane	C5H12	294.34	246.88	210.46
14	2,2-DiMth-Butane	C6H14	317.29	266.04	226.80
232	23-2Mth-2-Butene	C6H12	346.50	293.07	251.67
213	3-Mth-1-Butene	C5H10	297.16	249.57	212.96

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

212	2-Mth-1-Butene	C5H10	298.61	250.99	214.33
211	Trans-2-Pentene	C5H10	310.55	261.80	224.12
210	Cis-2-Pentene	C5H10	310.55	261.80	224.12
223	4-Mth-1-Pentene	C6H12	330.99	278.87	238.71
221	2-Mth-1-Pentene	C6H12	332.24	280.13	239.94
248	2-t-Butylpropene	C7H14	354.28	298.38	255.37
227	Cs-4-Mth-2-C5H10	C6H12	343.78	290.39	249.10
224	2-Mth-2-Pentene	C6H12	339.53	286.57	245.65
403	1-Butyne	C4H6	273.87	230.58	197.05
15	2,3-DiMth-Butane	C6H14	328.85	276.55	236.36
214	2-Mth-2-Butene	C5H10	306.38	257.83	220.38
228	Ts-4-Mth-2-C5H10	C6H12	343.78	290.39	249.10
225	Cs-3-Mth-2-C5H10	C6H12	339.53	286.57	245.65
218	Trans-2-Hexene	C6H12	343.18	290.10	249.01
2226	3-METH-Tr-2Pente	C6H12	339.53	286.57	245.65
222	3-Mth-1-Pentene	C6H12	330.99	278.87	238.71
257	2-Diisobutylene	C8H16	390.78	330.39	283.74
256	1-Diisobutylene	C8H16	383.96	324.35	278.37
217	Cis-2-Hexene	C6H12	343.18	290.10	249.01
2414	1-Heptyne	C7H12	372.44	315.94	272.05
13	3-Methylpentane	C6H14	328.31	276.32	236.34
219	Cis-3-Hexene	C6H12	343.18	290.10	249.01
12	2-Methylpentane	C6H14	328.31	276.32	236.34
220	Trans-3-Hexene	C6H12	343.18	290.10	249.01
405	1-Pentyne	C5H8	309.66	261.40	224.01
209	1-Pentene	C5H10	296.82	249.50	213.08
11	N-Hexane	C6H14	327.82	276.12	236.34
235	Cis-2-Heptene	C7H14	373.20	316.28	272.14
249	Cis-3-Heptene	C7H14	373.20	316.28	272.14
216	1-Hexene	C6H12	330.47	278.65	238.69
239	3-Eth-1-Pentene	C7H14	362.05	305.94	262.60
226	4-Mth-1-Hexene	C7H14	362.05	305.94	262.60
240	3-Mth-1-Hexene	C7H14	362.05	305.94	262.60
419	3-Mth-1-Butyne	C5H8	310.07	261.54	223.96
233	2-Eth-1-Pentene	C7H14	363.13	307.05	263.70
238	2-Mth-1-Hexene	C7H14	363.13	307.05	263.70
416	1-Octyne	C8H14	400.27	340.33	293.66
289	2,3Dimeth Hexene	C8H16	392.51	332.55	286.13
234	1-Heptene	C7H14	361.37	305.57	262.45
413	1-Hexyne	C6H10	342.35	289.73	248.91
237	Trans-3-Heptene	C7H14	373.20	316.28	272.14
236	Trans-2-Heptene	C7H14	373.20	316.28	272.14
251	Trans-2-Octene	C8H16	400.98	340.64	293.75
279	Trans-4-Octene	C8H16	400.98	340.64	293.75
277	Trans-3-Octene	C8H16	400.98	340.64	293.75

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

2252	2Methl-1-Heptene	C8H16	391.67	332.05	285.86
250	1-Octene	C8H16	389.91	330.58	284.61
258	2-Ethyl-1-Hexene	C8H16	391.67	332.05	285.86
280	3-Octene	C8H16	400.98	340.64	293.75
278	4-Octene	C8H16	400.98	340.64	293.75
276	2-Octene	C8H16	400.98	340.64	293.75
259	1-Nonene	C9H18	416.41	353.92	305.38
262	1-Dodecene	C12H24	485.93	415.73	360.80
263	1-Tridecene	C13H26	506.36	434.07	377.37
264	1-Tetradecene	C14H28	525.65	451.45	393.13
265	1-Pentadecene	C15H30	543.90	467.97	408.15
266	1-Hexadecene	C16H32	561.21	483.71	422.51
267	1-Octadecene	C18H36	593.34	513.06	449.40
281	1-Heptadecene	C17H34	577.67	498.72	436.24
284	1-Eicosene	C20H40	622.54	539.96	474.18
283	1-Nonadecene	C19H38	608.27	526.79	462.04
3	Propane	C3H8	216.11	179.93	152.24
4	I-Butane	C4H10	257.09	214.78	182.39
9	Neopentane	C5H12	281.89	235.41	199.91
5	N-Butane	C4H10	257.03	214.95	182.72
7	pentane	C5H12	294.05	246.85	210.62
44	Hexamethylethane	C8H18	371.31	312.18	266.86
25	223-TriMthButane	C7H16	350.42	294.63	251.82
24	3,3-DiMthPentane	C7H16	349.69	294.25	251.67
51	2,2,3,3-4Mth-C5	C9H20	399.99	337.39	289.26
21	2,2-DiMthPentane	C7H16	349.69	294.25	251.67
42	2,3,3-TriMth-C5	C8H18	380.38	320.86	275.05
22	2,3-DiMthPentane	C7H16	360.19	303.86	260.47
40	2,2,3-TriMth-C5	C8H18	380.38	320.86	275.05
23	2,4-DiMthPentane	C7H16	360.19	303.86	260.47
41	2,2,4-TriMth-C5	C8H18	380.38	320.86	275.05
39	3-Mth-3-Eth-C5	C8H18	379.53	320.36	274.80
20	3-Ethylpentane	C7H16	359.49	303.50	260.33
52	2,2,3,4-4Mth-C5	C9H20	409.13	345.88	297.11
54	2334TetrMethPent	C9H20	409.13	345.88	297.11
53	2,2,4,4-4Mth-C5	C9H20	399.99	337.39	289.26
43	2,3,4-TriMth-C5	C8H18	389.98	329.73	283.21
36	3,3-DiMth-Hexane	C8H18	379.53	320.36	274.80
19	3-Methylhexane	C7H16	359.49	303.50	260.33
18	2-Methylhexane	C7H16	359.49	303.50	260.33
38	2-Mth-3-Eth-C5	C8H18	389.11	329.21	282.94
190	2,2-2C1-3-C2-C5	C9H20	408.11	345.25	296.74
32	2,2-DiMth-Hexane	C8H18	379.53	320.36	274.80
37	3,4-DiMth-Hexane	C8H18	389.11	329.21	282.94
50	3,3-DiEthPentane	C9H20	407.14	344.65	296.40

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

34	2,4-DiMth-Hexane	C8H18	389.11	329.21	282.94
33	2,3-DiMth-Hexane	C8H18	389.11	329.21	282.94
17	N-Heptane	C7H16	358.84	303.16	260.20
49	244TriMethHexane	C9H20	408.11	345.25	296.74
192	2,4-2C1-3-C2-C5	C9H20	416.91	353.45	304.33
47	2,2,5-TriMth-C6	C9H20	408.11	345.25	296.74
35	2,5-DiMth-Hexane	C8H18	389.11	329.21	282.94
31	3-Ethylhexane	C8H18	388.28	328.72	282.68
30	4-Methylheptane	C8H18	388.28	328.72	282.68
29	3-Methylheptane	C8H18	388.28	328.72	282.68
28	2-Methylheptane	C8H18	388.28	328.72	282.68
96	2,2-DiMthHeptane	C9H20	407.14	344.65	296.40
176	2,6-DiMthHeptane	C9H20	415.93	352.84	303.97
27	N-Octane	C8H18	387.49	328.27	282.45
94	3-Ethylheptane	C9H20	414.99	352.25	303.62
92	3-Methyloctane	C9H20	414.99	352.25	303.62
93	4-Methyloctane	C9H20	414.99	352.25	303.62
91	2-Methyloctane	C9H20	414.99	352.25	303.62
72	2,2-DiMthOctane	C10H22	432.81	367.35	316.66
2095	2,3Dimethloctane	C10H22	440.90	374.95	323.72
2096	2,4Dimethloctane	C10H22	440.90	374.95	323.72
2098	2,6DimethlOctane	C10H22	440.90	374.95	323.72
2097	2,5Dimethloctane	C10H22	440.90	374.95	323.72
2099	2,7DimethlOctane	C10H22	440.90	374.95	323.72
46	N-Nonane	C9H20	414.07	351.68	303.29
88	5-Methylnonane	C10H22	439.86	374.28	323.30
85	3-Methylnonane	C10H22	439.86	374.28	323.30
87	4-Methylnonane	C10H22	439.86	374.28	323.30
86	2-Methylnonane	C10H22	439.86	374.28	323.30
56	N-Decane	C10H22	438.86	373.63	322.90
63	N-Undecane	C11H24	462.05	394.26	341.40
64	N-Dodecane	C12H26	483.81	413.71	358.91
65	N-Tridecane	C13H28	504.31	432.11	375.53
66	N-Tetradecane	C14H30	523.65	449.55	391.34
67	N-Pentadecane	C15H32	541.96	466.12	406.42
68	N-Hexadecane	C16H34	559.32	481.90	420.81
69	N-Heptadecane	C17H36	575.82	496.96	434.59
70	N-Octadecane	C18H38	591.53	511.34	447.79
71	N-Nonadecane	C19H40	606.51	525.12	460.46
73	N-Eicosane	C20H42	620.82	538.31	472.64
74	n-HENEICOSANE	C21H44	634.51	550.99	484.36
75	n-DOCOSANE	C22H46	647.61	563.16	495.65
76	n-TRICOSANE	C23H48	660.19	574.88	506.54
77	n-Tetracosane	C24H50	672.26	586.17	517.06
78	n-PENTACOSANE	C25H52	683.86	597.06	527.23

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

79	n-HEXACOSANE	C26H54	695.03	607.57	537.06
81	n-Octacosane	C28H58	716.15	627.56	555.81
2081	n-TRICONTANE	C30H62	735.81	646.27	573.44
2082	n-Dotriacontane	C32H66	754.17	663.87	590.07
2086	Hexatriacontane	C36H74	787.50	696.12	620.70

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Cyclic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
269	Cyclopentene	C5H8	306.28	257.34	219.50
270	Cyclohexene	C6H10	340.43	286.89	245.47
287	3MthCyclopentene	C6H10	341.33	287.40	245.72
286	1-MthCyclPentene	C6H10	336.94	283.45	242.14
288	4MthCyclopenten	C6H10	341.33	287.40	245.72
273	Cycloheptene	C7H12	371.79	314.17	269.54
274	Cyclooctene	C8H14	400.72	339.49	291.98
101	Cyclopropane	C3H6	208.34	172.55	145.06
810	ADAMANTANE	C10H16	453.99	381.96	326.45
102	Cyclobutane	C4H8	250.48	208.52	176.33
104	Cyclopentane	C5H10	289.16	241.79	205.42
137	Cyclohexane	C6H12	324.52	272.37	232.28
105	MthCyclopentane	C6H12	325.31	272.79	232.44
146	Cs-1,4-2C1-CycC6	C8H16	388.87	327.96	281.01
142	Cs-1,2-2C1-CycC6	C8H16	388.87	327.96	281.01
141	1,1-2C1-CycC6	C8H16	379.17	318.97	272.70
145	Ts-1,3-2C1-CycC6	C8H16	388.87	327.96	281.01
144	Cs-1,3-2C1-CycC6	C8H16	388.87	327.96	281.01
147	Ts-1,4-2C1-CycC6	C8H16	388.87	327.96	281.01
143	Ts-1,2-2C1-CycC6	C8H16	388.87	327.96	281.01
138	MthCyclohexane	C7H14	357.84	301.09	257.41
159	Cycloheptane	C7H14	356.93	300.56	257.15
140	Ethylcyclohexane	C8H16	387.80	327.30	280.63
154	Trans-Decalin	C10H18	445.24	376.44	323.25
149	N-PropylCyc-C6	C9H18	415.52	351.67	302.30
109	Cs-1,2-2C1-CycC5	C7H14	358.82	301.67	257.71
110	Ts-1,2-2C1-CycC5	C7H14	358.82	301.67	257.71
112	Ts-1,3-2C1-CycC5	C7H14	358.82	301.67	257.71
107	Eth-Cyclopentane	C7H14	357.84	301.09	257.41
114	N-PropCycPentane	C8H16	387.80	327.30	280.63

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

108	1,1-DiMthCycC5	C7H14	348.20	291.90	248.73
111	Cs-1,3-2C1-CycC5	C7H14	358.82	301.67	257.71
152	N-ButylCycHexane	C10H20	441.27	374.44	322.63
160	Cyclooctane	C8H16	386.78	326.67	280.27
153	Cis-Decalin	C10H18	445.24	376.44	323.25
115	ISOPROPYLCYCLOPENTANE	C8H16	388.87	327.96	281.01
150	Isopropyl-CycC6	C9H18	416.68	352.42	302.77
116	1-C1-1-C2-CycC5	C8H16	379.17	318.97	272.70
122	Butylcyclpentane	C9H18	415.52	351.67	302.30
155	1,1-Bicyclohexyl	C12H22	493.10	419.03	361.51
158	N-Decylcyclo-C6	C16H32	565.32	485.84	423.32

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Aromatic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
307	1,4-Pentadiene	C5H8	299.51	252.08	215.49
306	1-ts3-Pentadiene	C5H8	313.06	264.25	226.43
414	2-Methyl-1-Butenyne	C5H6	313.77	265.21	227.49
305	Cs1,3-Pentadiene	C5H8	313.06	264.25	226.43
309	Isoprene	C5H8	301.28	253.57	216.75
421	1-Pentene-4-yne	C5H6	312.06	263.77	226.26
303	1,3-Butadiene	C4H6	262.78	220.46	187.84
332	1,4-CyclHexadien	C6H8	355.38	300.64	258.03
501	Benzene	C6H6	337.11	284.04	242.87
315	Cyclopentadiene	C5H6	322.19	271.94	232.82
319	Diisopropenyl	C6H10	336.59	284.10	243.51
615	Ethynylbezene	C8H6	419.63	356.64	307.39
601	Styrene	C8H8	409.97	347.32	298.57
331	1,3-CycHexadiene	C6H8	355.38	300.64	258.03
310	1,5-Hexadiene	C6H10	333.04	281.12	241.00
312	MthCycPentadiene	C6H8	352.20	297.46	254.94
420	1-Pentene-3-yne	C5H6	329.26	277.93	238.07
502	Toluene	C7H8	375.91	318.01	273.00
521	T-Butylbenzene	C10H14	455.47	386.03	332.15
320	Dipropylene	C6H10	357.69	303.41	261.14
520	Sec-Butylbenzene	C10H14	448.41	380.42	327.63
313	1,4-Hexadiene	C6H10	345.60	292.46	251.23
314	Dipropylene	C6H10	357.69	303.41	261.14
316	DiCycPentadiene	C10H12	462.51	395.53	343.05

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

333	1,5-CycOctadiene	C8H12	414.39	353.82	306.45
701	Naphthalene	C10H8	481.35	408.57	351.77
504	Ethylbenzene	C8H10	399.72	338.17	290.41
820	Indan	C9H10	431.30	364.31	312.36
505	O-Xylene	C8H10	411.14	349.05	300.65
612	P-Methylstyrene	C9H10	442.72	376.34	324.54
330	DIISOCROTYL	C8H14	408.66	347.26	299.47
507	P-Xylene	C8H10	411.14	349.05	300.65
329	DIISOBUTENYL	C8H14	395.81	335.81	289.25
506	M-Xylene	C8H10	411.14	349.05	300.65
603	Methylstyrene	C9H10	442.72	376.34	324.54
613	Alpha-MthStyrene	C9H10	439.04	372.76	321.13
510	Isopropylbenzene	C9H12	422.42	357.48	307.15
724	2-Methylindene	C10H10	474.85	403.06	347.08
285	Vinylcyclohexene	C8H12	404.18	342.48	294.57
803	Indene	C9H8	451.92	382.38	328.26
706	Tetralin	C10H12	457.54	387.47	333.06
511	O-Ethyltoluene	C9H12	433.06	367.69	316.81
723	1-Methylindene	C10H10	488.83	416.93	360.52
738	Fluorene	C13H10	572.04	486.93	420.34
619	Tr-1PropenylBz	C9H10	447.31	380.55	328.39
525	O-Diethylbenzene	C10H14	453.93	385.52	332.31
618	Propenyl Bz(cis)	C9H10	447.31	380.55	328.39
602	O-Methylstyrene	C9H10	442.72	376.34	324.54
702	1-MthNaphthalene	C11H10	509.84	434.13	374.89
509	N-Propylbenzene	C9H12	427.23	362.32	311.87
526	M-Diethylbenzene	C10H14	453.93	385.52	332.31
583	Cs-2-PhnButene-2	C10H12	470.21	400.37	345.81
543	M-DiisopropylBz	C12H18	492.91	419.04	361.63
584	Ts-2-PhnButene-2	C10H12	470.21	400.37	345.81
580	1,2-DiC1-3C2-Bz	C10H14	463.62	394.91	341.26
704	1-EthNaphthalene	C12H12	529.05	450.57	389.22
512	M-Ethyltoluene	C9H12	433.06	367.69	316.81
522	1-Mth-2-iC3-Benz	C10H14	454.00	385.59	332.38
513	P-Ethyltoluene	C9H12	433.06	367.69	316.81
514	1,2,3-Mesitylene	C9H12	443.34	377.58	326.18
614	M-Divinylbenzene	C10H10	472.91	402.49	347.50
524	1-Mth-4-iC3-Benz	C10H14	454.00	385.59	332.38
822	Gamma-Terpinene	C10H16	461.94	393.01	339.29
821	Alpha-Terpinene	C10H16	461.94	393.01	339.29
523	1-Mth-3-iC3-Benz	C10H14	454.00	385.59	332.38
703	2-MthNaphthalene	C11H10	509.84	434.13	374.89
557	CycHexylBenzene	C12H16	499.85	424.88	366.54
515	1,2,4-Mesitylene	C9H12	443.34	377.58	326.18
519	Isobutylbenzene	C10H14	454.19	385.84	332.66

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

424	DiPhnAcetylene	C14H10	597.21	512.04	444.88
544	P-DiisopropylBz	C12H18	492.91	419.04	361.63
518	N-Butylbenzene	C10H14	452.78	384.88	332.01
516	1,3,5-Mesitylene	C9H12	443.34	377.58	326.18
809	Acenaphthalene	C12H8	559.43	475.33	409.57
725	123-TriMthIndene	C12H14	522.57	445.10	384.58
527	1,4-DiEthBenzene	C10H14	453.93	385.52	332.31
558	Diphenyl	C12H10	530.96	452.84	391.64
576	2-Ethyl-m-Xylene	C10H14	463.62	394.91	341.26
620	p-ISOPROPENYLSTY	C11H12	498.08	424.75	367.39
585	o-PropylToluene	C10H14	458.25	389.94	336.67
577	2-Ethyl-p-Xylene	C10H14	463.62	394.91	341.26
579	4-Ethyl-o-Xylene	C10H14	463.62	394.91	341.26
586	m-Propyltoluene	C10H14	458.25	389.94	336.67
587	p-Propyltoluene	C10H14	458.25	389.94	336.67
578	4-Ethyl-m-Xylene	C10H14	463.62	394.91	341.26
575	5-Ethyl-m-Xylene	C10H14	463.62	394.91	341.26
530	Prehnitene	C10H14	472.90	403.94	349.87
709	2,6-2Mth-Naphtha	C12H12	536.24	457.92	396.49
715	2,7-2Mth-Naphtha	C12H12	536.24	457.92	396.49
719	2-ETHYLNAPHTHALENE	C12H12	529.05	450.57	389.22
621	p-tert-BUTYLSTY	C12H16	512.93	436.81	377.45
532	1,2,4,5-TetMthBz	C10H14	472.90	403.94	349.87
531	1,2,3,5-TetMthBz	C10H14	472.90	403.94	349.87
533	p-tert-BUTYL ET	C12H18	510.75	434.69	375.45
567	N-Pentylbenzene	C11H16	476.62	406.03	350.96
718	1-n-PROPYLNAPHTH	C13H14	556.65	475.15	411.32
562	1,1-DiPhnEthane	C14H14	562.15	480.38	416.29
616	4-ISOBUTYLSTYRE	C12H16	517.46	441.68	382.40
260	1-Decene	C10H20	441.12	375.78	324.92
735	Cis-Stilbene	C14H12	580.64	498.02	432.88
568	Hexylbenzene	C12H18	498.92	425.92	368.85
563	Diphenylmethane	C13H12	544.82	465.43	403.16
564	1,2-DiPhnEthane	C14H14	557.95	477.41	414.18
804	Anthracene	C14H10	602.30	514.13	444.93
736	Trans-Stilbene	C14H12	580.64	498.02	432.88
805	Phenanthrene	C14H10	602.30	514.13	444.93
713	1-ButNaphthalene	C14H16	569.27	486.75	422.02
807	Pyrene	C16H10	673.23	575.08	497.96
261	1-Undecene	C11H22	464.23	396.34	343.35
581	23-2C1-23-2PhnC4	C18H22	639.33	548.64	477.29
549	N-Heptylbenzene	C13H20	519.85	444.68	385.78
710	1-PhnNaphthalene	C16H12	640.73	549.18	477.05
566	2,4-Diphenyl-4-M	C18H20	642.70	552.94	482.05
561	O-Terphenyl	C18H14	675.38	581.03	506.40

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

569	N-Octylbenzene	C14H22	539.56	462.42	401.86
565	Triphenylmethane	C19H16	683.62	589.05	514.12
714	N-C6-Naphthalene	C16H20	605.03	519.23	451.69
717	Fluoranthene	C16H10	673.23	575.08	497.96
716	1-Hexyl-Tetralin	C16H24	597.56	512.52	445.69
731	TriPhnEthylene	C20H16	702.94	607.26	531.20
806	Chrysene	C18H12	706.32	605.78	526.46
588	1,1,2TriPhenEth	C20H18	697.36	601.80	525.98
711	1-n-NonylNaphtha	C19H26	651.95	562.32	491.36
570	N-Nonylbenzene	C15H24	558.17	479.25	417.16
712	1-Decyl Naphtha	C20H28	666.10	575.42	503.50
559	P-Terphenyl	C18H14	675.38	581.03	506.40
560	M-Terphenyl	C18H14	675.38	581.03	506.40
589	TetraPhenylMetha	C25H20	787.21	682.21	598.45
554	Decylbenzene	C16H26	575.78	495.24	431.75
732	TetraPhnEthylene	C26H20	802.06	698.03	614.55
574	N-Dodecylbenzene	C18H30	608.34	524.99	459.02
571	N-Undecylbenzene	C17H28	592.47	510.46	445.68
572	Tridecylbenzene	C19H32	623.43	538.87	471.80
573	n-TETRADECYLBENZ	C20H34	642.99	556.71	488.12
2575	n-PENTADECYLBENZ	C21H36	656.60	569.33	499.81
2576	n-HEXADECYLBENZ	C22H38	669.62	581.44	511.07
2577	n-HEPTADECYLBENZ	C23H40	682.10	593.09	521.92
2578	n-OCTADECYLBENZE	C24H42	694.06	604.30	532.39

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

Halocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1544	Allyl Chloride	C3H5Cl	315.79	266.51	228.18
1531	3-Chloropropyne	C3H3Cl	327.20	277.39	238.37
1535	T-Butyl Chloride	C4H9Cl	322.41	271.58	232.32
1530	Isopropyl Cl	C3H7Cl	287.24	241.21	205.69
1572	O-DiCl-Benzene	C6H4Cl2	456.46	387.62	333.81
1585	Propyl Chloride	C3H7Cl	313.42	264.13	225.90
1684	Isopropyl Iodide	C3H7I	351.91	296.21	253.10
1651	2-Bromopropane	C3H7Br	317.45	267.25	228.38
1691	Iodobenzene	C6H5I	461.70	391.61	336.87
1860	Fluorobenzene	C6H5F	354.99	301.62	260.00
1571	Chlorobenzene	C6H5Cl	399.42	337.98	290.12

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

1680	Bromobenzene	C6H5Br	429.76	364.66	313.78
1526	1,2-DiCl-Propane	C3H6Cl2	373.39	316.37	271.91
1683	Propyl Iodide	C3H7I	350.76	295.49	252.69
1536	2,3-DICHLOROBUT	C4H8Cl2	380.71	322.45	277.16
2638	2-Bromobutane	C4H9Br	350.61	295.98	253.65
1586	1-Chlorobutane	C4H9Cl	346.83	293.05	251.31
1573	M-DiCl-Benzene	C6H4Cl2	456.46	387.62	333.81
2634	Benzotrifluoride	C7H5F3	377.82	318.30	272.30
1574	P-DiCl-Benzene	C6H4Cl2	456.46	387.62	333.81
1650	1-Bromopropane	C3H7Br	316.74	266.88	228.25
1587	2-Chlorobutane	C4H9Cl	322.41	271.58	232.32
1678	M-Dibromobenzene	C6H4Br2	511.10	436.00	376.95
1537	1,2-DiCl-Butane	C4H8Cl2	402.81	342.01	294.57
1597	34-DiCl-1-Butene	C4H6Cl2	404.91	344.13	296.61
1577	O-Chlorotoluene	C7H7Cl	433.45	368.04	316.99
1532	123-3Cl-Propane	C3H5Cl3	448.03	382.10	330.27
1578	P-Chlorotoluene	C7H7Cl	433.45	368.04	316.99
1562	Benzyl Chloride	C7H7Cl	454.12	386.13	332.92
2661	P-Bromotoluene	C7H7Br	461.69	392.97	339.16
1508	1,4-DiCl-Butane	C4H8Cl2	424.07	360.89	311.42
1655	1-Bromobutane	C4H9Br	349.78	295.50	253.43
2652	Perfluoropropane	C3F8	218.08	181.57	153.89
1505	2-Butylene DiCl	C4H6Cl2	429.55	364.13	312.96
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	436.19	372.28	322.00
1588	1-Chloropentane	C5H11Cl	377.52	319.75	274.88
1592	1,2,4-TriCl-Bz	C6H3Cl3	509.09	433.65	374.49
1579	2,4-2Cl-Toluene	C7H6Cl2	486.54	414.43	357.95
2593	1,3,5-TriCl-BZ	C6H3Cl3	509.09	433.65	374.49
1697	1-Br-Naphthalene	C10H7Br	557.89	476.01	411.71
1622	Perfluorobutane	C4F10	262.02	220.31	188.39
1857	P-Cl-Benzo-TriF	C7H4ClF3	436.62	369.40	317.21
1509	1,5-DiCl-Pentane	C5H10Cl2	450.16	383.79	331.78
1589	1-Cl-Naphthalene	C10H7Cl	532.64	453.53	391.57
1864	Perfluorobenzene	C6F6	428.20	373.25	329.11
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	490.69	416.64	358.91
1667	1-Bromoheptane	C7H15Br	434.25	369.48	319.03
1575	HexaCl-Benzene	C6Cl6	646.19	554.58	482.13
2640	Freon 123B1	C2HBrClF3	344.27	290.31	248.45
1504	Vinyl Chloride	C2H3Cl	244.04	203.35	171.78
1672	1,1-DiBr-Ethane	C2H4Br2	372.58	315.54	270.99
1580	Acetylene DiCl	C2H2Cl2	314.48	264.16	224.95
1692	Diiodomethane	CH2I2	408.77	345.34	295.84
1698	Bromoform	CHBr3	423.50	360.42	310.81
2687	Freon 13B1	CBrF3	240.15	200.37	169.70
1649	Tetrabromoethane	C2H2Br4	521.12	446.21	387.02

Table C.6 Boiling Temperatures Calculated by the Tihic et al. Method using FOGs. (Continued)

1503	Ethyl Chloride	C2H5Cl	276.80	232.64	198.36
1641	Methyl Bromide	CH3Br	240.82	201.74	171.38
2688	Freon 12B2	CBr2F2	336.83	286.08	246.33
1673	1,2-DiBr-Ethane	C2H4Br2	371.39	314.76	270.52
2637	Dibromomethane	CH2Br2	338.85	286.65	245.81
1612	Cl-2F-Ethylene	C2HClF2	243.31	204.07	173.66
2639	Br-Cl-Methane	CH2BrCl	335.40	283.85	243.44
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	314.48	264.16	224.95
1682	Ethyl Iodide	C2H5I	316.98	266.24	226.95
2693	Perfluoroethane	C2F6	165.17	135.50	113.17
1645	Ethyl Bromide	C2H5Br	280.59	235.75	201.01
1619	111-3F-Ethane	C2H3F3	168.08	138.51	116.08
2694	Vinyl Bromide	C2H3Br	283.04	238.22	203.37
1523	1,2-DiCl-Ethane	C2H4Cl2	365.28	309.76	266.26
2527	1,3-DiCl-Propane	C3H6Cl2	395.90	336.30	289.65

Table C. 7 Boiling Temperatures Calculated by the Tihic et al. Method using SOGs.

Nitrates

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1761	Nitroethane	C2H5NO2	380.47	324.85	280.87
1763	2-Nitropropane	C3H7NO2	410.35	351.00	304.15
1762	1-Nitropropane	C3H7NO2	409.98	350.37	303.31
1779	P-Nitrotoluene	C7H7NO2	505.62	436.03	380.56
1886	Nitrobenzene	C6H5NO2	478.13	411.61	358.64
1778	O-Nitrotoluene	C7H7NO2	505.62	436.03	380.56
1780	M-Nitrotoluene	C7H7NO2	505.62	436.03	380.56
1891	O-Nitroanisole	C7H7NO3	533.73	462.56	405.43
2740	M-Dinitrobenzene	C6H4N2O4	578.62	504.47	444.39
2742	P-Dinitrobenzene	C6H4N2O4	578.62	504.47	444.39
2741	O-Dinitrobenzene	C6H4N2O4	578.62	504.47	444.39
2749	3,5-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2743	DNT	C7H6N2O4	599.81	523.50	461.65
2745	3,4-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2744	2,6-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2748	2,5-DiNitToluene	C7H6N2O4	599.81	523.50	461.65
2746	1,3,5-TrinitroBz	C6H3N3O6	656.09	577.20	512.49
2747	Trinitrotoluene	C7H5N3O6	673.23	592.72	526.69

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Thiols

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1802	Ethyl Mercaptan	C2H6S	275.50	230.81	196.17
1820	Dimethyl Sulfide	C2H6S	299.07	251.97	215.35
1843	Thiacyclopentane	C4H8S	365.77	310.28	266.96
1803	1-Propanethiol	C3H8S	312.53	262.66	224.05
1805	Isobut Mercaptan	C4H10S	342.02	287.99	246.20
6860	Ethylenedithiol	C2H6S2	367.59	310.20	265.35
1811	Cyclohexanethiol	C6H12S	416.23	353.36	304.38
1828	DiMth Disulfide	C2H6S2	367.59	310.20	265.35
1841	Butanethiol	C4H10S	346.45	292.02	249.87
1814	Methylproylsulf	C4H10S	346.45	292.02	249.87
2816	ETHYLtBUTYL SUL	C6H14S	394.55	333.57	286.41
1818	Diethyl Sulfide	C4H10S	347.42	293.30	251.39
1812	Benzyl Mercaptan	C7H8S	456.69	387.55	333.54
1838	T-OctylMercaptan	C8H18S	448.22	380.34	327.66
1827	1-Pentanethiol	C5H12S	377.62	319.15	273.82
2815	METHnBUTYL SULFD	C5H12S	390.58	331.39	285.34

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

1824	DiethylDisulfide	C4H10S2	425.13	361.32	311.50
1807	N-Hexylmercaptan	C6H14S	406.39	344.33	296.14
6857	Dimercaptoethyl	C4H10OS2	452.60	386.94	335.19
1839	1-Heptanethiol	C7H16S	433.06	367.79	317.03
1829	DiProp Disulfide	C6H14S2	475.03	405.34	350.78
1809	1-Octanethiol	C8H18S	457.87	389.74	336.65
1808	N-Nonanethiol	C9H20S	481.06	410.35	355.14
1826	1-Decanethiol	C10H22S	502.79	429.77	372.62
2838	tertDodecanThiol	C12H26S	535.60	458.48	398.08
1825	1-Undecanethiol	C11H24S	523.22	448.11	389.20
1837	Dodecylthiol	C12H26S	542.49	465.48	404.96

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Aldehydes

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1037	Methacrolein	C4H6O	341.84	292.09	252.84
1002	Acetaldehyde	C2H4O	272.15	232.32	200.82
1003	Propionaldehyde	C3H6O	307.16	262.30	226.92
1041	Benzaldehyde	C7H6O	447.44	382.97	332.02
1034	Acrolein	C3H4O	307.57	262.63	227.11
1005	N-Butyraldehyde	C4H8O	339.04	289.79	250.99
1036	Trans-2-Butenal	C4H6O	351.56	301.04	261.06
1007	Valeraldehyde	C5H10O	368.36	315.23	273.38
1006	Isobutyraldehyde	C4H8O	339.39	289.91	250.96
1009	1-Hexanal	C6H12O	395.49	338.92	294.33
1040	P-Tolualdehyde	C8H8O	477.41	409.51	355.78
1016	2-Methylhexanal	C7H14O	421.52	361.57	314.30
1017	3-Methylhexanal	C7H14O	421.52	361.57	314.30
1008	1-Heptanal	C7H14O	420.75	361.09	314.02
1013	2-Ethylhexanal	C8H16O	445.23	382.48	332.96
1010	1-Octanal	C8H16O	444.37	381.92	332.60
1011	1-Nonanal	C9H18O	466.52	401.56	350.18
1020	1-Decanal	C10H20O	487.38	420.13	366.88
1021	1-Undecanal	C11H22O	507.06	437.74	382.76
1025	Dodecanal	C12H24O	525.69	454.48	397.90
1026	1-Tridecanal	C13H26O	543.36	470.42	412.37
1014	1,2-Ethanedione	C2H2O2	341.30	295.56	258.59
1044	1,4BenzDicarboxAldehy	C8H6O2	533.35	461.22	403.44

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Epoxides

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1440	ISOBUTYLENE OXID	C4H8O	284.97	239.60	204.45
1479	Tetrahydrofuran	C4H8O	296.38	250.41	214.64
1477	2,5-Dihydrofuran	C4H6O	311.63	264.45	227.48
1408	1-Methoxypropane	C4H10O	312.01	264.60	227.65
1411	2-Methoxypropane	C4H10O	307.42	260.46	223.92
1421	1,4-Dioxane	C4H8O2	335.63	286.52	247.83
2422	1,3-DIOXANE	C4H8O2	335.63	286.52	247.83
1426	2-Methoxybutane	C5H12O	344.24	292.32	251.86
1413	1-Methoxybutane	C5H12O	343.78	292.12	251.83
1461	Methoxybenzene	C7H8O	417.38	356.05	307.86
1448	1-Ethoxybutane	C6H14O	364.57	310.13	267.69
1429	1-MethoxyPentane	C6H14O	364.57	310.13	267.69
6885	Ethyl-3-Ethoxypr	C7H14O3	438.18	376.95	328.51

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Ether

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1401	Dimethyl Ether	C2H6O	239.11	202.04	173.10
1407	MethylEthylEther	C3H8O	267.27	225.91	193.76
1470	VinylMethylEther	C3H6O	279.49	236.93	203.67
1405	MTBE	C5H12O	329.70	279.09	239.82
1445	VinylEthyl Ether	C4H8O	304.80	258.52	222.43
1402	Diethyl Ether	C4H10O	302.54	256.27	220.29
1431	Methylal	C3H8O2	326.97	279.83	242.56
1428	T-But EthylEther	C6H14O	351.40	297.87	256.35
1427	TAME	C6H14O	364.68	309.44	266.50
1410	Mth Isobut Ether	C5H12O	339.55	288.29	248.36
1430	Eth-t-Pent-Ether	C7H16O	384.44	326.66	281.73
1403	DiisopropylEther	C6H14O	364.02	311.09	269.58
1415	Eth Propyl Ether	C5H12O	334.82	284.22	244.84
1455	Dimethyl Acetal	C4H10O2	340.78	291.39	252.50
1446	Dipropyl Ether	C6H14O	364.57	310.13	267.69
1447	Butyl VinylEther	C6H12O	366.75	312.27	269.72
1462	EthylPhenylEther	C8H10O	435.61	371.91	321.89
1406	Di-sec-But Ether	C8H18O	419.47	359.73	312.73
1432	Acetal	C6H14O2	396.80	340.04	295.33
1460	BenzylEthylEther	C9H12O	453.50	387.71	336.05
1050	Paraldehyde	C6H12O3	424.73	370.19	326.10

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

1404	Di-n-Butyl Ether	C8H18O	417.77	356.83	309.15
1420	Anethole	C10H12O	508.87	436.92	380.06
1456	DimethylCarbitol	C6H14O3	437.61	378.11	330.67
1463	Dibenzyl Ether	C14H14O	579.38	498.90	435.15
1425	Di-n-PentylEther	C10H22O	464.23	398.01	346.00
1458	Diethyl Carbitol	C8H18O3	467.89	404.70	354.36
1412	Dihexyl Ether	C12H26O	505.34	434.79	379.14
1454	Triglyme	C8H18O4	500.92	435.85	383.55
1459	Dibutyl Carbitol	C12H26O3	542.31	471.33	414.52
1424	Di-n-Octyl Ether	C16H34O	575.26	498.09	436.76
1457	Tetraglyme	C10H22O5	542.24	474.25	419.26
1418	Dinonyl Ether	C18H38O	605.39	525.69	462.09
2432	ETHYLAL	C5H12O2	369.52	316.37	274.52
2405	DIISOBUTYL ETHER	C8H18O	410.82	350.44	303.29
2456	Ethyl Glyme	C6H14O2	396.18	339.68	295.16
2417	ETHYLHEXYL ETHER	C8H18O	417.77	356.83	309.15
2415	ETHYLISOPROPETH	C5H12O	335.17	286.13	247.67

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

	Formate				
Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1301	Methyl Formate	C2H4O2	275.67	233.89	201.11
1311	Vinyl Formate	C3H4O2	313.28	266.51	229.77
1302	Ethyl Formate	C3H6O2	311.34	264.48	227.78
2306	t-Butyl Formate	C5H10O2	361.04	306.63	264.21
1303	Propyl Formate	C4H8O2	343.83	292.53	252.38
2305	sec-ButylFormate	C5H10O2	374.36	318.85	275.41
2311	CYCLOHEXL FORMAT	C7H12O2	428.06	365.07	315.73
1304	N-Butyl Formate	C5H10O2	373.68	318.46	275.22
1305	Isobutyl Formate	C5H10O2	374.36	318.85	275.41
2350	Benzyl Formate	C8H8O2	469.72	402.25	349.05
2307	n-Hexyl Formate	C7H14O2	426.92	365.11	316.59
1306	N-Pentyl Formate	C6H12O2	401.27	342.58	296.56
2308	n-Heptyl Formate	C8H16O2	450.86	386.26	335.47
1308	N-Octyl Formate	C9H18O2	473.30	406.17	353.31
1309	n-Nonyl Formate	C10H20O2	494.38	424.97	370.22
1310	n-Decyl Formate	C11H22O2	514.26	442.78	386.30

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Ester

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1351	Mth Methacrylate	C5H8O2	370.32	316.52	274.19
1312	Methyl Acetate	C3H6O2	293.34	249.86	215.72
1331	Vinyl Propionate	C5H8O2	356.25	303.93	262.90
1321	Vinyl Acetate	C4H6O2	339.15	289.49	250.43
1352	Eth MthAcrylate	C6H10O2	385.99	329.84	285.75
1322	MethylPropionate	C4H8O2	337.24	287.52	248.52
1341	Methyl Acrylate	C4H6O2	327.79	278.84	240.52
1313	Ethyl Acetate	C4H8O2	312.17	265.69	229.34
1319	IsopropylAcetate	C5H10O2	356.17	304.04	263.15
1332	Methyl Butyrate	C5H10O2	342.97	292.40	252.81
1342	Ethyl Acrylate	C5H8O2	358.50	305.46	263.93
1318	Allyl Acetate	C5H8O2	357.69	305.81	265.01
1314	N-Propyl Acetate	C5H10O2	355.75	303.86	263.12
1323	Ethyl Propionate	C5H10O2	354.22	301.90	260.95
1360	I-But I-Butyrate	C8H16O2	429.13	366.86	318.08
1320	Sec-ButylAcetate	C6H12O2	384.00	328.33	284.62
1336	PropylI-Butyrate	C7H14O2	407.64	348.05	301.40
1353	N-C3-Mthacrylate	C7H12O2	400.71	340.91	294.24
1333	Ethyl Butyrate	C6H12O2	382.44	326.52	282.71
1347	EthylIsovalerate	C7H14O2	405.17	346.32	300.19
1315	N-Butyl Acetate	C6H12O2	383.44	328.02	284.49
1390	Methyl Benzoate	C8H8O2	461.08	395.52	343.72
1388	Isobutyl mthacr	C8H14O2	436.07	373.25	323.93
1343	1-PropylAcrylate	C6H10O2	384.45	328.52	284.62
1316	Isobutyl Acetate	C6H12O2	379.76	324.67	281.42
1344	N-Butyl Acrylate	C7H12O2	408.48	348.42	301.38
1357	Pentyl Acetate	C7H14O2	419.84	359.65	312.30
1327	N-PropN-Butyrate	C7H14O2	408.66	349.53	303.12
1324	N-PropPropionate	C6H12O2	382.44	326.52	282.71
1291	Acetic Anhydride	C4H6O3	405.55	348.60	303.37
1389	N-ButMthacrylate	C8H14O2	439.31	376.26	326.69
1359	Benzyl Acetate	C9H10O2	477.74	410.27	356.94
1326	N-But Propionate	C7H14O2	408.66	349.53	303.12
1391	Ethyl Benzoate	C9H10O2	477.56	409.23	355.38
1897	CH3OC3H600CH3	C6H12O3	420.28	362.10	315.91
1392	DiethylCarbonate	C5H10O3	386.43	331.92	288.79
1385	N-But N-Butyrate	C8H16O2	433.14	371.11	322.36
1317	IsopentylAcetate	C7H14O2	405.77	347.49	301.68
1363	N-Hexyl Acetate	C8H16O2	425.04	363.91	315.92
1387	Ethylene Acetate	C6H10O4	427.48	369.79	323.73
1393	Diethyl Oxalate	C6H10O4	426.76	368.03	321.34
1365	Butyl Benzoate	C11H14O2	520.53	447.43	389.69
1361	I-C5 I-Valerate	C10H20O2	471.83	405.21	352.75
1367	Heptyl Acetate	C9H18O2	448.29	384.50	334.33

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

1346	N-Butyl Valerate	C9H18O2	456.06	391.42	340.53
1358	2-C2-C6 Acetate	C10H20O2	478.09	411.47	358.84
1394	Diethyl Malonate	C7H12O4	468.66	404.36	353.25
1292	Propionyl Oxide	C6H10O3	435.88	374.80	326.42
1364	Benzyl Benzoate	C14H12O2	589.69	508.22	443.60
1381	2Mth p-Phthalate	C10H10O4	543.85	471.22	413.13
1368	n-Octyl Acetate	C10H20O2	470.14	403.93	351.77
1377	DiMthI-Phthalate	C10H10O4	533.67	460.63	402.54
1896	Ethylene DiAcr	C8H10O4	479.61	414.33	362.37
1386	2-Ethylhexyl Acr	C11H20O2	503.74	433.43	377.93
1395	Methyl Decanoate	C11H22O2	497.93	428.77	374.12
1369	n-Nonyl Acetate	C11H22O2	490.73	422.33	368.34
1370	n-Decyl Acetate	C12H24O2	510.18	439.78	384.11
1345	N-ButylNonanoate	C13H26O2	535.31	462.40	404.58
1375	DiProp Phthalate	C14H18O4	603.25	523.33	459.47
1376	Diisobutyl Phtha	C16H22O4	629.33	546.91	480.95
1396	IsopropMyristate	C17H34O2	600.55	521.22	457.95
1383	Butyl Stearate	C22H44O2	665.25	581.62	514.19
1362	Methyl Oleate	C19H36O2	634.94	553.66	488.37
1355	Diisooctyl Phtha	C24H38O4	726.47	637.18	564.80
1382	DioctylTerephtha	C24H38O4	729.12	639.84	567.41
1384	Dibutyl Sebacate	C18H34O4	633.74	554.33	490.23
1371	Diisodecyl Phtha	C28H46O4	764.89	673.66	599.15
1354	DioctylPhthalate	C24H38O4	732.29	642.29	569.34
2375	DiethylPhthalate	C12H14O4	563.63	488.46	428.42
2388	Dipropyl Maleate	C10H16O4	524.99	454.93	399.00
2381	Diallyl Maleate	C10H12O4	522.48	453.85	398.84
2370	Glyceryl Triacet	C9H14O6	520.30	454.73	401.73
2382	Dibutyl Maleate	C12H20O4	559.86	486.31	427.45
2376	DibutylPhthalate	C16H22O4	633.02	550.51	484.40
2353	CetylMthacrylate	C20H38O2	646.63	563.75	497.21
2379	Dihexyl Adipate	C18H34O4	633.74	554.33	490.23
2321	T-Butyl Acetate	C6H12O2	372.59	316.70	273.18
2332	Methl.I-butyrate	C5H10O2	356.95	303.65	262.02
2354	AllylMthacrylate	C7H10O2	416.74	356.58	309.29
2364	Cyclohexl Acetat	C8H14O2	444.80	380.02	329.22
2337	EthylIsobutyrate	C6H12O2	381.02	324.70	280.69
2384	IsobutylAcrylate	C7H12O2	409.69	350.07	303.32
2380	1,1-Diacetoxy C2	C6H10O4	422.14	363.28	316.64
2392	n-PropylBenzoate	C10H12O2	499.73	428.89	373.00
2377	DiMth Phthalate	C10H10O4	543.85	471.22	413.13
2386	Diethyl Maleate	C8H12O4	486.12	420.25	367.77
2385	Mth Dodecanoate	C13H26O2	535.31	462.40	404.58
3379	Dioctyl Adipate	C22H42O4	691.06	606.03	537.11
5886	Mth Acetoacetate	C5H8O3	439.37	377.93	329.15
5884	Ethoxy Acetate	C6H12O3	412.48	355.31	309.96

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

5887	EthAcetoAcetate	C6H10O3	444.73	382.78	333.62
5885	Carbitol Acetate	C8H16O4	479.96	416.64	365.93

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Ketone

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1096	Methyl Isopropen	C5H8O	378.72	322.37	278.23
1079	Cyclopentanone	C5H8O	377.42	320.19	275.45
1051	Acetone	C3H6O	309.30	262.01	225.02
1052	MEK	C4H8O	342.91	290.97	250.40
1065	Mesityl Oxide	C6H10O	413.14	352.53	304.97
1066	T-But Mth Ketone	C6H12O	391.67	332.56	286.52
1060	2-Pentanone	C5H10O	373.68	317.67	273.90
1061	Mth iC3 Ketone	C5H10O	374.52	318.17	274.17
1053	Diethyl Ketone	C5H10O	364.03	309.42	266.78
1059	3-Hexanone	C6H12O	392.69	334.41	288.87
1099	Diketene	C4H4O2	306.75	261.38	225.72
1055	Sec-ButMthKetone	C6H12O	403.01	343.04	296.17
1054	MIBK	C6H12O	398.35	339.04	292.69
1095	EthIsopropKetone	C6H12O	388.92	330.97	285.72
1063	2-Heptanone	C7H14O	428.35	365.52	316.31
1064	5-Mth-2-Hexanone	C7H14O	424.91	362.34	313.39
1058	4-Heptanone	C7H14O	419.25	357.72	309.56
1057	3-Heptanone	C7H14O	419.25	357.72	309.56
1076	2,4-Pentanedione	C5H8O2	442.09	379.43	329.78
1068	DiisobutylKetone	C9H18O	460.97	394.32	342.06
1097	2-CycC6 CycC6one	C12H20O	552.96	473.67	411.34
1083	2-Octanone	C8H16O	452.85	387.13	335.59
1073	Dibutyl Ketone	C9H18O	467.13	400.04	347.37
1062	2-Hexanone	C6H12O	402.05	342.43	295.80
1077	Isophorone	C9H14O	488.23	416.66	360.57
1090	Acetophenone	C8H8O	474.14	405.24	351.01
1080	Cyclohexanone	C6H10O	406.73	345.71	298.00
1074	2-Nonanone	C9H18O	475.76	407.45	353.79

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
404	DiMth-Acetylene	C4H6	291.60	245.13	209.13
202	Propylene	C3H6	219.52	183.16	155.24
412	2-Pentyne	C5H8	388.80	329.44	283.36
207	2-Methylpropene	C4H8	261.75	219.25	186.57
204	1-Butene	C4H8	259.96	217.75	185.31
205	Cis-2-Butene	C4H8	275.07	231.24	197.39
402	Propyne	C3H4	234.40	196.81	167.67
406	3-Hexyne	C6H10	359.10	303.52	260.43
206	Trans-2-Butene	C4H8	275.07	231.24	197.39
407	2-Hexyne	C6H10	359.10	303.52	260.43
231	33-2Mth-1-Butene	C6H12	315.19	264.57	225.75
230	23-2Mth-1-Butene	C6H12	327.67	276.01	236.22
229	2-Ethyl-1-Butene	C6H12	332.24	280.13	239.94
8	I-Pentane	C5H12	294.34	246.88	210.47
14	2,2-DiMth-Butane	C6H14	312.32	261.86	223.25
232	23-2Mth-2-Butene	C6H12	346.50	293.07	251.67
213	3-Mth-1-Butene	C5H10	291.81	245.01	209.04
212	2-Mth-1-Butene	C5H10	298.61	250.99	214.33
211	Trans-2-Pentene	C5H10	310.16	261.33	223.62
210	Cis-2-Pentene	C5H10	310.16	261.33	223.62
223	4-Mth-1-Pentene	C6H12	325.89	274.52	234.96
221	2-Mth-1-Pentene	C6H12	332.24	280.13	239.94
248	2-t-Butylpropene	C7H14	349.46	294.31	251.90
227	Cs-4-Mth-2-C5H10	C6H12	338.89	286.24	245.53
224	2-Mth-2-Pentene	C6H12	339.53	286.57	245.65
403	1-Butyne	C4H6	273.87	230.58	197.05
15	2,3-DiMth-Butane	C6H14	318.49	267.73	228.76
214	2-Mth-2-Butene	C5H10	306.53	257.98	220.54
228	Ts-4-Mth-2-C5H10	C6H12	338.89	286.24	245.53
225	Cs-3-Mth-2-C5H10	C6H12	339.63	286.68	245.77
218	Trans-2-Hexene	C6H12	343.28	290.21	249.13
2226	3-METH-Tr-2Pente	C6H12	339.63	286.68	245.77
222	3-Mth-1-Pentene	C6H12	330.99	278.87	238.71
257	2-Diisobutylene	C8H16	386.10	326.44	280.36
256	1-Diisobutylene	C8H16	379.29	320.40	274.99
217	Cis-2-Hexene	C6H12	342.87	289.70	248.57
2414	1-Heptyne	C7H12	372.44	315.94	272.05
13	3-Methylpentane	C6H14	328.31	276.32	236.34
219	Cis-3-Hexene	C6H12	342.37	289.08	247.89
12	2-Methylpentane	C6H14	323.19	271.96	232.58
220	Trans-3-Hexene	C6H12	342.37	289.08	247.89
405	1-Pentyne	C5H8	309.65	261.40	224.01
209	1-Pentene	C5H10	296.83	249.50	213.08
11	N-Hexane	C6H14	327.82	276.13	236.34

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

235	Cis-2-Heptene	C7H14	372.97	315.95	271.76
249	Cis-3-Heptene	C7H14	372.61	315.46	271.20
216	1-Hexene	C6H12	330.47	278.65	238.69
239	3-Eth-1-Pentene	C7H14	362.05	305.94	262.60
226	4-Mth-1-Hexene	C7H14	361.70	305.48	262.09
240	3-Mth-1-Hexene	C7H14	362.05	305.94	262.60
419	3-Mth-1-Butyne	C5H8	304.88	257.11	220.14
233	2-Eth-1-Pentene	C7H14	363.13	307.05	263.70
238	2-Mth-1-Hexene	C7H14	363.13	307.05	263.70
416	1-Octyne	C8H14	400.27	340.33	293.67
289	2,3Dimeth Hexene	C8H16	392.51	332.55	286.13
234	1-Heptene	C7H14	361.37	305.57	262.45
413	1-Hexyne	C6H10	342.35	289.73	248.91
237	Trans-3-Heptene	C7H14	372.61	315.46	271.20
236	Trans-2-Heptene	C7H14	372.97	315.95	271.76
251	Trans-2-Octene	C8H16	400.81	340.37	293.43
279	Trans-4-Octene	C8H16	400.58	339.99	292.96
277	Trans-3-Octene	C8H16	400.58	339.99	292.96
2252	2Methl-1-Heptene	C8H16	391.67	332.05	285.86
250	1-Octene	C8H16	389.91	330.58	284.61
258	2-Ethyl-1-Hexene	C8H16	391.67	332.05	285.86
280	3-Octene	C8H16	400.58	339.99	292.96
278	4-Octene	C8H16	400.58	339.99	292.96
276	2-Octene	C8H16	400.81	340.37	293.43
259	1-Nonene	C9H18	416.41	353.92	305.38
262	1-Dodecene	C12H24	485.93	415.73	360.80
263	1-Tridecene	C13H26	506.36	434.07	377.37
264	1-Tetradecene	C14H28	525.65	451.45	393.13
265	1-Pentadecene	C15H30	543.90	467.98	408.15
266	1-Hexadecene	C16H32	561.22	483.71	422.51
267	1-Octadecene	C18H36	593.33	513.06	449.40
281	1-Heptadecene	C17H34	577.67	498.72	436.24
284	1-Eicosene	C20H40	622.54	539.96	474.18
283	1-Nonadecene	C19H38	608.27	526.79	462.04
3	Propane	C3H8	216.11	179.92	152.24
4	I-Butane	C4H10	257.09	214.79	182.39
9	Neopentane	C5H12	276.71	231.06	196.22
5	N-Butane	C4H10	257.02	214.95	182.72
7	pentane	C5H12	294.05	246.85	210.62
44	Hexamethylethane	C8H18	361.51	303.94	259.85
25	223-TriMthButane	C7H16	340.40	286.14	244.55
24	3,3-DiMthPentane	C7H16	349.69	294.25	251.67
51	2,2,3,3-4Mth-C5	C9H20	390.33	329.20	282.23
21	2,2-DiMthPentane	C7H16	344.89	290.20	248.22
42	2,3,3-TriMth-C5	C8H18	370.50	312.42	267.77

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

22	2,3-DiMthPentane	C7H16	355.23	299.63	256.82
40	2,2,3-TriMth-C5	C8H18	375.66	316.87	271.65
23	2,4-DiMthPentane	C7H16	350.28	295.41	253.17
41	2,2,4-TriMth-C5	C8H18	370.74	312.67	268.02
39	3-Mth-3-Eth-C5	C8H18	379.53	320.36	274.79
20	3-Ethylpentane	C7H16	359.49	303.50	260.33
52	2,2,3,4-4Mth-C5	C9H20	399.70	337.87	290.23
54	2334TetrMethPent	C9H20	394.75	333.60	286.49
53	2,2,4,4-4Mth-C5	C9H20	390.51	329.40	282.45
43	2,3,4-TriMth-C5	C8H18	380.36	321.50	276.10
36	3,3-DiMth-Hexane	C8H18	379.53	320.36	274.79
19	3-Methylhexane	C7H16	359.49	303.50	260.33
18	2-Methylhexane	C7H16	354.59	299.31	256.71
38	2-Mth-3-Eth-C5	C8H18	384.34	325.13	279.41
190	2,2-2C1-3-C2-C5	C9H20	403.52	341.38	293.43
32	2,2-DiMth-Hexane	C8H18	374.87	316.43	271.44
37	3,4-DiMth-Hexane	C8H18	389.11	329.21	282.94
50	3,3-DiEthPentane	C9H20	407.14	344.65	296.39
34	2,4-DiMth-Hexane	C8H18	384.34	325.13	279.41
33	2,3-DiMth-Hexane	C8H18	384.34	325.13	279.41
17	N-Heptane	C7H16	358.84	303.16	260.20
49	244TriMethHexane	C9H20	398.62	337.14	289.72
192	2,4-2C1-3-C2-C5	C9H20	407.65	345.52	297.46
47	2,2,5-TriMth-C6	C9H20	398.80	337.34	289.93
35	2,5-DiMth-Hexane	C8H18	379.59	321.07	275.90
31	3-Ethylhexane	C8H18	388.28	328.72	282.68
30	4-Methylheptane	C8H18	388.28	328.72	282.68
29	3-Methylheptane	C8H18	388.28	328.72	282.68
28	2-Methylheptane	C8H18	383.57	324.69	279.19
96	2,2-DiMthHeptane	C9H20	402.61	340.83	293.12
176	2,6-DiMthHeptane	C9H20	406.76	344.98	297.16
27	N-Octane	C8H18	387.49	328.26	282.45
94	3-Ethylheptane	C9H20	414.98	352.25	303.62
92	3-Methyloctane	C9H20	414.98	352.25	303.62
93	4-Methyloctane	C9H20	414.98	352.25	303.62
91	2-Methyloctane	C9H20	414.98	352.25	303.62
72	2,2-DiMthOctane	C10H22	428.40	363.62	313.46
2095	2,3Dimethloctane	C10H22	436.47	371.14	320.42
2096	2,4Dimethloctane	C10H22	436.47	371.14	320.42
2098	2,6DimethlOctane	C10H22	436.47	371.14	320.42
2097	2,5Dimethloctane	C10H22	436.47	371.14	320.42
2099	2,7DimethlOctane	C10H22	432.05	367.35	317.13
46	N-Nonane	C9H20	414.07	351.69	303.30
88	5-Methylnonane	C10H22	439.87	374.28	323.30
85	3-Methylnonane	C10H22	439.87	374.28	323.30
87	4-Methylnonane	C10H22	439.87	374.28	323.30

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

86	2-Methylnonane	C10H22	435.48	370.51	320.03
56	N-Decane	C10H22	438.86	373.63	322.90
63	N-Undecane	C11H24	462.05	394.26	341.40
64	N-Dodecane	C12H26	483.81	413.71	358.91
65	N-Tridecane	C13H28	504.31	432.11	375.53
66	N-Tetradecane	C14H30	523.65	449.55	391.34
67	N-Pentadecane	C15H32	541.96	466.12	406.42
68	N-Hexadecane	C16H34	559.32	481.90	420.81
69	N-Heptadecane	C17H36	575.82	496.96	434.59
70	N-Octadecane	C18H38	591.53	511.34	447.79
71	N-Nonadecane	C19H40	606.51	525.11	460.46
73	N-Eicosane	C20H42	620.82	538.31	472.64
74	n-HENEICOSANE	C21H44	634.51	550.99	484.36
75	n-DOCOSANE	C22H46	647.62	563.16	495.65
76	n-TRICOSANE	C23H48	660.19	574.88	506.55
77	n-Tetracosane	C24H50	672.26	586.17	517.06
78	n-PENTACOSANE	C25H52	683.86	597.06	527.23
79	n-HEXACOSANE	C26H54	695.03	607.57	537.06
81	n-Octacosane	C28H58	716.15	627.55	555.81
2081	n-TRICONTANE	C30H62	735.81	646.27	573.44
2082	n-Dotriacontane	C32H66	754.17	663.87	590.07
2086	Hexatriacontane	C36H74	787.50	696.12	620.70

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Cyclic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
269	Cyclopentene	C5H8	306.27	257.33	219.49
270	Cyclohexene	C6H10	340.43	286.89	245.47
287	3MthCyclopentene	C6H10	346.74	291.53	248.89
286	1-MthCyclPentene	C6H10	342.35	287.57	245.31
288	4MthCyclopenten	C6H10	346.74	291.53	248.89
273	Cycloheptene	C7H12	371.79	314.17	269.55
274	Cyclooctene	C8H14	400.72	339.48	291.98
101	Cyclopropane	C3H6	240.33	201.76	171.87
810	Adamantane	C10H16	453.99	381.96	326.45
102	Cyclobutane	C4H8	277.14	232.92	198.71
104	Cyclopentane	C5H10	303.54	255.12	217.75
137	Cyclohexane	C6H12	334.83	281.48	240.36
105	MthCyclopentane	C6H12	343.09	288.60	246.57
146	Cs-1,4-2C1-CycC6	C8H16	409.35	344.80	295.06
142	Cs-1,2-2C1-CycC6	C8H16	409.35	344.80	295.06

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

141	1,1-2C1-CycC6	C8H16	400.28	336.28	287.10
145	Ts-1,3-2C1-CycC6	C8H16	409.35	344.80	295.06
144	Cs-1,3-2C1-CycC6	C8H16	409.35	344.80	295.06
147	Ts-1,4-2C1-CycC6	C8H16	409.35	344.80	295.06
143	Ts-1,2-2C1-CycC6	C8H16	409.35	344.80	295.06
138	MthCyclohexane	C7H14	372.90	313.78	268.23
159	Cycloheptane	C7H14	356.93	300.56	257.15
140	Ethylcyclohexane	C8H16	407.89	343.83	294.44
154	Trans-Decalin	C10H18	445.24	376.44	323.25
149	N-PropylCyc-C6	C9H18	440.94	372.32	319.35
109	Cs-1,2-2C1-CycC5	C7H14	380.89	320.69	274.26
110	Ts-1,2-2C1-CycC5	C7H14	380.89	320.69	274.26
112	Ts-1,3-2C1-CycC5	C7H14	380.89	320.69	274.26
107	Eth-Cyclopentane	C7H14	379.65	319.90	273.79
114	N-PropCycPentane	C8H16	414.10	349.51	299.62
108	1,1-DiMthCycC5	C7H14	371.03	311.52	265.77
111	Cs-1,3-2C1-CycC5	C7H14	380.89	320.69	274.26
152	N-ButylCycHexane	C10H20	472.23	399.40	343.10
160	Cyclooctane	C8H16	386.78	326.67	280.27
153	Cis-Decalin	C10H18	445.24	376.44	323.25
115	Isopropylcyclopentane	C8H16	394.31	333.71	286.80
150	Isopropyl-CycC6	C9H18	425.31	360.12	309.66
116	1-C1-1-C2-CycC5	C8H16	406.67	342.11	292.43
122	Butylcyclpentane	C9H18	446.66	377.59	324.19
155	1,1-Bicyclohexyl	C12H22	493.10	419.03	361.50
158	N-Decylcyclo-C6	C16H32	631.27	538.55	466.26

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Aromatic Hydrocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
307	1,4-Pentadiene	C5H8	299.51	252.08	215.49
306	1-ts3-Pentadiene	C5H8	309.12	260.55	222.98
414	2-Methyl-1-Butenyne	C5H6	313.77	265.22	227.49
305	Cs1,3-Pentadiene	C5H8	309.12	260.55	222.98
309	Isoprene	C5H8	301.28	253.57	216.74
421	1-Pentene-4-yne	C5H6	312.06	263.77	226.26
303	1,3-Butadiene	C4H6	257.99	216.05	183.78
332	1,4-CyclHexadien	C6H8	355.38	300.64	258.03
501	Benzene	C6H6	337.11	284.04	242.87
315	Cyclopentadiene	C5H6	322.19	271.94	232.82
319	Diisopropenyl	C6H10	336.59	284.10	243.51

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

615	Ethynylbezene	C8H6	419.63	356.64	307.39
601	Styrene	C8H8	409.97	347.31	298.57
331	1,3-CycHexadiene	C6H8	355.38	300.64	258.03
310	1,5-Hexadiene	C6H10	332.14	280.03	239.82
312	MthCycPentadiene	C6H8	352.20	297.46	254.94
420	1-Pentene-3-yne	C5H6	329.26	277.93	238.07
502	Toluene	C7H8	375.91	318.01	273.00
521	T-Butylbenzene	C10H14	450.55	381.87	328.59
320	Dipropylene	C6H10	354.42	300.27	258.18
520	Sec-Butylbenzene	C10H14	448.41	380.42	327.63
313	1,4-Hexadiene	C6H10	345.32	292.08	250.81
314	Dipropylene	C6H10	354.42	300.27	258.18
316	DiCycPentadiene	C10H12	462.51	395.53	343.05
333	1,5-CycOctadiene	C8H12	414.39	353.82	306.45
701	Naphthalene	C10H8	481.35	408.57	351.77
504	Ethylbenzene	C8H10	399.72	338.17	290.40
820	Indan	C9H10	431.29	364.31	312.36
505	O-Xylene	C8H10	411.15	349.05	300.65
612	P-Methylstyrene	C9H10	442.72	376.34	324.54
330	DIISOCROTYL	C8H14	406.03	344.66	296.96
507	P-Xylene	C8H10	411.15	349.05	300.65
329	DIISOBUTENYL	C8H14	395.81	335.81	289.25
506	M-Xylene	C8H10	411.15	349.05	300.65
603	Methylstyrene	C9H10	442.72	376.34	324.54
613	Alpha-MthStyrene	C9H10	438.99	372.75	321.14
510	Isopropylbenzene	C9H12	417.41	353.20	303.45
724	2-Methylindene	C10H10	474.85	403.05	347.08
285	Vinylcyclohexene	C8H12	404.17	342.48	294.57
803	Indene	C9H8	451.91	382.38	328.26
706	Tetralin	C10H12	457.54	387.47	333.06
511	O-Ethyltoluene	C9H12	433.06	367.69	316.81
723	1-Methylindene	C10H10	488.83	416.93	360.52
738	Fluorene	C13H10	572.04	486.92	420.34
619	Tr-1PropenylBz	C9H10	447.31	380.55	328.39
525	O-Diethylbenzene	C10H14	453.93	385.52	332.31
618	Propenyl Bz(cis)	C9H10	447.31	380.55	328.39
602	O-Methylstyrene	C9H10	442.72	376.34	324.54
702	1-MthNaphthalene	C11H10	509.85	434.13	374.89
509	N-Propylbenzene	C9H12	427.23	362.32	311.87
526	M-Diethylbenzene	C10H14	453.93	385.52	332.31
583	Cs-2-PhnButene-2	C10H12	470.21	400.37	345.81
543	M-DiisopropylBz	C12H18	483.68	411.13	354.78
584	Ts-2-PhnButene-2	C10H12	470.06	400.31	345.81
580	1,2-DiC1-3C2-Bz	C10H14	463.62	394.91	341.26
704	1-EthNaphthalene	C12H12	529.05	450.57	389.22
512	M-Ethyltoluene	C9H12	433.06	367.69	316.81

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

522	1-Mth-2-iC3-Benz	C10H14	454.00	385.59	332.39
513	P-Ethyltoluene	C9H12	433.06	367.69	316.81
514	1,2,3-Mesitylene	C9H12	443.33	377.58	326.18
614	M-Divinylbenzene	C10H10	472.91	402.49	347.50
524	1-Mth-4-iC3-Benz	C10H14	449.25	381.51	328.85
822	Gamma-Terpinene	C10H16	457.30	389.03	335.84
821	Alpha-Terpinene	C10H16	457.30	389.03	335.84
523	1-Mth-3-iC3-Benz	C10H14	449.25	381.51	328.85
703	2-MthNaphthalene	C11H10	509.85	434.13	374.89
557	CycHexylBenzene	C12H16	507.47	431.75	372.74
515	1,2,4-Mesitylene	C9H12	443.33	377.58	326.18
519	Isobutylbenzene	C10H14	449.44	381.77	329.13
424	DiPhnAcetylene	C14H10	597.21	512.05	444.89
544	P-DiisopropylBz	C12H18	483.68	411.13	354.78
518	N-Butylbenzene	C10H14	452.78	384.88	332.01
516	1,3,5-Mesitylene	C9H12	443.33	377.58	326.18
809	Acenaphthalene	C12H8	559.44	475.33	409.57
725	123-TriMthIndene	C12H14	522.56	445.09	384.58
527	1,4-DiEthBenzene	C10H14	453.93	385.52	332.31
558	Diphenyl	C12H10	530.96	452.85	391.64
576	2-Ethyl-m-Xylene	C10H14	463.62	394.91	341.26
620	p-ISOPROPENYLSTY	C11H12	498.08	424.75	367.39
585	o-PropylToluene	C10H14	458.25	389.94	336.67
577	2-Ethyl-p-Xylene	C10H14	463.62	394.91	341.26
579	4-Ethyl-o-Xylene	C10H14	463.62	394.91	341.26
586	m-Propyltoluene	C10H14	458.25	389.94	336.67
587	p-Propyltoluene	C10H14	458.25	389.94	336.67
578	4-Ethyl-m-Xylene	C10H14	463.62	394.91	341.26
575	5-Ethyl-m-Xylene	C10H14	463.62	394.91	341.26
530	Prehnitene	C10H14	472.90	403.94	349.87
709	2,6-2Mth-Naphtha	C12H12	536.24	457.93	396.49
715	2,7-2Mth-Naphtha	C12H12	536.24	457.93	396.49
719	2-ETHYLNAPHTHALENE	C12H12	531.54	452.70	391.07
621	p-tert-BUTYLSTY	C12H16	508.22	432.82	374.02
532	1,2,4,5-TetMthBz	C10H14	472.90	403.94	349.87
531	1,2,3,5-TetMthBz	C10H14	472.90	403.94	349.87
533	p-tert-BUTYL ET	C12H18	506.03	430.69	372.02
567	N-Pentylbenzene	C11H16	476.61	406.02	350.96
718	1-n-PROPYLNAPHTH	C13H14	556.64	475.15	411.31
562	1,1-DiPhnEthane	C14H14	562.15	480.38	416.29
616	4-ISOBUTYLSTYRE	C12H16	512.98	437.82	379.05
260	1-Decene	C10H20	441.11	375.78	324.91
735	Cis-Stilbene	C14H12	580.64	498.02	432.89
568	Hexylbenzene	C12H18	498.92	425.91	368.85
563	Diphenylmethane	C13H12	544.82	465.43	403.16
564	1,2-DiPhnEthane	C14H14	557.95	477.41	414.18

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

804	Anthracene	C14H10	604.75	516.23	446.76
736	Trans-Stilbene	C14H12	580.64	498.02	432.89
805	Phenanthrene	C14H10	602.30	514.13	444.93
713	1-ButNaphthalene	C14H16	569.27	486.75	422.03
807	Pyrene	C16H10	673.23	575.09	497.96
261	1-Undecene	C11H22	464.23	396.34	343.35
581	23-2C1-23-2PhnC4	C18H22	657.21	563.79	490.28
549	N-Heptylbenzene	C13H20	519.86	444.68	385.78
710	1-PhnNaphthalene	C16H12	640.74	549.19	477.05
566	2,4-Diphenyl-4-M	C18H20	642.70	552.94	482.05
561	O-Terphenyl	C18H14	675.38	581.03	506.40
569	N-Octylbenzene	C14H22	539.57	462.42	401.86
565	Triphenylmethane	C19H16	683.63	589.05	514.12
714	N-C6-Naphthalene	C16H20	605.04	519.23	451.69
717	Fluoranthene	C16H10	673.23	575.09	497.96
716	1-Hexyl-Tetralin	C16H24	597.56	512.52	445.69
731	TriPhnEthylene	C20H16	702.94	607.27	531.21
806	Chrysene	C18H12	706.31	605.77	526.46
588	1,1,2TriPhenEth	C20H18	697.36	601.80	525.97
711	1-n-NonylNaphtha	C19H26	651.96	562.32	491.36
570	N-Nonylbenzene	C15H24	558.17	479.25	417.16
712	1-Decyl Naphtha	C20H28	666.10	575.42	503.50
559	P-Terphenyl	C18H14	675.38	581.03	506.40
560	M-Terphenyl	C18H14	675.38	581.03	506.40
589	TetraPhenylMetha	C25H20	787.20	682.21	598.45
554	Decylbenzene	C16H26	575.78	495.24	431.75
732	TetraPhnEthylene	C26H20	802.07	698.03	614.55
574	N-Dodecylbenzene	C18H30	608.33	524.99	459.02
571	N-Undecylbenzene	C17H28	592.47	510.46	445.69
572	Tridecylbenzene	C19H32	623.43	538.87	471.80
573	n-TETRADECYLBENZ	C20H34	642.99	556.71	488.12
2575	n-PENTADECYLBENZ	C21H36	656.60	569.33	499.82
2576	n-HEXADECYLBENZ	C22H38	669.62	581.44	511.07
2577	n-HEPTADECYLBENZ	C23H40	682.10	593.09	521.92
2578	n-OCTADECYLBENZE	C24H42	694.06	604.30	532.39

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

Halocarbons

Dip ID	Name	Formula	$T_{b,760\,mmHg}^{Calc}$	$T_{b,100\,mmHg}^{Calc}$	$T_{b,10\,mmHg}^{Calc}$
1544	Allyl Chloride	C3H5Cl	315.78	266.51	228.18
1531	3-Chloropropyne	C3H3Cl	327.21	277.39	238.37

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

1535	T-Butyl Chloride	C4H9Cl	322.41	271.58	232.32
at1530	Isopropyl Cl	C3H7Cl	287.24	241.21	205.69
1572	O-DiCl-Benzene	C6H4Cl2	456.46	387.62	333.81
1585	Propyl Chloride	C3H7Cl	313.41	264.13	225.90
1684	Isopropyl Iodide	C3H7I	351.92	296.21	253.10
1651	2-Bromopropane	C3H7Br	317.45	267.24	228.38
1691	Iodobenzene	C6H5I	461.69	391.60	336.86
1860	Fluorobenzene	C6H5F	354.99	301.62	260.00
1571	Chlorobenzene	C6H5Cl	399.41	337.97	290.12
1680	Bromobenzene	C6H5Br	420.76	356.38	306.17
1526	1,2-DiCl-Propane	C3H6Cl2	373.38	316.37	271.91
1683	Propyl Iodide	C3H7I	350.76	295.49	252.69
1536	2,3-DICHLOROBUT	C4H8Cl2	380.71	322.45	277.16
2638	2-Bromobutane	C4H9Br	350.61	295.98	253.65
1586	1-Chlorobutane	C4H9Cl	346.83	293.04	251.31
1573	M-DiCl-Benzene	C6H4Cl2	456.46	387.62	333.81
2634	Benzotrifluoride	C7H5F3	377.82	318.31	272.30
1574	P-DiCl-Benzene	C6H4Cl2	456.46	387.62	333.81
1650	1-Bromopropane	C3H7Br	316.74	266.88	228.25
1587	2-Chlorobutane	C4H9Cl	322.41	271.58	232.32
1678	M-Dibromobenzene	C6H4Br2	496.11	421.94	363.86
1537	1,2-DiCl-Butane	C4H8Cl2	402.81	342.01	294.57
1597	34-DiCl-1-Butene	C4H6Cl2	404.91	344.13	296.61
1577	O-Chlorotoluene	C7H7Cl	433.45	368.04	316.99
1532	123-3Cl-Propane	C3H5Cl3	448.02	382.09	330.26
1578	P-Chlorotoluene	C7H7Cl	433.45	368.04	316.99
1562	Benzyl Chloride	C7H7Cl	454.12	386.13	332.93
2661	P-Bromotoluene	C7H7Br	453.37	385.28	332.07
1508	1,4-DiCl-Butane	C4H8Cl2	424.08	360.89	311.42
1655	1-Bromobutane	C4H9Br	349.78	295.50	253.42
2652	Perfluoropropane	C3F8	218.07	181.57	153.88
1505	2-Butylene DiCl	C4H6Cl2	429.56	364.13	312.96
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	436.19	372.28	322.00
1588	1-Chloropentane	C5H11Cl	377.53	319.76	274.89
1592	1,2,4-TriCl-Bz	C6H3Cl3	509.09	433.65	374.49
1579	2,4-2Cl-Toluene	C7H6Cl2	486.54	414.43	357.95
2593	1,3,5-TriCl-BZ	C6H3Cl3	509.09	433.65	374.49
1697	1-Br-Naphthalene	C10H7Br	551.17	469.63	405.71
1622	Perfluorobutane	C4F10	262.02	220.31	188.39
1857	P-Cl-Benzo-TriF	C7H4ClF3	436.62	369.40	317.21
1509	1,5-DiCl-Pentane	C5H10Cl2	450.17	383.79	331.78
1589	1-Cl-Naphthalene	C10H7Cl	532.64	453.52	391.57
1864	Perfluorobenzene	C6F6	428.20	373.25	329.11
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	490.68	416.64	358.91
1667	1-Bromoheptane	C7H15Br	434.25	369.49	319.03
1575	HexaCl-Benzene	C6Cl6	646.19	554.58	482.14

Table C.7 Boiling Temperatures Calculated by the Tihic et al. Method using (Continued)

2640	Freon 123B1	C2HBrClF3	344.27	290.31	248.45
1504	Vinyl Chloride	C2H3Cl	244.03	203.35	171.78
1672	1,1-DiBr-Ethane	C2H4Br2	372.58	315.54	270.99
1580	Acetylene DiCl	C2H2Cl2	314.48	264.16	224.95
1692	Diiodomethane	CH2I2	408.77	345.34	295.84
1698	Bromoform	CHBr3	423.50	360.43	310.82
2687	Freon 13B1	CBrF3	240.14	200.37	169.70
1649	Tetrabromoethane	C2H2Br4	521.11	446.20	387.02
1503	Ethyl Chloride	C2H5Cl	276.80	232.65	198.37
1641	Methyl Bromide	CH3Br	240.81	201.73	171.38
2688	Freon 12B2	CBr2F2	336.82	286.08	246.33
1673	1,2-DiBr-Ethane	C2H4Br2	371.38	314.76	270.52
2637	Dibromomethane	CH2Br2	338.85	286.65	245.81
1612	Cl-2F-Ethylene	C2HClF2	243.31	204.06	173.66
2639	Br-Cl-Methane	CH2BrCl	335.40	283.85	243.44
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	314.48	264.16	224.95
1682	Ethyl Iodide	C2H5I	316.98	266.24	226.95
2693	Perfluoroethane	C2F6	165.17	135.50	113.17
1645	Ethyl Bromide	C2H5Br	280.59	235.75	201.01
1619	111-3F-Ethane	C2H3F3	168.08	138.51	116.08
2694	Vinyl Bromide	C2H3Br	283.04	238.22	203.37
1523	1,2-DiCl-Ethane	C2H4Cl2	365.29	309.77	266.27
2527	1,3-DiCl-Propane	C3H6Cl2	395.89	336.30	289.65

APPENDIX D.

BOILING AND CRITICAL TEMPERATURES CALCULATED BY THE METHODS GIVEN IN CHAPTER IV

Table D. 1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV

	Alcohols				
DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	$\boldsymbol{T_c}$
1181	Phenol	C6H6O	433.86	333.78	686.93
1182	O-Cresol	C7H8O	459.64	353.00	703.72
1183	M-Cresol	C7H8O	459.64	353.00	703.72
1176	2,6-Xylenol	C8H10O	483.67	371.04	718.50
1111	2-Mth-2-Butanol	C5H12O	387.17	289.06	568.10
1178	3,5-Xylenol	C8H10O	483.67	371.04	718.50
1133	2-Octanol	C8H18O	463.02	349.17	642.48
2885	4-HYDROXYSTYREN	C8H8O	497.84	372.53	714.52
1197	P-t-Butylphenol	C10H14O	510.45	388.00	745.73
1172	2,4-Xylenol	C8H10O	483.67	371.04	718.50
1184	P-Cresol	C7H8O	459.64	353.00	703.72
1151	Cyclohexanol	C6H12O	434.67	325.10	644.24
1170	2,3-Xylenol	C8H10O	477.01	366.62	716.46
1187	P-Ethyl Phenol	C8H10O	477.01	366.62	716.46
2859	P-Methoxyphenol	C7H8O2	487.08	373.88	727.88
1121	2-Ethylhexanol	C8H18O	463.02	349.17	642.48
1179	PropargylAlcohol	C3H4O	356.59	269.45	547.69
1123	3-Mth-1-Butanol	C5H12O	396.18	298.38	577.86

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

2196	P-t-Amylphenol	C11H16O	527.79	401.33	757.89
1174	2,5-Xylenol	C8H10O	483.67	371.04	718.50
1115	2-Hexanol	C6H14O	419.89	316.33	601.68
1152	1-MthCycHexanol	C7H14O	441.88	332.33	627.01
4854	Guaiacol	C7H8O2	487.08	373.88	727.88
1107	Sec-Butanol	C4H10O	370.76	279.21	551.15
1167	Allyl Alcohol	C3H6O	349.05	263.41	533.71
1130	4-Mth-2-Pentanol	C6H14O	413.33	310.77	592.23
1177	3,4-Xylenol	C8H10O	483.67	371.04	718.50
1114	1-Hexanol	C6H14O	426.33	321.78	610.89
1106	Isobutanol	C4H10O	370.76	279.21	551.15
1125	1-Heptanol	C7H16O	448.16	338.36	631.58
1105	N-Butanol	C4H10O	378.16	285.42	562.22
1109	1-Pentanol	C5H12O	403.06	304.18	587.92
1132	1-Octanol	C8H18O	468.73	354.04	650.35
1113	T-Butylcarbinol	C5H12O	387.17	289.06	568.10
1137	1-Undecanol	C11H24O	524.14	396.66	697.69
1108	Tert-Butanol	C4H10O	361.07	269.20	539.76
1103	N-Propanol	C3H8O	351.34	265.28	533.19
1134	1-Nonanol	C9H20O	488.17	368.94	667.48
2195	P-t-Octylphenol	C14H22O	565.55	428.60	782.16
1102	Ethanol	C2H6O	322.27	243.51	500.04
1124	3-Mth-2-Butanol	C5H12O	389.16	292.46	567.53
1136	1-Decanol	C10H22O	506.61	383.12	683.20
1140	Dodecanol	C12H26O	540.84	409.62	711.12
1104	Isopropanol	C3H8O	343.35	258.59	520.91
1110	2-Pentanol	C5H12O	396.18	298.38	577.86
1120	3-Pentanol	C5H12O	396.18	298.38	577.86
1112	2-Mth-1-Butanol	C5H12O	396.18	298.38	577.86
1154	Ts-2-Mth-CycC6OH	C7H14O	441.88	332.33	627.01
1153	Cs-2-Mth-CycC6OH	C7H14O	441.88	332.33	627.01
1156	Ts-3-Mth-CycC6OH	C7H14O	441.88	332.33	627.01
1157	Cs-4-Mth-CycC6OH	C7H14O	441.88	332.33	627.01
2197	P-Cumylphenol	C15H16O	604.70	459.21	845.89
1180	Benzyl Alcohol	C7H8O	470.27	352.36	687.24
1158	Ts-4-Mth-CycC6OH	C7H14O	441.88	332.33	627.01
1155	Cs-3-Mth-CycC6OH	C7H14O	441.88	332.33	627.01
1168	2-Phn-2-Propanol	C9H12O	496.24	370.08	707.16
1141	1-Tridecanol	C13H28O	556.79	422.04	723.61
1147	2-Eth-1-Butanol	C6H14O	419.89	316.33	601.68
1117	2-Mth-1-Pentanol	C6H14O	419.89	316.33	601.68
2115	2-Phenylethanol	C8H10O	481.21	362.55	691.47

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1142	1-Tetradecanol	C14H30O	572.05	433.98	735.26
2118	1-PHN-1-PROPANOL	C9H12O	502.88	377.16	711.03
2119	1-PHN-2-PROPANOL	C9H12O	502.88	377.16	711.03
1126	2-Heptanol	C7H16O	442.11	333.22	623.09
1143	1-Pentadecanol	C15H32O	586.67	445.47	746.19
1129	Isoheptanol	C7H16O	442.11	333.22	623.09
2117	2,6-DiMth-4-C7OH	C9H20O	471.71	354.82	645.05
1144	1-Hexadecanol	C16H34O	600.71	456.55	756.45
1145	Heptadecanol	C17H36O	614.21	467.24	766.12
1199	Nonylphenol	C15H24O	592.63	454.81	795.63
1146	1-Octadecanol	C18H38O	627.20	477.57	775.26
1135	2-Nonanol	C9H20O	482.77	364.31	660.16
1149	1-Nonadecanol	C19H40O	639.72	487.56	783.93
1139	Isodecanol	C10H22O	501.48	378.71	676.36
1148	1-Eicosanol	C20H42O	651.81	497.24	792.16
2198	Dinonylphenol	C24H42O	701.47	541.27	855.26
1159	Menthol	C10H20O	495.49	361.47	667.53
1202	DiethyleneGlycol	C4H10O3	476.27	368.80	657.27
1245	1,3-Benzenediol	C6H6O2	497.77	395.05	764.00
1186	P-Hydroquinone	C6H6O2	497.77	395.05	764.00
1244	1,2-Benzenediol	C6H6O2	497.77	395.05	764.00
1219	2MTH,13PROPNDIO	C4H10O2	450.45	347.37	635.27
1212	1,3-Propanediol	C3H8O2	435.04	336.48	624.07
1235	P-t-But-Catechol	C10H14O2	562.82	439.96	803.51
1203	Triglycol	C6H14O4	530.42	410.84	698.59
1198	Bisphenol A	C15H16O2	645.42	501.09	882.68
1238	2,3-Butanediol	C4H10O2	444.44	342.38	627.19
1211	1,2-Propanediol	C3H8O2	428.76	331.31	615.54
2219	2,4-PENTANEDIOL	C5H12O2	465.22	357.86	645.75
1215	1,4-Butynediol	C4H6O2	466.65	334.46	688.77
1214	Neopentyl Glycol	C5H12O2	463.61	355.16	647.28
1221	1,3-Butanediol	C4H10O2	450.45	347.37	635.27
1220	1,2-Butanediol	C4H10O2	450.45	347.37	635.27
1240	Ts2-C4H8-14-Diol	C4H8O2	458.16	352.68	644.62
1239	Cis-Butenediol	C4H8O2	458.16	352.68	644.62
1241	1,4-Butanediol	C4H10O2	456.36	352.27	643.17
1222	Hexylene Glycol	C6H14O2	477.85	365.38	657.15
1213	Dipropylene Gly	C6H14O3	503.26	388.04	675.15
1242	1,5-Pentanediol	C5H12O2	476.48	367.25	660.60
1243	1,6-Hexanediol	C6H14O2	495.51	381.51	676.61
1204	TetraC2H4 Glycol	C8H18O5	577.39	447.76	731.66
6886	C6H4(COOC2H4OH)2	C12H14O6	666.16	513.12	821.08

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1248	123-Benzenetriol	C6H6O3	551.91	445.91	818.65
1231	Glycerol	C3H8O3	497.52	389.31	678.67
1247	Hexaglycerol	C6H14O3	543.08	421.52	714.95
1246	Pentaerythritol	C5H12O4	579.87	454.82	743.51

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Amines

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1742	Ethyleneimine	C2H5N	271.20	206.91	487.42
1745	Piperidine	C5H11N	370.01	275.27	600.38
2726	Propyleneimine	C3H7N	292.94	224.41	512.58
1766	Pyrrolidine	C4H9N	340.17	254.43	568.43
1719	Isopropylamine	C3H9N	305.30	220.12	471.90
1711	N-Propylamine	C3H9N	321.63	237.20	496.95
1726	Sec-Butylamine	C4H11N	335.80	243.88	510.36
1704	Ethylamine	C2H7N	289.75	212.76	456.66
1702	Dimethylamine	C2H7N	266.12	198.64	437.71
1710	Diethylamine	C4H11N	329.45	240.78	503.91
1740	Allylamine	C3H7N	319.13	235.11	497.07
1712	N-Butylamine	C4H11N	350.76	259.49	531.44
1794	HexMthyleneimine	C6H13N	397.50	294.61	628.26
1729	Cyclohexylamine	C6H13N	402.73	297.15	633.63
1714	Isobutylamine	C4H11N	342.75	252.64	518.66
2853	Acetamide	C2H5NO	483.69	338.40	757.18
2731	N-C1-CycC6-Amine	C7H15N	406.27	313.16	646.27
1743	Diisopropylamine	C6H15N	375.47	270.49	523.10
1796	N,N-DiMthAniline	C8H11N	496.75	367.80	729.27
1792	Aniline	C6H7N	448.87	330.10	699.00
1713	N-Pentylamine	C5H13N	377.61	280.04	561.47
1733	Benzylamine	C7H9N	449.35	332.10	672.64
1737	M-Toluidine	C7H9N	473.62	349.55	715.13
3796	N-Ethylaniline	C8H11N	454.80	334.64	677.13
1878	2-Methacrylamide	C4H7NO	519.11	367.11	795.02
1736	O-Toluidine	C7H9N	473.62	349.55	715.13
2739	Diallylamine	C6H11N	380.10	279.56	569.11
2706	Hexylamine	C6H15N	402.56	299.16	587.92
2724	O-Ethylaniline	C8H11N	490.34	363.33	727.53

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1707	Dipropylamine	C6H15N	384.28	283.09	567.05
1738	P-Toluidine	C7H9N	473.62	349.55	715.13
1795	N-Methylaniline	C7H9N	434.69	323.20	669.30
1718	Diisobutylamine	C8H19N	418.87	308.65	597.11
1879	Acrylamide	C3H5NO	500.86	352.72	775.99
2707	1-Aminoheptane	C7H17N	425.85	317.06	611.46
2730	DiCycHexylAmine	C12H23N	525.61	388.13	736.98
2787	P-Aminodiphenyl	C12H11N	581.38	432.02	843.26
1744	Dibutylamine	C8H19N	431.67	319.73	616.11
2708	1-Octylamine	C8H19N	447.71	333.90	632.59
2791	2,6-DiEthAniline	C10H15N	527.48	393.20	750.52
2709	1-Nonylamine	C9H21N	468.31	349.82	651.70
2710	1-Decylamine	C10H23N	487.78	364.92	669.09
3722	Diamylamine	C10H23N	473.48	352.22	655.67
3724	Undecylamine	C11H25N	506.23	379.29	685.01
2712	Dodecylamine	C12H27N	523.78	393.01	699.65
1720	Tetradecylamine	C14H31N	556.46	418.69	725.76
2752	Piperazine	C4H10N2	382.12	290.44	620.98
1752	Propylenediamine	C3H10N2	373.63	278.06	562.64
1741	Ethylenediamine	C2H8N2	360.96	272.20	551.35
2725	O-Aminoaniline	C6H8N2	522.51	389.04	790.09
2750	P-Aminoaniline	C6H8N2	522.51	389.04	790.09
2727	M-Aminoaniline	C6H8N2	522.51	389.04	790.09
1750	AEP	C6H15N3	444.29	350.31	693.18
1732	Toluene Diamine	C7H10N2	542.75	405.08	797.83
1731	hexamethyleneDiamine	C6H16N2	455.49	343.71	645.52
3750	P-Benzidine	C12H12N2	633.57	475.22	897.34

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Nitriles

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1773	Propionitrile	C3H5N	367.80	266.66	576.02
1782	Butyronitrile	C4H7N	393.42	286.69	604.23
2720	Allyl Cyanide	C4H5N	391.39	284.96	606.16
1783	Valeronitrile	C5H9N	417.31	305.38	628.93
3874	Benzyl Cyanide	C8H7N	500.84	368.30	750.00
1786	Hexanenitrile	C6H11N	439.68	322.90	650.80

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1776	Succinonitrile	C4H4N2	480.54	354.29	725.47
1781	Glutaronitrile	C5H6N2	499.37	369.17	740.04
2735	14-2Cyano-2-C4H8	C6H6N2	518.76	383.72	755.00
1777	Adiponitrile	C6H8N2	517.25	383.34	753.23

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Imines

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1767	N-MthPyrrolidine	C5H11N	328.45	258.42	550.00
2797	3-Methylpyridine	C6H7N	406.68	301.76	644.99
1797	2-Methylpyridine	C6H7N	406.68	301.76	644.99
2799	4-Methylpyridine	C6H7N	406.68	301.76	644.99
1753	N,N-DiEthAniline	C10H15N	464.19	348.61	694.42

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Tert-N

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1706	Triethylamine	C6H15N	342.79	260.16	535.15
2716	Tributylamine	C12H27N	482.40	365.39	672.01
2719	Tripropylamine	C9H21N	419.44	317.60	614.74
3723	Triamylamine	C15H33N	535.86	406.52	715.79

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Nitrates

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1761	Nitroethane	C2H5NO2	381.09	279.06	587.98
1763	2-Nitropropane	C3H7NO2	393.95	288.28	593.99
1762	1-Nitropropane	C3H7NO2	405.79	298.24	614.09

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Thiols

DipID	Name	Formula	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1802	Ethyl Mercaptan	C2H6S	313.66	224.25	500.38
1820	Dimethyl Sulfide	C2H6S	304.36	222.65	500.20
1843	Thiacyclopentane	C4H8S	371.18	273.85	617.66
1803	1-Propanethiol	C3H8S	343.44	247.64	537.94
1805	Isobut Mercaptan	C4H10S	363.30	262.49	557.57
6860	Ethylenedithiol	C2H6S2	398.99	290.24	629.79
1811	Cyclohexanethiol	C6H12S	430.62	312.62	657.13
1828	DiMth Disulfide	C2H6S2	398.99	290.24	629.79
1841	Butanethiol	C4H10S	370.85	269.09	570.09
1814	Methylproylsulf	C4H10S	370.85	269.09	570.09
2816	ETHYLtBUTYL SUL	C6H14S	396.26	285.31	586.58
1818	Diethyl Sulfide	C4H10S	361.40	261.19	550.98
1812	Benzyl Mercaptan	C7H8S	464.65	339.54	710.60
1838	T-OctylMercaptan	C8H18S	449.72	328.06	649.19
1827	1-Pentanethiol	C5H12S	396.26	288.95	598.03
2815	METHnBUTYL SULFD	C5H12S	388.97	287.70	598.74
1824	DiethylDisulfide	C4H10S2	429.11	313.03	642.10
1807	N-Hexylmercaptan	C6H14S	419.96	307.49	622.60
6857	Dimercaptoethyl	C4H10OS2	465.13	344.05	686.70
1839	1-Heptanethiol	C7H16S	442.18	324.89	644.42
1829	DiProp Disulfide	C6H14S2	471.20	346.23	681.36
1809	1-Octanethiol	C8H18S	463.08	341.30	663.97
1808	N-Nonanethiol	C9H20S	482.83	356.83	681.62
1826	1-Decanethiol	C10H22S	501.54	371.59	697.66
2838	tertDodecanThiol	C12H26S	525.40	388.23	715.77
1825	1-Undecanethiol	C11H24S	519.31	385.65	712.33
1837	Dodecylthiol	C12H26S	536.24	399.08	725.80

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Aldehydes

DipID	Name	Formula	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1037	Methacrolein	C4H6O	343.47	249.91	523.70
1002	Acetaldehyde	C2H4O	282.93	204.58	441.65
1003	Propionaldehyde	C3H6O	315.44	229.82	484.10

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1041	Benzaldehyde	C7H6O	445.06	326.91	665.38
1034	Acrolein	C3H4O	312.90	227.67	484.01
1005	N-Butyraldehyde	C4H8O	345.08	252.73	520.23
1036	Trans-2-Butenal	C4H6O	347.54	253.32	522.27
1007	Valeraldehyde	C5H10O	372.36	273.78	551.54
1006	Isobutyraldehyde	C4H8O	336.94	245.70	506.99
1009	1-Hexanal	C6H12O	397.67	293.33	579.04
1040	P-Tolualdehyde	C8H8O	470.06	346.57	683.97
1016	2-Methylhexanal	C7H14O	414.75	305.94	593.70
1017	3-Methylhexanal	C7H14O	414.75	305.94	593.70
1008	1-Heptanal	C7H14O	421.28	311.59	603.45
1013	2-Ethylhexanal	C8H16O	437.28	323.43	616.36
1010	1-Octanal	C8H16O	443.41	328.74	625.31
1011	1-Nonanal	C9H18O	464.25	344.94	645.04
1020	1-Decanal	C10H20O	483.94	360.29	662.96
1021	1-Undecanal	C11H22O	502.59	374.88	679.33
1025	Dodecanal	C12H24O	520.31	388.79	694.38
1026	1-Tridecanal	C13H26O	537.19	402.08	708.27
1014	1,2-Ethanedione	C2H2O2	349.85	259.17	530.15
1044	1,4BenzDicarboxAldehy	C8H6O2	516.29	383.80	728.89

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Epoxides

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1440	ISOBUTYLENE OXID	C4H8O	292.79	220.62	499.32
1478	Furan	C4H4O	305.03	228.63	538.92
1443	1,3-Propylene Ox	C3H6O	280.83	215.87	490.24
1479	Tetrahydrofuran	C4H8O	321.17	239.69	534.15
1477	2,5-Dihydrofuran	C4H6O	340.65	244.90	542.00
1471	1,2-Epoxybutane	C4H8O	304.60	232.64	515.19
1408	1-Methoxypropane	C4H10O	312.71	226.91	476.40
1442	1,2-Propylene Ox	C3H6O	270.93	207.70	473.17
1411	2-Methoxypropane	C4H10O	303.74	219.11	461.21
1421	1,4-Dioxane	C4H8O2	343.04	264.32	559.57
2422	1,3-DIOXANE	C4H8O2	343.04	264.32	559.57
1426	2-Methoxybutane	C5H12O	334.38	242.97	499.80
1422	Trioxane	C3H6O3	342.74	266.54	555.70

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1413	1-Methoxybutane	C5H12O	342.58	250.07	513.18
1461	Methoxybenzene	C7H8O	421.04	307.48	637.90
1448	1-Ethoxybutane	C6H14O	367.61	269.89	539.61
1429	1-MethoxyPentane	C6H14O	367.61	269.89	539.61
6885	Ethyl-3-Ethoxypr	C7H14O3	442.15	329.62	616.14

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Ether

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1401	Dimethyl Ether	C2H6O	243.33	172.43	380.77
1407	MethylEthylEther	C3H8O	276.72	199.43	426.61
1470	VinylMethylEther	C3H6O	277.07	198.90	432.12
1405	MTBE	C5H12O	323.59	231.45	484.60
1445	VinylEthyl Ether	C4H8O	307.23	223.00	469.95
1402	Diethyl Ether	C4H10O	309.82	225.20	470.31
1431	Methylal	C3H8O2	315.25	231.16	480.58
1428	T-But EthylEther	C6H14O	349.98	252.68	514.66
1427	TAME	C6H14O	352.55	254.22	520.35
1410	Mth Isobut Ether	C5H12O	334.38	242.97	499.80
1430	Eth-t-Pent-Ether	C7H16O	376.90	273.74	546.00
1403	DiisopropylEther	C6H14O	351.19	247.44	500.05
1415	Eth Propyl Ether	C5H12O	339.93	248.51	507.45
1455	Dimethyl Acetal	C4H10O2	339.63	250.87	505.23
1446	Dipropyl Ether	C6H14O	367.61	269.89	539.61
1447	Butyl VinylEther	C6H12O	365.42	268.04	540.19
1462	EthylPhenylEther	C8H10O	441.20	323.69	653.72
1406	Di-sec-But Ether	C8H18O	402.93	288.78	560.86
1432	Acetal	C6H14O2	385.90	285.66	554.20
1460	BenzylEthylEther	C9H12O	453.06	334.91	659.81
1050	Paraldehyde	C6H12O3	396.67	282.80	567.15
1404	Di-n-Butyl Ether	C8H18O	417.15	308.19	592.89
1420	Anethole	C10H12O	495.23	363.92	706.49
1456	DimethylCarbitol	C6H14O3	420.90	314.44	595.93
1463	Dibenzyl Ether	C14H14O	561.59	418.09	786.86
1425	Di-n-PentylEther	C10H22O	460.59	341.92	635.57
1458	Diethyl Carbitol	C8H18O3	460.16	345.28	628.89
1412	Dihexyl Ether	C12H26O	499.30	372.15	670.76

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1454	Triglyme	C8H18O4	483.41	364.28	651.93
1459	Dibutyl Carbitol	C12H26O3	533.86	402.37	693.68
1424	Di-n-Octyl Ether	C16H34O	565.98	424.74	725.98
1457	Tetraglyme	C10H22O5	533.51	405.12	687.56
1418	Dinonyl Ether	C18H38O	595.13	447.97	748.25
2432	ETHYLAL	C5H12O2	367.33	272.07	536.93
2405	DIISOBUTYL ETHER	C8H18O	403.80	296.64	572.91
2456	Ethyl Glyme	C6H14O2	392.99	291.72	564.84
2417	ETHYLHEXYL ETHER	C8H18O	417.15	308.19	592.89
2415	ETHYLISOPROPETH	C5H12O	330.60	231.67	477.34

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Formates

DipID	Name	Formula	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1301	Methyl Formate	C2H4O2	289.64	211.20	453.78
1311	Vinyl Formate	C3H4O2	319.03	233.69	494.54
1302	Ethyl Formate	C3H6O2	321.53	235.79	494.46
2306	t-Butyl Formate	C5H10O2	360.41	262.22	536.13
1303	Propyl Formate	C4H8O2	350.66	258.19	529.26
2305	sec-ButylFormate	C5H10O2	370.12	272.48	547.99
2311	CYCLOHEXL FORMAT	C7H12O2	434.13	319.40	644.98
1304	N-Butyl Formate	C5H10O2	377.53	278.84	559.53
1305	Isobutyl Formate	C5H10O2	370.12	272.48	547.99
2350	Benzyl Formate	C8H8O2	469.78	347.18	689.38
2307	n-Hexyl Formate	C7H14O2	425.78	316.01	609.89
1306	N-Pentyl Formate	C6H12O2	402.48	298.04	586.18
2308	n-Heptyl Formate	C8H16O2	447.64	332.91	631.16
1308	N-Octyl Formate	C9H18O2	468.24	348.89	650.39
1309	n-Nonyl Formate	C10H20O2	487.71	364.04	667.88
1310	n-Decyl Formate	C11H22O2	506.17	378.45	683.88

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Esters

DipID	Name	Formula	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1351	Mth Methacrylate	C5H8O2	373.57	274.61	562.26

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1312	Methyl Acetate	C3H6O2	318.60	233.84	492.28
1331	Vinyl Propionate	C5H8O2	366.28	270.83	542.09
1321	Vinyl Acetate	C4H6O2	345.66	254.46	528.06
1352	Eth MthAcrylate	C6H10O2	392.64	289.84	573.15
1322	MethylPropionate	C4H8O2	347.98	256.40	527.51
1341	Methyl Acrylate	C4H6O2	341.37	249.57	513.82
1313	Ethyl Acetate	C4H8O2	340.85	251.50	509.94
1319	IsopropylAcetate	C5H10O2	367.58	270.78	546.45
1332	Methyl Butyrate	C5H10O2	368.46	272.65	541.52
1342	Ethyl Acrylate	C5H8O2	368.94	270.87	545.76
1318	Allyl Acetate	C5H8O2	372.90	275.39	559.01
1314	N-Propyl Acetate	C5H10O2	375.04	277.19	558.11
1323	Ethyl Propionate	C5H10O2	368.46	272.65	541.52
1360	I-But I-Butyrate	C8H16O2	429.97	317.08	601.44
1320	Sec-ButylAcetate	C6H12O2	393.23	290.53	574.47
1336	PropylI-Butyrate	C7H14O2	413.63	304.96	587.73
1353	N-C3-Mthacrylate	C7H12O2	405.51	307.28	624.46
1333	Ethyl Butyrate	C6H12O2	394.04	292.27	569.30
1347	EthylIsovalerate	C7H14O2	411.29	304.93	584.28
1315	N-Butyl Acetate	C6H12O2	400.16	296.49	585.02
1390	Methyl Benzoate	C8H8O2	467.87	345.87	689.08
1388	ISOBUTYL MTHACR	C8H14O2	434.99	320.33	614.90
1343	1-PropylAcrylate	C6H10O2	392.01	290.57	570.15
1316	Isobutyl Acetate	C6H12O2	393.23	290.53	574.47
1344	N-Butyl Acrylate	C7H12O2	414.07	316.03	631.90
1357	Pentyl Acetate	C7H14O2	423.61	314.56	608.93
1327	N-PropN-Butyrate	C7H14O2	417.88	310.60	594.00
1324	N-PropPropionate	C6H12O2	394.04	292.27	569.30
1291	Acetic Anhydride	C4H6O3	406.30	302.59	601.87
1389	N-ButMthacrylate	C8H14O2	441.17	325.70	624.00
1359	Benzyl Acetate	C9H10O2	478.89	356.28	693.10
1326	N-But Propionate	C7H14O2	417.88	310.60	594.00
1391	Ethyl Benzoate	C9H10O2	484.49	357.83	694.44
1897	CH3OC3H600CH3	C6H12O3	419.00	312.10	600.71
1392	DiethylCarbonate	C5H10O3	393.78	294.28	566.36
1385	N-But N-Butyrate	C8H16O2	440.22	327.81	616.16
1317	IsopentylAcetate	C7H14O2	417.12	308.97	599.31
1363	N-Hexyl Acetate	C8H16O2	442.38	327.85	619.56
1387	Ethylene Acetate	C6H10O4	451.36	339.14	641.37
1393	Diethyl Oxalate	C6H10O4	440.69	331.82	613.77
1365	Butyl Benzoate	C11H14O2	520.81	386.56	724.18
1361	I-C5 I-Valerate	C10H20O2	469.98	349.81	638.93

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1367	Heptyl Acetate	C9H18O2	463.28	344.09	639.50
1346	N-Butyl Valerate	C9H18O2	461.24	344.06	636.18
1358	2-C2-C6 Acetate	C10H20O2	480.46	358.08	659.76
1394	Diethyl Malonate	C7H12O4	463.71	347.89	636.64
1292	Propionyl Oxide	C6H10O3	439.97	331.17	621.55
1364	Benzyl Benzoate	C14H12O2	578.59	431.80	799.27
1381	2Mth p-Phthalate	C10H10O4	552.89	414.49	761.06
1368	n-Octyl Acetate	C10H20O2	483.01	359.48	657.63
1377	DiMthI-Phthalate	C10H10O4	548.11	408.87	742.73
1896	Ethylene DiAcr	C8H10O4	482.20	360.45	660.50
1386	2-Ethylhexyl Acr	C11H20O2	495.00	368.26	668.51
1395	Methyl Decanoate	C11H22O2	499.89	374.08	671.05
1369	n-Nonyl Acetate	C11H22O2	501.71	374.11	674.20
1370	n-Decyl Acetate	C12H24O2	519.48	388.06	689.44
1345	N-ButylNonanoate	C13H26O2	534.74	401.36	700.53
1375	DiProp Phthalate	C14H18O4	606.85	455.91	784.27
1376	Diisobutyl Phtha	C16H22O4	625.71	470.46	792.37
1396	IsopropMyristate	C17H34O2	593.00	445.96	745.69
1383	Butyl Stearate	C22H44O2	659.20	500.63	793.40
1362	Methyl Oleate	C19H36O2	623.56	471.25	768.70
1355	Diisooctyl Phtha	C24H38O4	715.37	544.11	848.26
1382	DioctylTerephtha	C24H38O4	720.91	549.25	854.77
1384	DIBUTYL SEBACATE	C18H34O4	635.40	483.59	773.50
1371	Diisodecyl Phtha	C28H46O4	752.62	575.27	869.87
1354	DioctylPhthalate	C24H38O4	715.37	544.11	848.26
2375	DiethylPhthalate	C12H14O4	575.77	433.25	758.36
2388	Dipropyl Maleate	C10H16O4	523.07	391.72	690.36
2381	Diallyl Maleate	C10H12O4	516.78	389.25	687.22
2370	Glyceryl Triacet	C9H14O6	543.12	412.13	720.84
2382	Dibutyl Maleate	C12H20O4	555.82	417.51	717.11
2376	DibutylPhthalate	C16H22O4	632.89	476.97	801.37
2353	CetylMthacrylate	C20H38O2	635.68	479.91	783.06
2379	Dihexyl Adipate	C18H34O4	635.40	483.59	773.50
2321	T-Butyl Acetate	C6H12O2	380.30	276.51	551.40
2332	Methl.I-butyrate	C5H10O2	363.56	266.18	533.26
2354	AllylMthacrylate	C7H10O2	417.00	306.75	603.06
2364	CYCLOHEXL ACETAT	C8H14O2	450.36	331.10	652.69
2337	EthylIsobutyrate	C6H12O2	389.48	286.25	562.14
2384	IsobutylAcrylate	C7H12O2	411.71	303.34	588.75
2380	1,1-Diacetoxy C2	C6H10O4	438.88	326.63	611.54
2392	n-PropylBenzoate	C10H12O2	503.12	372.54	709.99
2387	Dimethyl Maleate	C6H8O4	446.84	332.33	621.84

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

2377	DiMth Phthalate	C10H10O4	552.89	414.49	761.06
2386	Diethyl Maleate	C8H12O4	487.00	363.51	659.10
2385	Mth Dodecanoate	C13H26O2	534.74	401.36	700.53
3379	Dioctyl Adipate	C22H42O4	674.78	512.62	798.60
5886	Mth Acetoacetate	C5H8O3	423.72	316.40	609.53
5884	Ethoxy Acetate	C6H12O3	423.37	316.41	605.35
5887	EthAcetoAcetate	C6H10O3	445.71	333.28	630.77
5885	Carbitol Acetate	C8H16O4	485.49	365.94	660.00

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Ketones

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1096	Methyl Isopropen	C5H8O	373.14	271.85	565.59
1079	Cyclopentanone	C5H8O	377.19	284.03	609.42
1051	Acetone	C3H6O	318.10	230.61	493.97
1052	MEK	C4H8O	347.51	253.44	529.96
1065	Mesityl Oxide	C6H10O	402.16	295.07	594.13
1066	T-But Mth Ketone	C6H12O	383.72	278.24	567.38
1060	2-Pentanone	C5H10O	374.61	274.45	561.08
1061	Mth iC3 Ketone	C5H10O	367.15	267.98	549.16
1053	Diethyl Ketone	C5H10O	367.58	271.85	549.91
1059	3-Hexanone	C6H12O	393.22	291.52	577.72
1099	Diketene	C4H4O2	342.64	262.23	570.70
1055	Sec-ButMthKetone	C6H12O	392.82	287.92	577.59
1054	MIBK	C6H12O	392.82	287.92	577.59
1095	EthIsopropKetone	C6H12O	386.14	285.45	566.91
1063	2-Heptanone	C7H14O	423.24	312.16	612.51
1064	5-Mth-2-Hexanone	C7H14O	416.74	306.53	602.71
1058	4-Heptanone	C7H14O	417.12	309.89	602.38
1057	3-Heptanone	C7H14O	417.12	309.89	602.38
1076	2,4-Pentanedione	C5H8O2	428.99	317.93	628.79
1068	DiisobutylKetone	C9H18O	448.79	333.24	627.48
1097	2-CycC6 CycC6one	C12H20O	527.22	392.92	755.14
1083	2-Octanone	C8H16O	445.26	329.29	634.11
1073	Dibutyl Ketone	C9H18O	460.57	343.43	644.33
1062	2-Hexanone	C6H12O	399.76	293.94	588.35
1077	Isophorone	C9H14O	449.67	338.79	640.81
1090	Acetophenone	C8H8O	467.54	343.73	694.98
1080	Cyclohexanone	C6H10O	404.15	302.79	635.82
1074	2-Nonanone	C9H18O	465.99	345.46	653.57

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Alcohol-Ethers

DipID	Name	Formula	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
2862	2-Butoxyethanol	C6H14O2	447.93	340.07	628.14
4857	butyl carbitol	C8H18O3	506.23	386.05	676.35
2898	2-Chloroethanol	C2H5ClO	385.68	293.53	589.59
2864	Carbitol	C6H14O3	468.31	357.28	643.56
3854	Methyl propasol	C4H10O2	398.18	301.64	579.66
2860	2-Methoxyethanol	C3H8O2	380.25	288.82	564.32
2854	DiacetoneAlcohol	C6H12O2	455.33	344.59	641.06
2861	2-Ethoxyethanol	C4H10O2	402.81	306.11	584.74
2889	HydroxyAcetone	C3H6O2	402.78	307.82	594.01
3856	1tButoxy2Propnol	C7H16O2	449.43	338.02	624.26
3858	PROPGLYC2tBUTYL	C7H16O2	448.66	331.24	614.69
4855	2-Propoxyethanol	C5H12O2	426.09	323.59	607.55
4849	Acetovanillone	C9H10O3	567.85	435.40	793.71
5883	Ethyl Lactate	C5H10O3	442.57	337.15	620.59
6883	2-HydroxyEth Acr	C5H8O3	448.99	340.83	633.34
2863	Methyl Carbitol	C5H12O3	447.71	341.77	624.91
3855	Dowanol DPM	C7H16O3	489.51	373.02	664.53
3857	TriPropGlymEthlE	C10H22O4	557.73	426.75	717.07

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Hydrocarbons

DipID	Name	Formula	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
404	DiMth-Acetylene	C4H6	294.19	162.83	441.53
202	Propylene	C3H6	236.90	163.97	370.33
412	2-Pentyne	C5H8	381.05	243.31	587.42
207	2-Methylpropene	C4H8	275.11	192.94	428.45
204	1-Butene	C4H8	274.22	194.02	426.22
205	Cis-2-Butene	C4H8	280.10	197.25	429.76
402	Propyne	C3H4	247.51	173.18	392.80
406	3-Hexyne	C6H10	354.47	219.50	549.00
206	Trans-2-Butene	C4H8	280.10	197.25	429.76
407	2-Hexyne	C6H10	354.47	219.50	549.00
231	33-2Mth-1-Butene	C6H12	318.61	225.03	480.37
230	23-2Mth-1-Butene	C6H12	330.31	235.94	499.05

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

229	2-Ethyl-1-Butene	C6H12	338.61	243.23	513.15
8	I-Pentane	C5H12	301.12	214.65	456.43
14	2,2-DiMth-Butane	C6H14	321.11	227.21	480.50
232	23-2Mth-2-Butene	C6H12	322.59	222.35	512.36
213	3-Mth-1-Butene	C5H10	298.46	212.36	455.85
212	2-Mth-1-Butene	C5H10	308.38	219.41	474.47
211	Trans-2-Pentene	C5H10	312.89	223.26	474.29
210	Cis-2-Pentene	C5H10	312.89	223.26	474.29
223	4-Mth-1-Pentene	C6H12	329.56	236.84	496.24
221	2-Mth-1-Pentene	C6H12	338.61	243.23	513.15
248	2-t-Butylpropene	C7H14	348.70	247.49	520.68
227	Cs-4-Mth-2-C5H10	C6H12	334.54	239.54	498.27
224	2-Mth-2-Pentene	C6H12	343.08	247.47	516.06
403	1-Butyne	C4H6	283.63	201.99	445.49
15	2,3-DiMth-Butane	C6H14	323.52	231.50	481.95
214	2-Mth-2-Butene	C5H10	313.26	224.06	478.55
228	Ts-4-Mth-2-C5H10	C6H12	334.54	239.54	498.27
225	Cs-3-Mth-2-C5H10	C6H12	343.08	247.47	516.06
218	Trans-2-Hexene	C6H12	342.74	246.74	511.96
2226	3-METH-Tr-2Pente	C6H12	343.08	247.47	516.06
222	3-Mth-1-Pentene	C6H12	329.56	236.84	496.24
257	2-Diisobutylene	C8H16	379.73	272.80	554.88
256	1-Diisobutylene	C8H16	375.71	268.95	553.00
217	Cis-2-Hexene	C6H12	342.74	246.74	511.96
2414	1-Heptyne	C7H12	372.90	271.82	557.26
13	3-Methylpentane	C6H14	331.98	238.92	496.17
219	Cis-3-Hexene	C6H12	342.74	246.74	511.96
12	2-Methylpentane	C6H14	331.98	238.92	496.17
220	Trans-3-Hexene	C6H12	342.74	246.74	511.96
405	1-Pentyne	C5H8	316.08	227.50	488.86
209	1-Pentene	C5H10	307.57	220.37	471.78
11	N-Hexane	C6H14	340.24	246.13	509.89
235	Cis-2-Heptene	C7H14	370.20	268.25	544.46
249	Cis-3-Heptene	C7H14	370.20	268.25	544.46
216	1-Hexene	C6H12	337.87	244.11	510.18
239	3-Eth-1-Pentene	C7H14	358.04	259.15	530.81
226	4-Mth-1-Hexene	C7H14	358.04	259.15	530.81
240	3-Mth-1-Hexene	C7H14	358.04	259.15	530.81
419	3-Mth-1-Butyne	C5H8	307.20	219.72	473.43
233	2-Eth-1-Pentene	C7H14	366.39	265.03	546.36
238	2-Mth-1-Hexene	C7H14	366.39	265.03	546.36
416	1-Octyne	C8H14	398.17	291.50	584.98

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

289	2,3Dimeth Hexene	C8H16	385.01	278.97	564.04
234	1-Heptene	C7H14	365.71	265.83	543.21
413	1-Hexyne	C6H10	345.66	250.60	525.58
237	Trans-3-Heptene	C7H14	370.20	268.25	544.46
236	Trans-2-Heptene	C7H14	370.20	268.25	544.46
251	Trans-2-Octene	C8H16	395.66	288.18	572.90
279	Trans-4-Octene	C8H16	395.66	288.18	572.90
277	Trans-3-Octene	C8H16	395.66	288.18	572.90
2252	2Methl-1-Heptene	C8H16	392.11	285.18	575.29
250	1-Octene	C8H16	391.48	285.93	572.05
258	2-Ethyl-1-Hexene	C8H16	392.11	285.18	575.29
280	3-Octene	C8H16	395.66	288.18	572.90
278	4-Octene	C8H16	395.66	288.18	572.90
276	2-Octene	C8H16	395.66	288.18	572.90
259	1-Nonene	C9H18	415.49	304.66	597.53
262	1-Dodecene	C12H24	479.09	354.45	659.20
263	1-Tridecene	C13H26	497.99	369.32	676.07
264	1-Tetradecene	C14H28	515.94	383.48	691.52
265	1-Pentadecene	C15H30	533.02	397.01	705.76
266	1-Hexadecene	C16H32	549.32	409.95	718.93
267	1-Octadecene	C18H36	579.82	434.29	742.60
281	1-Heptadecene	C17H34	564.90	422.37	731.18
284	1-Eicosene	C20H40	607.88	456.83	763.33
283	1-Nonadecene	C19H38	594.13	445.77	753.29
3	Propane	C3H8	240.14	166.86	372.78
4	I-Butane	C4H10	267.06	187.59	409.09
9	Neopentane	C5H12	289.18	201.67	437.24
5	N-Butane	C4H10	277.08	196.51	427.34
7	pentane	C5H12	310.16	222.59	472.07
44	Hexamethylethane	C8H18	360.04	254.49	524.42
25	223-TriMthButane	C7H16	342.26	243.25	503.81
24	3,3-DiMthPentane	C7H16	350.28	250.34	517.24
51	2,2,3,3-4Mth-C5	C9H20	386.22	275.41	555.38
21	2,2-DiMthPentane	C7H16	350.28	250.34	517.24
42	2,3,3-TriMth-C5	C8H18	369.76	265.04	537.03
22	2,3-DiMthPentane	C7H16	352.49	254.26	517.67
40	2,2,3-TriMth-C5	C8H18	369.76	265.04	537.03
23	2,4-DiMthPentane	C7H16	352.49	254.26	517.67
41	2,2,4-TriMth-C5	C8H18	369.76	265.04	537.03
39	3-Mth-3-Eth-C5	C8H18	377.17	271.58	549.02
20	3-Ethylpentane	C7H16	360.28	261.06	530.29
52	2,2,3,4-4Mth-C5	C9H20	388.21	278.98	554.92

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

54	2334TetrMethPent	C9H20	388.21	278.98	554.92
53	2,2,4,4-4Mth-C5	C9H20	386.22	275.41	555.38
43	2,3,4-TriMth-C5	C8H18	371.85	268.75	537.02
36	3,3-DiMth-Hexane	C8H18	377.17	271.58	549.02
19	3-Methylhexane	C7H16	360.28	261.06	530.29
18	2-Methylhexane	C7H16	360.28	261.06	530.29
38	2-Mth-3-Eth-C5	C8H18	379.22	275.20	548.71
190	2,2-2C1-3-C2-C5	C9H20	395.25	285.19	566.06
32	2,2-DiMth-Hexane	C8H18	377.17	271.58	549.02
37	3,4-DiMth-Hexane	C8H18	379.22	275.20	548.71
50	3,3-DiEthPentane	C9H20	402.15	291.27	576.88
34	2,4-DiMth-Hexane	C8H18	379.22	275.20	548.71
33	2,3-DiMth-Hexane	C8H18	379.22	275.20	548.71
17	N-Heptane	C7H16	367.89	267.69	542.51
49	244TriMethHexane	C9H20	395.25	285.19	566.06
192	2,4-2C1-3-C2-C5	C9H20	397.19	288.64	565.46
47	2,2,5-TriMth-C6	C9H20	395.25	285.19	566.06
35	2,5-DiMth-Hexane	C8H18	379.22	275.20	548.71
31	3-Ethylhexane	C8H18	386.44	281.50	560.04
30	4-Methylheptane	C8H18	386.44	281.50	560.04
29	3-Methylheptane	C8H18	386.44	281.50	560.04
28	2-Methylheptane	C8H18	386.44	281.50	560.04
96	2,2-DiMthHeptane	C9H20	402.15	291.27	576.88
176	2,6-DiMthHeptane	C9H20	404.05	294.64	576.03
27	N-Octane	C8H18	393.51	287.66	571.06
94	3-Ethylheptane	C9H20	410.78	300.52	586.31
92	3-Methyloctane	C9H20	410.78	300.52	586.31
93	4-Methyloctane	C9H20	410.78	300.52	586.31
91	2-Methyloctane	C9H20	410.78	300.52	586.31
72	2,2-DiMthOctane	C10H22	425.47	309.66	601.59
2095	2,3Dimethloctane	C10H22	427.26	312.82	600.32
2096	2,4Dimethloctane	C10H22	427.26	312.82	600.32
2098	2,6DimethlOctane	C10H22	427.26	312.82	600.32
2097	2,5Dimethloctane	C10H22	427.26	312.82	600.32
2099	2,7DimethlOctane	C10H22	427.26	312.82	600.32
46	N-Nonane	C9H20	417.39	306.28	596.33
88	5-Methylnonane	C10H22	433.56	318.34	609.73
85	3-Methylnonane	C10H22	433.56	318.34	609.73
87	4-Methylnonane	C10H22	433.56	318.34	609.73
86	2-Methylnonane	C10H22	433.56	318.34	609.73
56	N-Decane	C10H22	439.76	323.75	618.90
63	N-Undecane	C11H24	460.81	340.22	639.23

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

64	N-Dodecane	C12H26	480.68	355.81	657.66
65	N-Tridecane	C13H28	499.50	370.61	674.48
66	N-Tetradecane	C14H30	517.37	384.72	689.90
67	N-Pentadecane	C15H32	534.39	398.19	704.12
68	N-Hexadecane	C16H34	550.62	411.08	717.29
69	N-Heptadecane	C17H36	566.14	423.45	729.54
70	N-Octadecane	C18H38	581.01	435.34	740.97
71	N-Nonadecane	C19H40	595.27	446.78	751.68
73	N-Eicosane	C20H42	608.98	457.81	761.75
74	n-HENEICOSANE	C21H44	622.16	468.45	771.23
75	n-DOCOSANE	C22H46	634.87	478.74	780.20
76	n-TRICOSANE	C23H48	647.12	488.70	788.69
77	n-Tetracosane	C24H50	658.95	498.35	796.76
78	n-PENTACOSANE	C25H52	670.39	507.70	804.45
79	n-HEXACOSANE	C26H54	681.46	516.78	811.78
81	n-Octacosane	C28H58	702.57	534.18	825.49
2081	n-TRICONTANE	C30H62	722.43	550.66	838.12
2082	n-Dotriacontane	C32H66	741.19	566.30	849.81

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Cyclic Hydrocarbons

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
269	Cyclopentene	C5H8	324.13	237.85	520.72
270	Cyclohexene	C6H10	355.33	259.98	556.35
287	3MthCyclopentene	C6H10	346.36	251.41	528.90
286	1-MthCyclPentene	C6H10	353.38	260.78	542.00
288	4MthCyclopenten	C6H10	346.36	251.41	528.90
273	Cycloheptene	C7H12	383.96	280.40	587.33
274	Cyclooctene	C8H14	410.42	299.41	614.59
101	Cyclopropane	C3H6	254.20	185.47	448.35
810	ADAMANTANE	C10H16	444.62	327.56	701.96
102	Cyclobutane	C4H8	292.34	212.66	499.28
104	Cyclopentane	C5H10	326.47	237.00	541.51
137	Cyclohexane	C6H12	357.47	259.20	577.37
105	MthCyclopentane	C6H12	348.55	250.60	547.72
146	Cs-1,4-2C1-CycC6	C8H16	396.85	283.69	583.92
142	Cs-1,2-2C1-CycC6	C8H16	396.85	283.69	583.92

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

141	1,1-2C1-CycC6	C8H16	386.17	280.43	564.03
145	Ts-1,3-2C1-CycC6	C8H16	396.85	283.69	583.92
144	Cs-1,3-2C1-CycC6	C8H16	396.85	283.69	583.92
147	Ts-1,4-2C1-CycC6	C8H16	396.85	283.69	583.92
143	Ts-1,2-2C1-CycC6	C8H16	396.85	283.69	583.92
138	MthCyclohexane	C7H14	377.71	271.72	580.57
159	Cycloheptane	C7H14	385.93	279.67	608.32
140	Ethylcyclohexane	C8H16	402.65	291.40	607.90
154	Trans-Decalin	C10H18	452.22	330.47	690.68
149	N-PropylCyc-C6	C9H18	425.94	309.79	631.92
109	Cs-1,2-2C1-CycC5	C7H14	369.31	263.53	553.57
110	Ts-1,2-2C1-CycC5	C7H14	369.31	263.53	553.57
112	Ts-1,3-2C1-CycC5	C7H14	369.31	263.53	553.57
107	Eth-Cyclopentane	C7H14	375.58	271.82	579.18
114	N-PropCycPentane	C8H16	400.66	291.50	606.52
108	1,1-DiMthCycC5	C7H14	357.74	260.01	533.00
111	Cs-1,3-2C1-CycC5	C7H14	369.31	263.53	553.57
152	N-ButylCycHexane	C10H20	447.80	327.05	653.25
160	Cyclooctane	C8H16	412.25	298.73	635.38
153	Cis-Decalin	C10H18	452.22	330.47	690.68
115	ISOPROPYLCYCLOPENTANE	C8H16	393.73	285.42	595.37
150	Isopropyl-CycC6	C9H18	419.50	304.10	621.78
116	1-C1-1-C2-CycC5	C8H16	384.08	280.53	562.92
122	Butylcyclpentane	C9H18	424.08	309.87	630.57
155	1,1-Bicyclohexyl	C12H22	494.88	361.70	726.99
158	N-Decylcyclo-C6	C16H32	556.52	413.55	744.86

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Aromatic Hydrocarbons

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
307	1,4-Pentadiene	C5H8	304.96	218.13	471.53
306	1-ts3-Pentadiene	C5H8	310.32	221.04	474.06
414	2-Methyl-1-Butenyne	C5H6	314.33	224.38	492.00
305	Cs1,3-Pentadiene	C5H8	310.32	221.04	474.06
309	Isoprene	C5H8	305.78	217.16	474.30
421	1-Pentene-4-yne	C5H6	313.54	225.32	488.94
303	1,3-Butadiene	C4H6	271.33	191.50	425.08

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

332	1,4-CyclHexadien	C6H8	353.18	260.77	576.00
501	Benzene	C6H6	355.84	255.88	568.09
315	Cyclopentadiene	C5H6	321.77	238.71	540.54
319	Diisopropenyl	C6H10	336.97	240.31	516.80
615	Ethynylbezene	C8H6	423.50	307.91	653.30
601	Styrene	C8H8	417.28	302.66	639.86
331	1,3-CycHexadiene	C6H8	353.18	260.77	576.00
310	1,5-Hexadiene	C6H10	335.49	242.07	510.52
312	MthCycPentadiene	C6H8	348.91	261.66	577.90
420	1-Pentene-3-yne	C5H6	323.20	190.51	503.08
502	Toluene	C7H8	387.71	280.95	599.87
521	T-Butylbenzene	C10H14	448.99	325.09	664.06
320	Dipropylene	C6H10	345.22	247.34	514.05
520	Sec-Butylbenzene	C10H14	443.97	324.99	652.70
313	1,4-Hexadiene	C6H10	340.39	244.72	512.30
314	Dipropylene	C6H10	345.22	247.34	514.05
316	DiCycPentadiene	C10H12	441.27	328.79	699.27
333	1,5-CycOctadiene	C8H12	408.58	300.09	633.55
701	Naphthalene	C10H8	480.85	353.39	745.63
504	Ethylbenzene	C8H10	408.88	298.33	621.76
820	Indan	C9H10	437.99	328.92	699.07
505	O-Xylene	C8H10	416.92	303.91	626.44
612	P-Methylstyrene	C9H10	444.24	323.99	661.85
330	DIISOCROTYL	C8H14	398.37	289.95	582.41
507	P-Xylene	C8H10	416.92	303.91	626.44
329	DIISOBUTENYL	C8H14	390.71	282.68	579.94
506	M-Xylene	C8H10	416.92	303.91	626.44
603	Methylstyrene	C9H10	444.24	323.99	661.85
613	Alpha-MthStyrene	C9H10	440.21	319.69	666.34
510	Isopropylbenzene	C9H12	421.87	307.60	631.13
724	2-Methylindene	C10H10	473.55	352.61	728.55
285	Vinylcyclohexene	C8H12	398.78	290.40	609.07
803	Indene	C9H8	459.71	338.58	730.92
706	Tetralin	C10H12	460.82	345.03	718.05
511	O-Ethyltoluene	C9H12	436.46	319.97	645.23
723	1-Methylindene	C10H10	449.46	340.53	716.75
738	Fluorene	C13H10	548.66	410.79	839.59
619	Tr-1PropenylBz	C9H10	443.30	322.34	661.17
525	O-Diethylbenzene	C10H14	454.98	335.17	662.11
618	Propenyl Bz(cis)	C9H10	443.30	322.34	661.17
602	O-Methylstyrene	C9H10	444.24	323.99	661.85
702	1-MthNaphthalene	C11H10	503.53	371.41	757.37

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

509	N-Propylbenzene	C9H12	431.77	316.28	644.60
526	M-Diethylbenzene	C10H14	454.98	335.17	662.11
583	Cs-2-PhnButene-2	C10H12	464.39	339.42	684.57
543	M-DiisopropylBz	C12H18	477.50	351.29	675.98
584	Ts-2-PhnButene-2	C10H12	464.39	339.42	684.57
580	1,2-DiC1-3C2-Bz	C10H14	462.05	340.09	665.51
704	1-EthNaphthalene	C12H12	518.94	384.23	767.01
512	M-Ethyltoluene	C9H12	436.46	319.97	645.23
522	1-Mth-2-iC3-Benz	C10H14	448.50	328.57	653.21
513	P-Ethyltoluene	C9H12	436.46	319.97	645.23
514	1,2,3-Mesitylene	C9H12	443.90	325.14	649.12
614	M-Divinylbenzene	C10H10	469.60	342.76	694.09
524	1-Mth-4-iC3-Benz	C10H14	448.50	328.57	653.21
822	Gamma-Terpinene	C10H16	446.75	329.29	660.98
821	Alpha-Terpinene	C10H16	446.75	329.29	660.98
523	1-Mth-3-iC3-Benz	C10H14	448.50	328.57	653.21
703	2-MthNaphthalene	C11H10	503.53	371.41	757.37
557	CycHexylBenzene	C12H16	494.45	365.88	747.14
515	1,2,4-Mesitylene	C9H12	443.90	325.14	649.12
519	Isobutylbenzene	C10H14	447.32	327.93	655.92
424	DiPhnAcetylene	C14H10	560.93	393.62	891.77
544	P-DiisopropylBz	C12H18	477.50	351.29	675.98
518	N-Butylbenzene	C10H14	453.28	333.17	664.92
516	1,3,5-Mesitylene	C9H12	443.90	325.14	649.12
809	Acenaphthalene	C12H8	539.63	402.14	845.04
725	123-TriMthIndene	C12H14	506.88	377.93	745.68
527	1,4-DiEthBenzene	C10H14	454.98	335.17	662.11
558	Diphenyl	C12H10	520.05	381.68	773.02
576	2-Ethyl-m-Xylene	C10H14	462.05	340.09	665.51
620	p-ISOPROPENYLSTY	C11H12	489.48	357.64	715.19
585	o-PropylToluene	C10H14	457.69	336.65	665.19
577	2-Ethyl-p-Xylene	C10H14	462.05	340.09	665.51
579	4-Ethyl-o-Xylene	C10H14	462.05	340.09	665.51
586	m-Propyltoluene	C10H14	457.69	336.65	665.19
587	p-Propyltoluene	C10H14	457.69	336.65	665.19
578	4-Ethyl-m-Xylene	C10H14	462.05	340.09	665.51
575	5-Ethyl-m-Xylene	C10H14	462.05	340.09	665.51
530	Prehnitene	C10H14	468.98	344.92	668.81
709	2,6-2Mth-Naphtha	C12H12	524.86	388.40	767.82
715	2,7-2Mth-Naphtha	C12H12	524.86	388.40	767.82
719	2-ETHYLNAPHTHALENE	C12H12	518.94	384.23	767.01
621	p-tert-BUTYLSTY	C12H16	497.14	362.38	711.81

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

532	1,2,4,5-TetMthBz	C10H14	468.98	344.92	668.81
531	1,2,3,5-TetMthBz	C10H14	468.98	344.92	668.81
533	p-tert-BUTYL ET	C12H18	498.64	363.71	709.19
567	N-Pentylbenzene	C11H16	473.57	349.13	683.16
718	1-n-PROPYLNAPHTH	C13H14	543.11	401.98	790.14
562	1,1-DiPhnEthane	C14H14	538.89	397.71	775.15
616	4-ISOBUTYLSTYRE	C12H16	503.77	369.64	715.49
260	1-Decene	C10H20	437.98	322.23	620.26
735	Cis-Stilbene	C14H12	554.43	408.65	796.24
568	Hexylbenzene	C12H18	492.76	364.26	699.64
563	Diphenylmethane	C13H12	529.58	390.93	772.19
564	1,2-DiPhnEthane	C14H14	538.87	399.90	771.77
804	Anthracene	C14H10	573.11	426.36	860.38
736	Trans-Stilbene	C14H12	554.43	408.65	796.24
805	Phenanthrene	C14H10	573.11	426.36	860.38
713	1-ButNaphthalene	C14H16	552.05	410.63	788.88
807	Pyrene	C16H10	619.21	465.31	935.63
261	1-Undecene	C11H22	459.13	338.78	640.69
581	23-2C1-23-2PhnC4	C18H22	593.34	437.18	817.78
549	N-Heptylbenzene	C13H20	510.96	378.66	714.64
710	1-PhnNaphthalene	C16H12	603.68	448.79	873.50
566	2,4-Diphenyl-4-M	C18H20	601.53	444.99	831.01
561	O-Terphenyl	C18H14	631.78	469.69	884.96
569	N-Octylbenzene	C14H22	528.28	392.40	728.37
565	Triphenylmethane	C19H16	634.22	472.14	880.66
714	N-C6-Naphthalene	C16H20	582.32	434.92	807.44
717	Fluoranthene	C16H10	619.21	465.31	935.63
716	1-Hexyl-Tetralin	C16H24	578.23	429.97	798.26
731	TriPhnEthylene	C20H16	651.07	486.05	894.74
806	Chrysene	C18H12	646.13	485.15	941.25
588	1,1,2TriPhenEth	C20H18	646.49	482.31	885.35
711	1-n-NonylNaphtha	C19H26	623.33	468.08	830.84
570	N-Nonylbenzene	C15H24	544.79	405.54	741.00
712	1-Decyl Naphtha	C20H28	635.99	478.38	837.73
559	P-Terphenyl	C18H14	631.78	469.69	884.96
560	M-Terphenyl	C18H14	631.78	469.69	884.96
589	TetraPhenylMetha	C25H20	709.28	532.06	951.70
554	Decylbenzene	C16H26	560.57	418.13	752.68
732	TetraPhnEthylene	C26H20	719.64	538.81	996.01
574	N-Dodecylbenzene	C18H30	590.15	441.85	773.64
571	N-Undecylbenzene	C17H28	575.67	430.22	763.53
572	Tridecylbenzene	C19H32	604.05	453.06	783.11

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

573	n-TETRADECYLBENZ	C20H34	623.16	467.30	800.02
2575	n-PENTADECYLBENZ	C21H36	635.83	477.63	808.07
2576	n-HEXADECYLBENZ	C22H38	648.05	487.62	815.68
2577	n-HEPTADECYLBENZ	C23H40	659.85	497.30	822.91
2578	n-OCTADECYLBENZE	C24H42	671.26	506.69	829.78

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Halocarbons

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1544	Allyl Chloride	C3H5Cl	316.79	230.71	506.40
1595	2-Chloropropene	C3H5Cl	293.53	208.38	461.12
1531	3-Chloropropyne	C3H3Cl	325.07	237.55	523.49
1535	T-Butyl Chloride	C4H9Cl	315.46	217.88	454.14
1583	Chloroprene	C4H5Cl	322.59	231.13	503.12
1530	Isopropyl Cl	C3H7Cl	294.82	206.86	452.04
1572	O-DiCl-Benzene	C6H4Cl2	446.95	325.05	684.16
1585	Propyl Chloride	C3H7Cl	319.31	232.84	505.95
1684	Isopropyl Iodide	C3H7I	365.04	263.65	580.24
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	391.90	288.68	599.80
1651	2-Bromopropane	C3H7Br	290.97	199.89	470.82
1691	Iodobenzene	C6H5I	465.95	340.42	737.06
1860	Fluorobenzene	C6H5F	355.49	256.72	557.71
1571	Chlorobenzene	C6H5Cl	404.33	292.61	631.93
1680	Bromobenzene	C6H5Br	412.00	293.94	679.03
1526	1,2-DiCl-Propane	C3H6Cl2	363.03	263.67	561.32
1683	Propyl Iodide	C3H7I	372.55	270.22	592.99
1576	Benzotrichloride	C7H5Cl3	487.82	353.76	732.68
1536	2,3-DICHLOROBUT	C4H8Cl2	369.14	262.82	549.13
2638	2-Bromobutane	C4H9Br	322.74	225.62	515.34
1586	1-Chlorobutane	C4H9Cl	348.62	255.48	541.43
1573	M-DiCl-Benzene	C6H4Cl2	446.95	325.05	684.16
2634	Benzotrifluoride	C7H5F3	371.50	271.86	681.13
1574	P-DiCl-Benzene	C6H4Cl2	446.95	325.05	684.16
1650	1-Bromopropane	C3H7Br	300.29	208.34	489.04
1587	2-Chlorobutane	C4H9Cl	326.24	231.88	494.00
2653	8F-2-Butene	C4F8	192.89	141.98	392.38
1678	M-Dibromobenzene	C6H4Br2	460.44	327.41	790.52
1537	1,2-DiCl-Butane	C4H8Cl2	389.00	283.92	590.27
1597	34-DiCl-1-Butene	C4H6Cl2	386.94	282.17	591.87
1577	O-Chlorotoluene	C7H7Cl	432.25	314.68	655.34

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1532	123-3Cl-Propane	C3H5Cl3	420.00	310.41	644.89
1578	P-Chlorotoluene	C7H7Cl	432.25	314.68	655.34
1562	Benzyl Chloride	C7H7Cl	447.74	329.02	688.79
2661	P-Bromotoluene	C7H7Br	439.34	315.90	698.99
1508	1,4-DiCl-Butane	C4H8Cl2	407.79	303.52	627.91
1655	1-Bromobutane	C4H9Br	331.23	233.21	531.00
1599	BenzylDichloride	C7H6Cl2	475.49	347.49	714.49
2652	Perfluoropropane	C3F8	134.62	44.01	209.69
1505	2-Butylene DiCl	C4H6Cl2	397.00	303.39	666.38
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	409.85	304.01	629.94
1588	1-Chloropentane	C5H11Cl	375.64	276.33	572.07
2654	OctaF-CycButane	C4F8	241.34	76.72	388.36
1592	1,2,4-TriCl-Bz	C6H3Cl3	485.01	354.21	727.86
1579	2,4-2Cl-Toluene	C7H6Cl2	471.83	344.84	701.62
2593	1,3,5-TriCl-BZ	C6H3Cl3	485.01	354.21	727.86
1697	1-Br-Naphthalene	C10H7Br	521.23	380.97	831.99
1622	Perfluorobutane	C4F10	177.01	58.39	386.36
1857	P-Cl-Benzo-TriF	C7H4ClF3	418.01	306.64	740.34
1509	1,5-DiCl-Pentane	C5H10Cl2	430.75	321.16	650.01
1589	1-Cl-Naphthalene	C10H7Cl	515.61	379.98	782.62
1864	Perfluorobenzene	C6F6	353.69	260.88	516.74
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	459.11	337.61	787.85
1667	1-Bromoheptane	C7H15Br	410.18	296.00	622.73
1575	HexaCl-Benzene	C6Cl6	579.50	427.63	824.94
2640	Freon 123B1	C2HBrClF3	286.49	200.23	580.52
1504	Vinyl Chloride	C2H3Cl	264.38	196.75	473.19
1672	1,1-DiBr-Ethane	C2H4Br2	313.25	211.55	548.03
1580	Acetylene DiCl	C2H2Cl2	315.34	232.09	543.59
1692	Diiodomethane	CH2I2	425.45	310.66	707.84
1698	Bromoform	CHBr3	334.13	222.66	651.14
2687	Freon 13B1	CBrF3	185.78	120.77	387.81
2690	Br-3F-Ethylene	C2BrF3	254.27	155.90	418.72
1649	Tetrabromoethane	C2H2Br4	398.36	270.30	824.14
2686	Freon 12B1	CBrClF2	275.69	170.00	464.12
1503	Ethyl Chloride	C2H5Cl	287.19	207.92	464.11
2641	Br-TriCl-Methane	CBrCl3	367.55	255.29	609.09
1641	Methyl Bromide	CH3Br	227.72	147.93	371.95
2688	Freon 12B2	CBr2F2	280.90	165.88	523.61
2545	2,3-DiCl-Propene	C3H4Cl2	356.64	264.79	582.86
1673	1,2-DiBr-Ethane	C2H4Br2	321.97	219.59	566.43
2637	Dibromomethane	CH2Br2	290.12	193.15	519.31
1542	TetraCl-Ethylene	C2Cl4	382.64	273.19	620.00
1541	TriCl-Ethylene	C2HCl3	360.42	262.84	556.14
1527	111-TriCl-Ethane	C2H3Cl3	348.66	245.57	541.21
1612	Cl-2F-Ethylene	C2HClF2	254.36	169.99	461.47
1617	Ethyl Fluoride	C2H5F	195.28	136.72	309.80
2639	Br-Cl-Methane	CH2BrCl	309.71	219.20	531.21

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	315.34	232.09	543.59
1682	Ethyl Iodide	C2H5I	345.28	248.87	561.41
1522	1,1-DiCl-Ethane	C2H4Cl2	330.20	236.26	516.23
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	155.39	116.18	332.10
1525	Hexachloroethane	C2Cl6	452.37	322.91	684.96
1528	1112-4Cl-Ethane	C2H2Cl4	407.81	295.24	633.49
1590	Penta-Cl-Ethane	C2HCl5	438.73	315.93	664.98
1529	1122-4Cl-Ethane	C2H2Cl4	424.54	308.77	645.00
2693	Perfluoroethane	C2F6	1.16	0.75	2.89
1611	Freon 114B2	C2Br2F4	305.02	168.74	617.41
2692	Cl-PentaF-Ethane	C2ClF5	70.12	74.96	302.16
2655	122-3Cl-112-3FC2	C2Cl3F3	260.67	197.98	521.08
1609	12-2Cl-1122-4FC2	C2Cl2F4	89.89	98.31	418.85
2526	1,1-DiCl-Propane	C3H6Cl2	358.63	258.62	550.91
1645	Ethyl Bromide	C2H5Br	266.14	180.44	437.74
2658	1112-4Cl-22-2FC2	C2Cl4F2	324.71	237.59	634.04
1619	111-3F-Ethane	C2H3F3	148.39	98.91	275.11
1524	1,1,2-3Cl-Ethane	C2H3Cl3	392.30	287.53	612.03
1640	1,1-DiF-Ethane	C2H4F2	187.58	103.85	278.28
2691	Genetron 1113	C2ClF3	248.59	160.27	386.78
2694	Vinyl Bromide	C2H3Br	263.17	177.75	437.02
1694	Refrigerant 123	C2HCl2F3	301.09	219.66	565.16
1523	1,2-DiCl-Ethane	C2H4Cl2	356.81	264.52	574.34
2656	1122-4Cl-12-2FC2	C2Cl4F2	360.59	263.61	550.53
2527	1,3-DiCl-Propane	C3H6Cl2	383.22	284.71	602.92

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

Acids

DipID	**Name**	**Formula**	$T_{b,GC}^{760\,mmHg}$	$T_{b,GC}^{10\,mmHg}$	T_c
1277	Acrylic Acid	C3H4O2	404.43	313.02	618.28
1274	Ts-Crotonic Acid	C4H6O2	419.30	331.46	668.92
1279	Oleic Acid	C18H34O2	654.48	503.01	807.46
1278	Methacrylic Acid	C4H6O2	417.47	328.50	672.51
2271	Cinnamic Acid	C9H8O2	545.75	415.91	767.75
1266	n-UNDECANOIC ACI	C11H22O2	558.95	429.08	742.59
1282	O-Toluic Acid	C8H8O2	531.39	405.63	753.97
2283	IBUPROFEN	C13H18O2	603.06	459.68	799.75
1261	Isovaleric Acid	C5H10O2	445.08	342.64	648.96
1264	1,4-CychexDicarboxAcid	C8H12O4	598.02	465.64	796.70

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

1283	P-Toluic Acid	C8H8O2	531.39	405.63	753.97
1257	3-MthButyricAcid	C5H10O2	445.08	342.64	648.96
1288	Isophthalic Acid	C8H6O4	617.75	481.51	828.75
2871	4CarboxAcidBzldhyde	C8H6O3	570.67	436.55	785.95
1256	N-Butyric Acid	C4H8O2	429.44	331.58	638.01
1276	Stearic Acid	C18H36O2	653.45	502.76	806.52
1285	Adipic Acid	C6H10O4	567.08	446.06	765.89
1273	Cs-Crotonic Acid	C4H6O2	431.38	332.02	639.69
4851	Diglycolic Acid	C4H6O5	551.43	435.84	751.59
1286	Maleic Acid	C4H4O4	536.85	423.01	745.93
2277	Citraconic Acid	C5H6O4	538.53	428.67	779.42
2278	Itaconic Acid	C5H6O4	550.70	433.10	760.77
2281	Glutaric Acid	C5H8O4	551.60	434.60	755.63
1271	TetradecylicAcid	C14H28O2	602.61	462.84	773.17
1259	N-Nonanoic Acid	C9H18O2	526.50	404.30	718.50
1280	Linoleic Acid	C18H32O2	655.50	503.27	808.39
1260	Isobutyric Acid	C4H8O2	423.06	326.31	629.11
2268	Fumaric Acid	C4H4O4	527.91	422.59	770.99
1287	Phthalic Acid	C8H6O4	617.75	481.51	828.75
1289	TerephthalicAcid	C8H6O4	617.75	481.51	828.75
2280	Succinic Acid	C4H6O4	535.41	422.68	744.65
1270	Tridecanoic Acid	C13H26O2	588.65	451.99	763.61
1254	N-Decanoic Acid	C10H20O2	543.10	416.94	730.98
2270	Suberic Acid	C8H14O4	596.13	467.79	784.59
2255	Linolenic Acid	C18H30O2	656.53	503.52	809.33
1262	N-Hexanoic Acid	C6H12O2	471.49	362.83	674.57
4852	Levulinic Acid	C5H8O3	495.55	381.93	703.35
2275	Sebacic Acid	C10H18O4	622.96	488.08	801.26
1255	Oxalic Acid	C2H2O4	500.62	397.35	720.15
2259	PentadecylicAcid	C15H30O2	616.04	473.31	782.20
2266	NonadecanoicAcid	C19H38O2	665.07	511.99	813.85
2269	Pimelic Acid	C7H12O4	581.90	457.12	775.53
1252	Acetic Acid	C2H4O2	381.72	296.53	593.01
3268	Malonic Acid	C3H4O4	518.44	410.28	732.86
2279	2-EthButyricAcid	C6H12O2	465.83	358.11	666.95
1265	N-Octanoic Acid	C8H16O2	509.09	391.10	705.04
2258	NeopentanoicAcid	C5H10O2	437.25	334.68	642.61
2257	Azelaic Acid	C9H16O4	609.80	478.10	793.16
1281	Benzoic Acid	C7H6O2	510.47	389.62	742.81
1269	Dodecanoic Acid	C12H24O2	574.11	440.75	753.44
2261	Heptanoic Acid	C7H14O2	490.79	377.30	690.45
1258	N-Valeric Acid	C5H10O2	451.09	347.62	657.17

Table D.1 Boiling and Critical Temperatures Calculated by the Suggested Correlations in Chapter IV (Continued)

2265	HeptadecylicAcid	C17H34O2	641.42	493.25	798.83
2267	N-Eicosanic Acid	C20H40O2	676.31	520.94	820.85
1253	Propionic Acid	C3H6O2	406.38	314.59	616.76
5877	Ascorbic Acid	C6H8O6	638.70	508.51	822.21
1272	HexadecanoicAcid	C16H32O2	628.96	483.44	790.73

Table D. 2 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method

DipID	Alcohols Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1181	Phenol	C6H6O	439.20	322.26	43.58
1182	O-Cresol	C7H8O	467.06	342.94	46.47
1183	M-Cresol	C7H8O	467.06	342.94	46.47
1176	2,6-Xylenol	C8H10O	494.92	363.63	49.35
1111	2-Mth-2-Butanol	C5H12O	402.95	299.69	42.11
1178	3,5-Xylenol	C8H10O	494.92	363.63	49.35
1133	2-Octanol	C8H18O	474.38	353.04	49.69
2885	4-HYDROXYSTYREN	C8H8O	503.16	373.80	52.35
1197	P-t-Butylphenol	C10H14O	532.47	388.73	51.85
1172	2,4-Xylenol	C8H10O	494.92	363.63	49.35
1184	P-Cresol	C7H8O	467.06	342.94	46.47
1151	Cyclohexanol	C6H12O	448.61	332.13	46.06
1170	2,3-Xylenol	C8H10O	489.94	359.65	48.69
1187	P-Ethyl Phenol	C8H10O	489.94	359.65	48.69
2859	P-Methoxyphenol	C7H8O2	489.48	359.76	48.88
1121	2-Ethylhexanol	C8H18O	474.38	353.04	49.69
1179	PropargylAlcohol	C3H4O	350.54	264.52	38.81
1123	3-Mth-1-Butanol	C5H12O	405.74	302.88	43.02
2196	P-t-Amylphenol	C11H16O	555.35	405.43	54.07
1174	2,5-Xylenol	C8H10O	494.92	363.63	49.35
1115	2-Hexanol	C6H14O	428.62	319.60	45.24
1152	1-MthCycHexanol	C7H14O	471.73	346.77	47.13
4854	Guaiacol	C7H8O2	489.48	359.76	48.88
1107	Sec-Butanol	C4H10O	382.86	286.15	40.79
1167	Allyl Alcohol	C3H6O	357.10	267.32	38.28
1130	4-Mth-2-Pentanol	C6H14O	428.18	318.65	44.85
1177	3,4-Xylenol	C8H10O	494.92	363.63	49.35
1114	1-Hexanol	C6H14O	429.06	320.54	45.63
1106	Isobutanol	C4H10O	382.86	286.15	40.79
1125	1-Heptanol	C7H16O	451.94	337.26	47.86
1105	N-Butanol	C4H10O	383.30	287.08	41.18
1109	1-Pentanol	C5H12O	406.18	303.81	43.40
1132	1-Octanol	C8H18O	474.82	353.98	50.08
1113	T-Butylcarbinol	C5H12O	402.95	299.69	42.11
1137	1-Undecanol	C11H24O	543.46	404.14	56.76
1108	Tert-Butanol	C4H10O	380.07	282.97	39.88
1103	N-Propanol	C3H8O	360.42	270.35	38.95
1134	1-Nonanol	C9H20O	497.70	370.70	52.31
2195	P-t-Octylphenol	C14H22O	620.76	451.16	59.46
1102	Ethanol	C2H6O	337.54	253.61	36.73
1124	3-Mth-2-Butanol	C5H12O	405.30	301.94	42.63
1136	1-Decanol	C10H22O	520.58	387.42	54.53
1140	Dodecanol	C12H26O	566.34	420.85	58.99
1104	Isopropanol	C3H8O	359.98	269.43	38.56
1110	2-Pentanol	C5H12O	405.74	302.88	43.02
1120	3-Pentanol	C5H12O	405.74	302.88	43.02

Table D. 3 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1112	2-Mth-1-Butanol	C5H12O	405.74	302.88	43.02
1154	Ts-2-Mth-CycC6OH	C7H14O	471.73	346.77	47.13
1153	Cs-2-Mth-CycC6OH	C7H14O	471.73	346.77	47.13
1156	Ts-3-Mth-CycC6OH	C7H14O	471.73	346.77	47.13
1157	Cs-4-Mth-CycC6OH	C7H14O	471.73	346.77	47.13
2197	P-Cumylphenol	C15H16O	673.55	491.05	65.25
1180	Benzyl Alcohol	C7H8O	478.62	356.18	50.13
1158	Ts-4-Mth-CycC6OH	C7H14O	471.73	346.77	47.13
1155	Cs-3-Mth-CycC6OH	C7H14O	471.73	346.77	47.13
1168	2-Phn-2-Propanol	C9H12O	521.15	385.43	53.29
1141	1-Tridecanol	C13H28O	589.22	437.57	61.21
1147	2-Eth-1-Butanol	C6H14O	428.62	319.60	45.24
1117	2-Mth-1-Pentanol	C6H14O	428.62	319.60	45.24
2115	2-Phenylethanol	C8H10O	501.50	372.90	52.36
1142	1-Tetradecanol	C14H30O	612.10	454.28	63.44
2118	1-PHN-1-PROPANOL	C9H12O	523.94	388.65	54.20
2119	1-PHN-2-PROPANOL	C9H12O	523.94	388.65	54.20
1126	2-Heptanol	C7H16O	451.50	336.32	47.47
1143	1-Pentadecanol	C15H32O	634.98	470.99	65.66
1129	Isoheptanol	C7H16O	451.50	336.32	47.47
2117	2,6-DiMth-4-C7OH	C9H20O	496.38	367.84	51.14
1144	1-Hexadecanol	C16H34O	657.86	487.70	67.89
1145	Heptadecanol	C17H36O	680.74	504.41	70.12
1199	Nonylphenol	C15H24O	650.10	476.55	64.27
1146	1-Octadecanol	C18H38O	703.62	521.12	72.34
1135	2-Nonanol	C9H20O	497.26	369.75	51.92
1149	1-Nonadecanol	C19H40O	726.50	537.83	74.57
1139	Isodecanol	C10H22O	520.14	386.47	54.15
1148	1-Eicosanol	C20H42O	749.38	554.54	76.79
2198	Dinonylphenol	C24H42O	861.00	630.84	84.97
1159	Menthol	C10H20O	509.71	364.85	46.22
1202	DiethyleneGlycol	C4H10O3	497.90	383.75	60.27
1245	1,3-Benzenediol	C6H6O2	519.82	390.63	56.59
1186	P-Hydroquinone	C6H6O2	519.82	390.63	56.59
1244	1,2-Benzenediol	C6H6O2	519.82	390.63	56.59
1219	2MTH,13PROPNDIO	C4H10O2	475.04	366.08	57.47
1212	1,3-Propanediol	C3H8O2	452.60	350.06	55.63
1235	P-t-But-Catechol	C10H14O2	613.09	457.42	64.86
1203	Triglycol	C6H14O4	566.08	434.23	67.13
1198	Bisphenol A	C15H16O2	754.17	559.91	78.27
1238	2,3-Butanediol	C4H10O2	474.60	365.25	57.08
1211	1,2-Propanediol	C3H8O2	452.16	349.24	55.24
2219	2,4-PENTANEDIOL	C5H12O2	497.48	382.08	59.31
1215	1,4-Butynediol	C4H6O2	484.48	375.36	60.01
1214	Neopentyl Glycol	C5H12O2	495.13	379.92	58.79
1221	1,3-Butanediol	C4H10O2	475.04	366.08	57.47
1220	1,2-Butanediol	C4H10O2	475.04	366.08	57.47

Table D. 4 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1240	Ts2-C4H8-14-Diol	C4H8O2	479.64	369.32	57.81
1239	Cis-Butenediol	C4H8O2	479.64	369.32	57.81
1241	1,4-Butanediol	C4H10O2	475.48	366.91	57.86
1222	Hexylene Glycol	C6H14O2	517.57	395.88	60.62
1213	Dipropylene Gly	C6H14O3	542.78	415.72	63.94
1242	1,5-Pentanediol	C5H12O2	498.36	383.75	60.08
1243	1,6-Hexanediol	C6H14O2	521.24	400.58	62.31
1204	TetraC2H4 Glycol	C8H18O5	634.26	484.67	73.99
6886	C6H4(COOC2H4OH)2	C12H14O6	806.62	615.32	93.42
1248	123-Benzenetriol	C6H6O3	600.44	458.14	69.61
1231	Glycerol	C3H8O3	544.34	427.77	71.92
1247	Hexaglycerol	C6H14O3	610.19	475.67	77.69
1246	Pentaerythritol	C5H12O4	679.49	536.93	92.14

Table D. 5 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Amines				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1742	Ethyleneimine	C2H5N	298.40	212.00	26.36
1745	Piperidine	C5H11N	382.50	272.34	34.05
2726	Propyleneimine	C3H7N	316.57	225.05	28.03
1766	Pyrrolidine	C4H9N	355.35	253.05	31.65
1719	Isopropylamine	C3H9N	340.33	247.20	32.53
1711	N-Propylamine	C3H9N	340.77	248.23	32.91
1726	Sec-Butylamine	C4H11N	363.21	263.90	34.75
1704	Ethylamine	C2H7N	317.89	231.53	30.69
1702	Dimethylamine	C2H7N	295.53	210.82	26.48
1710	Diethylamine	C4H11N	341.29	244.26	30.93
1740	Allylamine	C3H7N	337.45	245.09	32.24
1712	N-Butylamine	C4H11N	363.65	264.93	35.14
1794	HexMthyleneimine	C6H13N	409.65	291.63	36.45
1729	Cyclohexylamine	C6H13N	428.92	308.95	39.77
1714	Isobutylamine	C4H11N	363.21	263.90	34.75
2853	Acetamide	C2H5NO	371.76	273.84	37.43
2731	N-C1-CycC6-Amine	C7H15N	408.09	291.94	36.93
1743	Diisopropylamine	C6H15N	386.17	275.49	34.61
1796	N,N-DiMthAniline	C8H11N	491.81	358.55	47.64
1792	Aniline	C6H7N	436.09	317.15	41.87
1713	N-Pentylamine	C5H13N	386.53	281.63	37.37
1733	Benzylamine	C7H9N	458.97	333.85	44.09
1737	M-Toluidine	C7H9N	463.95	337.85	44.76

Table D. 6 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

3796	N-Ethylaniline	C8H11N	459.49	329.90	42.11
1878	2-Methacrylamide	C4H7NO	414.08	304.24	41.30
1736	O-Toluidine	C7H9N	463.95	337.85	44.76
2739	Diallylamine	C6H11N	380.41	271.28	34.05
2706	Hexylamine	C6H15N	409.41	298.33	39.59
2724	O-Ethylaniline	C8H11N	486.83	354.55	46.98
1707	Dipropylamine	C6H15N	387.05	277.69	35.39
1738	P-Toluidine	C7H9N	463.95	337.85	44.76
1795	N-Methylaniline	C7H9N	436.61	313.18	39.89
1718	Diisobutylamine	C8H19N	431.93	308.93	39.06
1879	Acrylamide	C3H5NO	391.32	287.45	38.99
2707	1-Aminoheptane	C7H17N	432.29	315.03	41.82
2730	DiCycHexylAmine	C12H23N	563.39	399.27	49.35
2787	P-Aminodiphenyl	C12H11N	605.03	426.50	52.04
1744	Dibutylamine	C8H19N	432.81	311.11	39.84
2708	1-Octylamine	C8H19N	455.17	331.73	44.04
2791	2,6-DiEthAniline	C10H15N	537.57	391.95	52.10
2709	1-Nonylamine	C9H21N	478.05	348.43	46.27
2710	1-Decylamine	C10H23N	500.93	365.13	48.50
3722	Diamylamine	C10H23N	478.57	344.53	44.29
3724	Undecylamine	C11H25N	523.81	381.83	50.72
2712	Dodecylamine	C12H27N	546.69	398.53	52.95
1720	Tetradecylamine	C14H31N	592.45	431.93	57.40
2752	Piperazine	C4H10N2	403.90	292.97	38.41
1752	Propylenediamine	C3H10N2	412.86	307.10	43.17
1741	Ethylenediamine	C2H8N2	390.42	291.33	41.33
2725	O-Aminoaniline	C6H8N2	513.60	381.07	53.17
2750	P-Aminoaniline	C6H8N2	513.60	381.07	53.17
2727	M-Aminoaniline	C6H8N2	513.60	381.07	53.17
1750	AEP	C6H15N3	514.35	380.98	52.90
1732	Toluene Diamine	C7H10N2	541.46	401.74	56.06
1731	hexamethyleneDiamine	C6H16N2	481.94	358.20	50.23
3750	P-Benzidine	C12H12N2	682.54	491.76	63.35

Table D. 7 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Nitriles				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1773	Propionitrile	C3H5N	370.32	263.18	32.75
1782	Butyronitrile	C4H7N	393.20	279.90	34.98
2720	Allyl Cyanide	C4H5N	389.88	276.67	34.31

Table D. 8 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1783	Valeronitrile	C5H9N	416.08	296.63	37.20
3874	Benzyl Cyanide	C8H7N	511.40	365.57	46.16
1786	Hexanenitrile	C6H11N	438.96	313.35	39.43
1776	Succinonitrile	C4H4N2	495.28	355.72	45.45
1781	Glutaronitrile	C5H6N2	518.16	372.43	47.68
2735	14-2Cyano-2-C4H8	C6H6N2	545.20	391.20	49.86
1777	Adiponitrile	C6H8N2	541.04	389.14	49.91

Table D. 9 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Imines				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1767	N-MthPyrrolidine	C5H11N	383.20	272.10	33.79
2797	3-Methylpyridine	C6H7N	417.26	297.76	37.44
1797	2-Methylpyridine	C6H7N	417.26	297.76	37.44
2799	4-Methylpyridine	C6H7N	417.26	297.76	37.44
1753	N,N-DiEthAniline	C10H15N	467.52	337.32	43.61

Table D. 10 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Tert-N				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1706	Triethylamine	C6H15N	349.32	251.71	32.43
2716	Tributylamine	C12H27N	486.60	351.94	45.79
2719	Tripropylamine	C9H21N	417.96	301.82	39.11
3723	Triamylamine	C15H33N	555.24	402.05	52.47

Table D. 11 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Nitrates				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1761	Nitroethane	C2H5NO2	397.20	285.68	36.64
1763	2-Nitropropane	C3H7NO2	419.64	301.31	38.48
1762	1-Nitropropane	C3H7NO2	420.08	302.39	38.86

Table D. 12 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

DipID	Thiols Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1802	Ethyl Mercaptan	C2H6S	308.22	217.92	26.78
1820	Dimethyl Sulfide	C2H6S	314.14	221.06	26.86
1843	Thiacyclopentane	C4H8S	371.31	260.77	31.54
1803	1-Propanethiol	C3H8S	331.10	234.67	29.01
1805	Isobut Mercaptan	C4H10S	353.54	250.27	30.85
6860	Ethylenedithiol	C2H6S2	371.08	265.32	33.52
1811	Cyclohexanethiol	C6H12S	420.39	296.92	36.40
1828	DiMth Disulfide	C2H6S2	371.08	265.32	33.52
1841	Butanethiol	C4H10S	353.98	251.40	31.24
1814	Methylproylsulf	C4H10S	353.98	251.40	31.24
2816	ETHYLtBUTYL SUL	C6H14S	402.43	283.33	34.47
1818	Diethyl Sulfide	C4H10S	359.90	254.56	31.32
1812	Benzyl Mercaptan	C7H8S	449.30	320.35	40.19
1838	T-OctylMercaptan	C8H18S	442.27	313.68	38.84
1827	1-Pentanethiol	C5H12S	376.86	268.13	33.46
2815	METHnBUTYL SULFD	C5H12S	382.78	271.30	33.54
1824	DiethylDisulfide	C4H10S2	428.68	305.16	38.13
1807	N-Hexylmercaptan	C6H14S	399.74	284.86	35.69
6857	Dimercaptoethyl	C4H10OS2	439.26	315.64	40.38
1839	1-Heptanethiol	C7H16S	422.62	301.58	37.91
1829	DiProp Disulfide	C6H14S2	474.44	338.61	42.58
1809	1-Octanethiol	C8H18S	445.50	318.30	40.14
1808	N-Nonanethiol	C9H20S	468.38	335.02	42.37
1826	1-Decanethiol	C10H22S	491.26	351.74	44.59
2838	tertDodecanThiol	C12H26S	533.79	380.59	47.75
1825	1-Undecanethiol	C11H24S	514.14	368.45	46.82
1837	Dodecylthiol	C12H26S	537.02	385.17	49.04

Table D. 13 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

DipID	Aldehydes Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1037	Methacrolein	C4H6O	336.34	241.04	30.63
1002	Acetaldehyde	C2H4O	294.02	210.69	26.77
1003	Propionaldehyde	C3H6O	316.90	227.40	28.99
1041	Benzaldehyde	C7H6O	435.10	313.03	40.17
1034	Acrolein	C3H4O	313.58	224.20	28.32
1005	N-Butyraldehyde	C4H8O	339.78	244.12	31.22

Table D. 14 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1036	Trans-2-Butenal	C4H6O	343.94	246.16	31.18
1007	Valeraldehyde	C5H10O	362.66	260.83	33.44
1006	Isobutyraldehyde	C4H8O	339.34	243.03	30.83
1009	1-Hexanal	C6H12O	385.54	277.53	35.67
1040	P-Tolualdehyde	C8H8O	462.96	333.76	43.06
1016	2-Methylhexanal	C7H14O	407.98	293.17	37.51
1017	3-Methylhexanal	C7H14O	407.98	293.17	37.51
1008	1-Heptanal	C7H14O	408.42	294.24	37.90
1013	2-Ethylhexanal	C8H16O	430.86	309.88	39.73
1010	1-Octanal	C8H16O	431.30	310.95	40.12
1011	1-Nonanal	C9H18O	454.18	327.66	42.35
1020	1-Decanal	C10H20O	477.06	344.36	44.57
1021	1-Undecanal	C11H22O	499.94	361.07	46.80
1025	Dodecanal	C12H24O	522.82	377.77	49.03
1026	1-Tridecanal	C13H26O	545.70	394.47	51.25
1014	1,2-Ethanedione	C2H2O2	342.68	250.41	33.49
1044	1,4BenzDicarboxAldehy	C8H6O2	511.62	373.43	49.78

Table D. 15 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

Epoxides					
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1440	ISOBUTYLENE OXID	C4H8O	308.91	214.63	25.32
1478	Furan	C4H4O	314.06	218.24	25.75
1443	1,3-Propylene Ox	C3H6O	289.26	202.70	24.39
1479	Tetrahydrofuran	C4H8O	324.95	227.04	27.13
1477	2,5-Dihydrofuran	C4H6O	320.57	229.73	29.19
1471	1,2-Epoxybutane	C4H8O	311.70	218.29	26.23
1408	1-Methoxypropane	C4H10O	313.54	220.88	26.91
1442	1,2-Propylene Ox	C3H6O	288.82	201.51	24.00
1411	2-Methoxypropane	C4H10O	313.10	219.71	26.52
1421	1,4-Dioxane	C4H8O2	334.56	236.43	29.02
2422	1,3-DIOXANE	C4H8O2	334.56	236.43	29.02
1426	2-Methoxybutane	C5H12O	335.98	236.47	28.75
1422	Trioxane	C3H6O3	334.10	236.64	29.21
1413	1-Methoxybutane	C5H12O	336.42	237.63	29.13
1461	Methoxybenzene	C7H8O	408.86	289.87	35.86
1448	1-Ethoxybutane	C6H14O	359.30	254.37	31.36
1429	1-MethoxyPentane	C6H14O	359.30	254.37	31.36
6885	Ethyl-3-Ethoxypr	C7H14O3	440.40	317.56	40.99

Table D. 16 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

DipID	Ether Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1401	Dimethyl Ether	C2H6O	267.78	187.35	22.46
1407	MethylEthylEther	C3H8O	290.66	204.12	24.68
1470	VinylMethylEther	C3H6O	287.34	200.82	24.01
1405	MTBE	C5H12O	333.19	232.85	27.84
1445	VinylEthyl Ether	C4H8O	310.22	217.59	26.24
1402	Diethyl Ether	C4H10O	313.54	220.88	26.91
1431	Methylal	C3H8O2	313.08	221.09	27.09
1428	T-But EthylEther	C6H14O	356.07	249.62	30.06
1427	TAME	C6H14O	356.07	249.62	30.06
1410	Mth Isobut Ether	C5H12O	335.98	236.47	28.75
1430	Eth-t-Pent-Ether	C7H16O	378.95	266.39	32.29
1403	DiisopropylEther	C6H14O	358.42	252.06	30.58
1415	Eth Propyl Ether	C5H12O	336.42	237.63	29.13
1455	Dimethyl Acetal	C4H10O2	335.96	237.83	29.32
1446	Dipropyl Ether	C6H14O	359.30	254.37	31.36
1447	Butyl VinylEther	C6H12O	355.98	251.11	30.69
1462	EthylPhenylEther	C8H10O	431.74	306.61	38.09
1406	Di-sec-But Ether	C8H18O	404.18	285.57	35.04
1432	Acetal	C6H14O2	381.28	270.17	33.38
1460	BenzylEthylEther	C9H12O	454.62	323.34	40.31
1050	Paraldehyde	C6H12O3	401.42	283.44	34.72
1404	Di-n-Butyl Ether	C8H18O	405.06	287.84	35.81
1420	Anethole	C10H12O	486.64	346.13	43.16
1456	DimethylCarbitol	C6H14O3	404.14	288.22	36.18
1463	Dibenzyl Ether	C14H14O	595.70	425.73	53.72
1425	Di-n-PentylEther	C10H22O	450.82	321.30	40.26
1458	Diethyl Carbitol	C8H18O3	449.90	321.66	40.63
1412	Dihexyl Ether	C12H26O	496.58	354.74	44.72
1454	Triglyme	C8H18O4	472.32	338.56	43.04
1459	Dibutyl Carbitol	C12H26O3	541.42	388.52	49.54
1424	Di-n-Octyl Ether	C16H34O	588.10	421.61	53.62
1457	Tetraglyme	C10H22O5	540.50	388.86	49.90
1418	Dinonyl Ether	C18H38O	633.86	455.03	58.07
2432	ETHYLAL	C5H12O2	358.84	254.57	31.54
2405	DIISOBUTYL ETHER	C8H18O	404.18	285.57	35.04
2456	Ethyl Glyme	C6H14O2	381.72	271.30	33.77
2417	ETHYLHEXYL ETHER	C8H18O	405.06	287.84	35.81
2415	ETHYLISOPROPETH	C5H12O	335.98	236.47	28.75

Table D. 17 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

DipID	Formates Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1301	Methyl Formate	C2H4O2	316.44	223.28	27.31
1311	Vinyl Formate	C3H4O2	336.00	236.76	28.86
1302	Ethyl Formate	C3H6O2	339.32	240.02	29.53
2306	t-Butyl Formate	C5H10O2	381.85	268.80	32.69
1303	Propyl Formate	C4H8O2	362.20	256.76	31.76
2305	sec-ButylFormate	C5H10O2	384.64	272.37	33.60
2311	CYCLOHEXL FORMAT	C7H12O2	450.39	317.79	38.87
1304	N-Butyl Formate	C5H10O2	385.08	273.50	33.98
1305	Isobutyl Formate	C5H10O2	384.64	272.37	33.60
2350	Benzyl Formate	C8H8O2	480.40	342.45	42.94
2307	n-Hexyl Formate	C7H14O2	430.84	306.96	38.44
1306	N-Pentyl Formate	C6H12O2	407.96	290.23	36.21
2308	n-Heptyl Formate	C8H16O2	453.72	323.68	40.66
1308	N-Octyl Formate	C9H18O2	476.60	340.40	42.89
1309	n-Nonyl Formate	C10H20O2	499.48	357.12	45.11
1310	n-Decyl Formate	C11H22O2	522.36	373.84	47.34

Table D. 18 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

DipID	Esters Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1351	Mth Methacrylate	C5H8O2	368.78	264.19	33.54
1312	Methyl Acetate	C3H6O2	326.46	233.85	29.68
1331	Vinyl Propionate	C5H8O2	368.90	264.08	33.46
1321	Vinyl Acetate	C4H6O2	346.02	247.36	31.24
1352	Eth MthAcrylate	C6H10O2	391.66	280.91	35.77
1322	MethylPropionate	C4H8O2	349.34	250.56	31.91
1341	Methyl Acrylate	C4H6O2	346.02	247.36	31.24
1313	Ethyl Acetate	C4H8O2	349.34	250.56	31.91
1319	IsopropylAcetate	C5H10O2	371.78	266.18	33.74
1332	Methyl Butyrate	C5H10O2	372.22	267.27	34.13
1342	Ethyl Acrylate	C5H8O2	368.90	264.08	33.46
1318	Allyl Acetate	C5H8O2	368.90	264.08	33.46
1314	N-Propyl Acetate	C5H10O2	372.22	267.27	34.13
1323	Ethyl Propionate	C5H10O2	372.22	267.27	34.13
1360	I-But I-Butyrate	C8H16O2	439.98	315.24	40.03
1320	Sec-ButylAcetate	C6H12O2	394.66	282.90	35.97
1336	PropylI-Butyrate	C7H14O2	417.54	299.61	38.20

Table D. 19 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1353	N-C3-Mthacrylate	C7H12O2	413.35	294.76	36.99
1333	Ethyl Butyrate	C6H12O2	395.10	283.98	36.36
1347	EthylIsovalerate	C7H14O2	417.54	299.61	38.20
1315	N-Butyl Acetate	C6H12O2	395.10	283.98	36.36
1390	Methyl Benzoate	C8H8O2	467.54	336.19	43.09
1388	ISOBUTYL MTHACR	C8H14O2	436.98	313.25	39.83
1343	1-PropylAcrylate	C6H10O2	391.78	280.79	35.69
1316	Isobutyl Acetate	C6H12O2	394.66	282.90	35.97
1344	N-Butyl Acrylate	C7H12O2	416.14	298.24	37.90
1357	Pentyl Acetate	C7H14O2	417.98	300.69	38.58
1327	N-PropN-Butyrate	C7H14O2	417.98	300.69	38.58
1324	N-PropPropionate	C6H12O2	395.10	283.98	36.36
1291	Acetic Anhydride	C4H6O3	403.21	293.11	38.65
1389	N-ButMthacrylate	C8H14O2	437.42	314.33	40.22
1359	Benzyl Acetate	C9H10O2	490.42	352.90	45.31
1326	N-But Propionate	C7H14O2	417.98	300.69	38.58
1391	Ethyl Benzoate	C9H10O2	490.42	352.90	45.31
1897	CH3OC3H600CH3	C6H12O3	417.08	299.78	38.38
1392	DiethylCarbonate	C5H10O3	394.64	284.15	36.54
1385	N-But N-Butyrate	C8H16O2	440.86	317.40	40.81
1317	IsopentylAcetate	C7H14O2	417.54	299.61	38.20
1363	N-Hexyl Acetate	C8H16O2	440.86	317.40	40.81
1387	Ethylene Acetate	C6H10O4	453.32	330.18	43.76
1393	Diethyl Oxalate	C6H10O4	453.32	330.18	43.76
1365	Butyl Benzoate	C11H14O2	536.18	386.31	49.76
1361	I-C5 I-Valerate	C10H20O2	485.74	348.66	44.49
1367	Heptyl Acetate	C9H18O2	463.74	334.11	43.04
1346	N-Butyl Valerate	C9H18O2	463.74	334.11	43.04
1358	2-C2-C6 Acetate	C10H20O2	486.18	349.74	44.87
1394	Diethyl Malonate	C7H12O4	476.20	346.88	45.99
1292	Propionyl Oxide	C6H10O3	448.97	326.52	43.10
1364	Benzyl Benzoate	C14H12O2	631.50	455.22	58.72
1381	2Mth p-Phthalate	C10H10O4	576.50	419.80	55.61
1368	n-Octyl Acetate	C10H20O2	486.62	350.82	45.26
1377	DiMthI-Phthalate	C10H10O4	576.50	419.80	55.61
1896	Ethylene DiAcr	C8H10O4	492.44	357.30	46.88
1386	2-Ethylhexyl Acr	C11H20O2	505.74	363.27	46.43
1395	Methyl Decanoate	C11H22O2	509.50	367.52	47.49
1369	n-Nonyl Acetate	C11H22O2	509.50	367.52	47.49
1370	n-Decyl Acetate	C12H24O2	532.38	384.23	49.71
1345	N-ButylNonanoate	C13H26O2	555.26	400.93	51.94
1375	DiProp Phthalate	C14H18O4	668.02	486.60	64.51
1376	Diisobutyl Phtha	C16H22O4	712.90	517.93	68.19
1396	IsopropMyristate	C17H34O2	646.34	466.69	60.46
1383	Butyl Stearate	C22H44O2	761.18	551.26	71.97
1362	Methyl Oleate	C19H36O2	696.70	503.24	65.25
1355	Diisooctyl Phtha	C24H38O4	895.94	651.53	85.99

Table D. 20 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1382	DioctylTerephtha	C24H38O4	896.82	653.59	86.77
1384	DIBUTYL SEBACATE	C18H34O4	727.88	530.58	70.48
1371	Diisodecyl Phtha	C28H46O4	987.46	718.33	94.90
1354	DioctylPhthalate	C24H38O4	895.94	651.53	85.99
2375	DiethylPhthalate	C12H14O4	622.26	453.20	60.06
2388	Dipropyl Maleate	C10H16O4	549.00	399.10	52.63
2381	Diallyl Maleate	C10H12O4	542.36	392.80	51.29
2370	Glyceryl Triacet	C9H14O6	579.74	425.26	57.46
2382	Dibutyl Maleate	C12H20O4	594.76	432.50	57.08
2376	DibutylPhthalate	C16H22O4	713.78	520.00	68.96
2353	CetylMthacrylate	C20H38O2	711.98	514.81	66.93
2379	Dihexyl Adipate	C18H34O4	727.88	530.58	70.48
2321	T-Butyl Acetate	C6H12O2	391.87	279.42	35.06
2332	Methl.I-butyrate	C5H10O2	371.78	266.18	33.74
2354	AllylMthacrylate	C7H10O2	411.22	294.42	37.32
2364	CYCLOHEXL ACETAT	C8H14O2	460.41	328.40	41.24
2337	EthylIsobutyrate	C6H12O2	394.66	282.90	35.97
2384	IsobutylAcrylate	C7H12O2	414.22	296.41	37.53
2380	1,1-Diacetoxy C2	C6H10O4	452.88	329.15	43.38
2392	n-PropylBenzoate	C10H12O2	513.30	369.61	47.54
2387	Dimethyl Maleate	C6H8O4	457.48	332.29	43.72
2377	DiMth Phthalate	C10H10O4	576.50	419.80	55.61
2386	Diethyl Maleate	C8H12O4	503.24	365.69	48.17
2385	Mth Dodecanoate	C13H26O2	555.26	400.93	51.94
3379	Dioctyl Adipate	C22H42O4	818.08	594.28	78.22
5886	Mth Acetoacetate	C5H8O3	426.09	309.81	40.88
5884	Ethoxy Acetate	C6H12O3	417.52	300.86	38.77
5887	EthAcetoAcetate	C6H10O3	448.97	326.52	43.10
5885	Carbitol Acetate	C8H16O4	485.70	351.13	45.63

Table D. 21 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Ketones				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1096	Methyl Isopropen	C5H8O	364.43	260.48	32.88
1079	Cyclopentanone	C5H8O	379.28	269.89	33.69
1051	Acetone	C3H6O	322.11	230.13	29.02
1052	MEK	C4H8O	344.99	246.85	31.24
1065	Mesityl Oxide	C6H10O	394.79	282.44	35.73
1066	T-But Mth Ketone	C6H12O	387.52	275.70	34.40
1060	2-Pentanone	C5H10O	367.87	263.57	33.47
1061	Mth iC3 Ketone	C5H10O	367.43	262.47	33.08

Table D. 22 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1053	Diethyl Ketone	C5H10O	367.87	263.57	33.47
1059	3-Hexanone	C6H12O	390.75	280.28	35.70
1099	Diketene	C4H4O2	344.50	246.10	31.02
1055	Sec-ButMthKetone	C6H12O	390.31	279.19	35.31
1054	MIBK	C6H12O	390.31	279.19	35.31
1095	EthIsopropKetone	C6H12O	390.31	279.19	35.31
1063	2-Heptanone	C7H14O	413.63	296.99	37.92
1064	5-Mth-2-Hexanone	C7H14O	413.19	295.91	37.53
1058	4-Heptanone	C7H14O	413.63	296.99	37.92
1057	3-Heptanone	C7H14O	413.63	296.99	37.92
1076	2,4-Pentanedione	C5H8O2	421.74	306.15	40.22
1068	DiisobutylKetone	C9H18O	458.51	328.24	41.60
1097	2-CycC6 CycC6one	C12H20O	558.59	397.36	49.57
1083	2-Octanone	C8H16O	436.51	313.71	40.15
1073	Dibutyl Ketone	C9H18O	459.39	330.42	42.37
1062	2-Hexanone	C6H12O	390.75	280.28	35.70
1077	Isophorone	C9H14O	466.14	330.75	41.00
1090	Acetophenone	C8H8O	463.19	332.49	42.42
1080	Cyclohexanone	C6H10O	406.43	289.18	36.09
1074	2-Nonanone	C9H18O	459.39	330.42	42.37

Table D. 23 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Alcohol-Ethers				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
2862	2-Butoxyethanol	C6H14O2	451.48	337.33	48.04
4857	butyl carbitol	C8H18O3	519.66	387.57	54.90
2898	2-Chloroethanol	C2H5ClO	374.97	282.27	41.11
2864	Carbitol	C6H14O3	473.90	354.13	50.45
3854	Methyl propasol	C4H10O2	405.28	302.95	43.20
2860	2-Methoxyethanol	C3H8O2	382.84	287.14	41.36
2854	DiacetoneAlcohol	C6H12O2	479.70	358.48	51.08
2861	2-Ethoxyethanol	C4H10O2	405.72	303.88	43.59
2889	HydroxyAcetone	C3H6O2	414.29	312.34	45.70
3856	1tButoxy2Propnol	C7H16O2	470.69	348.96	48.58
3858	PROPGLYC2tBUTYL	C7H16O2	470.69	348.96	48.58
4855	2-Propoxyethanol	C5H12O2	428.60	320.61	45.81
4849	Acetovanillone	C9H10O3	594.09	439.36	60.74
5883	Ethyl Lactate	C5H10O3	463.96	348.50	50.42
6883	2-HydroxyEth Acr	C5H8O3	461.08	346.39	50.14
2863	Methyl Carbitol	C5H12O3	451.02	337.40	48.22
3855	Dowanol DPM	C7H16O3	496.78	370.85	52.68
3857	TriPropGlymEthlE	C10H22O4	587.84	437.81	61.76

Table D. 24 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

DipID	Hydrocarbons Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
404	DiMth-Acetylene	C4H6	300.12	213.54	26.65
202	Propylene	C3H6	264.92	183.78	21.60
412	2-Pentyne	C5H8	368.76	263.71	33.33
207	2-Methylpropene	C4H8	287.68	200.72	23.91
204	1-Butene	C4H8	287.80	200.58	23.83
205	Cis-2-Butene	C4H8	295.28	205.81	24.46
402	Propyne	C3H4	258.36	181.90	22.13
406	3-Hexyne	C6H10	345.88	246.99	31.10
206	Trans-2-Butene	C4H8	295.28	205.81	24.46
407	2-Hexyne	C6H10	345.88	246.99	31.10
231	33-2Mth-1-Butene	C6H12	330.33	229.28	26.98
230	23-2Mth-1-Butene	C6H12	333.00	233.09	27.97
229	2-Ethyl-1-Butene	C6H12	333.44	234.27	28.36
8	I-Pentane	C5H12	313.56	219.48	26.34
14	2,2-DiMth-Butane	C6H14	333.65	232.61	27.65
232	23-2Mth-2-Butene	C6H12	340.80	239.64	29.07
213	3-Mth-1-Butene	C5H10	310.24	216.16	25.67
212	2-Mth-1-Butene	C5H10	310.56	217.50	26.13
211	Trans-2-Pentene	C5H10	318.16	222.59	26.68
210	Cis-2-Pentene	C5H10	318.16	222.59	26.68
223	4-Mth-1-Pentene	C6H12	333.12	232.95	27.89
221	2-Mth-1-Pentene	C6H12	333.44	234.27	28.36
248	2-t-Butylpropene	C7H14	353.09	246.22	29.29
227	Cs-4-Mth-2-C5H10	C6H12	340.60	238.18	28.52
224	2-Mth-2-Pentene	C6H12	340.92	239.50	28.99
403	1-Butyne	C4H6	281.24	198.65	24.36
15	2,3-DiMth-Butane	C6H14	336.00	235.07	28.17
214	2-Mth-2-Butene	C5H10	318.04	222.74	26.76
228	Ts-4-Mth-2-C5H10	C6H12	340.60	238.18	28.52
225	Cs-3-Mth-2-C5H10	C6H12	340.92	239.50	28.99
218	Trans-2-Hexene	C6H12	341.04	239.37	28.91
2226	3-METH-Tr-2Pente	C6H12	340.92	239.50	28.99
222	3-Mth-1-Pentene	C6H12	333.12	232.95	27.89
257	2-Diisobutylene	C8H16	383.45	268.24	32.14
256	1-Diisobutylene	C8H16	375.97	263.00	31.52
217	Cis-2-Hexene	C6H12	341.04	239.37	28.91
2414	1-Heptyne	C7H12	349.88	248.86	31.03
13	3-Methylpentane	C6H14	336.44	236.25	28.56
219	Cis-3-Hexene	C6H12	341.04	239.37	28.91
12	2-Methylpentane	C6H14	336.44	236.25	28.56
220	Trans-3-Hexene	C6H12	341.04	239.37	28.91
405	1-Pentyne	C5H8	304.12	215.39	26.58
209	1-Pentene	C5H10	310.68	217.36	26.05
11	N-Hexane	C6H14	336.88	237.41	28.95

Table D. 25 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

235	Cis-2-Heptene	C7H14	363.92	256.13	31.13
249	Cis-3-Heptene	C7H14	363.92	256.13	31.13
216	1-Hexene	C6H12	333.56	234.13	28.28
239	3-Eth-1-Pentene	C7H14	356.00	249.72	30.12
226	4-Mth-1-Hexene	C7H14	356.00	249.72	30.12
240	3-Mth-1-Hexene	C7H14	356.00	249.72	30.12
419	3-Mth-1-Butyne	C5H8	303.68	214.25	26.19
233	2-Eth-1-Pentene	C7H14	356.32	251.03	30.59
238	2-Mth-1-Hexene	C7H14	356.32	251.03	30.59
416	1-Octyne	C8H14	372.76	265.59	33.26
289	2,3Dimeth Hexene	C8H16	378.76	266.62	32.42
234	1-Heptene	C7H14	356.44	250.89	30.51
413	1-Hexyne	C6H10	327.00	232.13	28.81
237	Trans-3-Heptene	C7H14	363.92	256.13	31.13
236	Trans-2-Heptene	C7H14	363.92	256.13	31.13
251	Trans-2-Octene	C8H16	386.80	272.88	33.36
279	Trans-4-Octene	C8H16	386.80	272.88	33.36
277	Trans-3-Octene	C8H16	386.80	272.88	33.36
2252	2Methl-1-Heptene	C8H16	379.20	267.78	32.81
250	1-Octene	C8H16	379.32	267.65	32.73
258	2-Ethyl-1-Hexene	C8H16	379.20	267.78	32.81
280	3-Octene	C8H16	386.80	272.88	33.36
278	4-Octene	C8H16	386.80	272.88	33.36
276	2-Octene	C8H16	386.80	272.88	33.36
259	1-Nonene	C9H18	402.20	284.39	34.96
262	1-Dodecene	C12H24	470.84	334.60	41.64
263	1-Tridecene	C13H26	493.72	351.33	43.86
264	1-Tetradecene	C14H28	516.60	368.06	46.09
265	1-Pentadecene	C15H30	539.48	384.78	48.31
266	1-Hexadecene	C16H32	562.36	401.51	50.54
267	1-Octadecene	C18H36	608.12	434.94	54.99
281	1-Heptadecene	C17H34	585.24	418.23	52.77
284	1-Eicosene	C20H40	653.88	468.38	59.44
283	1-Nonadecene	C19H38	631.00	451.66	57.22
3	Propane	C3H8	268.24	187.11	22.27
4	I-Butane	C4H10	290.68	202.69	24.11
9	Neopentane	C5H12	310.77	215.81	25.43
5	N-Butane	C4H10	291.12	203.89	24.50
7	pentane	C5H12	314.00	220.65	26.72
44	Hexamethylethane	C8H18	376.18	261.31	30.81
25	223-TriMthButane	C7H16	356.09	248.19	29.49
24	3,3-DiMthPentane	C7H16	356.53	249.39	29.88
51	2,2,3,3-4Mth-C5	C9H20	399.06	278.11	33.04
21	2,2-DiMthPentane	C7H16	356.53	249.39	29.88
42	2,3,3-TriMth-C5	C8H18	378.97	264.98	31.72
22	2,3-DiMthPentane	C7H16	358.88	251.84	30.40
40	2,2,3-TriMth-C5	C8H18	378.97	264.98	31.72

Table D. 26 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

23	2,4-DiMthPentane	C7H16	358.88	251.84	30.40
41	2,2,4-TriMth-C5	C8H18	378.97	264.98	31.72
39	3-Mth-3-Eth-C5	C8H18	379.41	266.16	32.11
20	3-Ethylpentane	C7H16	359.32	253.01	30.79
52	2,2,3,4-4Mth-C5	C9H20	401.41	280.57	33.56
54	2334TetrMethPent	C9H20	401.41	280.57	33.56
53	2,2,4,4-4Mth-C5	C9H20	399.06	278.11	33.04
43	2,3,4-TriMth-C5	C8H18	381.32	267.43	32.24
36	3,3-DiMth-Hexane	C8H18	379.41	266.16	32.11
19	3-Methylhexane	C7H16	359.32	253.01	30.79
18	2-Methylhexane	C7H16	359.32	253.01	30.79
38	2-Mth-3-Eth-C5	C8H18	381.76	268.60	32.63
190	2,2-2C1-3-C2-C5	C9H20	401.85	281.75	33.94
32	2,2-DiMth-Hexane	C8H18	379.41	266.16	32.11
37	3,4-DiMth-Hexane	C8H18	381.76	268.60	32.63
50	3,3-DiEthPentane	C9H20	402.29	282.93	34.33
34	2,4-DiMth-Hexane	C8H18	381.76	268.60	32.63
33	2,3-DiMth-Hexane	C8H18	381.76	268.60	32.63
17	N-Heptane	C7H16	359.76	254.16	31.18
49	244TriMethHexane	C9H20	401.85	281.75	33.94
192	2,4-2C1-3-C2-C5	C9H20	404.20	284.19	34.46
47	2,2,5-TriMth-C6	C9H20	401.85	281.75	33.94
35	2,5-DiMth-Hexane	C8H18	381.76	268.60	32.63
31	3-Ethylhexane	C8H18	382.20	269.76	33.01
30	4-Methylheptane	C8H18	382.20	269.76	33.01
29	3-Methylheptane	C8H18	382.20	269.76	33.01
28	2-Methylheptane	C8H18	382.20	269.76	33.01
96	2,2-DiMthHeptane	C9H20	402.29	282.93	34.33
176	2,6-DiMthHeptane	C9H20	404.64	285.35	34.85
27	N-Octane	C8H18	382.64	270.90	33.40
94	3-Ethylheptane	C9H20	405.08	286.50	35.24
92	3-Methyloctane	C9H20	405.08	286.50	35.24
93	4-Methyloctane	C9H20	405.08	286.50	35.24
91	2-Methyloctane	C9H20	405.08	286.50	35.24
72	2,2-DiMthOctane	C10H22	425.17	299.68	36.56
2095	2,3Dimethloctane	C10H22	427.52	302.10	37.08
2096	2,4Dimethloctane	C10H22	427.52	302.10	37.08
2098	2,6DimethlOctane	C10H22	427.52	302.10	37.08
2097	2,5Dimethloctane	C10H22	427.52	302.10	37.08
2099	2,7DimethlOctane	C10H22	427.52	302.10	37.08
46	N-Nonane	C9H20	405.52	287.64	35.63
88	5-Methylnonane	C10H22	427.96	303.24	37.47
85	3-Methylnonane	C10H22	427.96	303.24	37.47
87	4-Methylnonane	C10H22	427.96	303.24	37.47
86	2-Methylnonane	C10H22	427.96	303.24	37.47
56	N-Decane	C10H22	428.40	304.38	37.85
63	N-Undecane	C11H24	451.28	321.11	40.08

Table D. 27 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

64	N-Dodecane	C12H26	474.16	337.83	42.31
65	N-Tridecane	C13H28	497.04	354.56	44.53
66	N-Tetradecane	C14H30	519.92	371.28	46.76
67	N-Pentadecane	C15H32	542.80	388.00	48.98
68	N-Hexadecane	C16H34	565.68	404.72	51.21
69	N-Heptadecane	C17H36	588.56	421.43	53.44
70	N-Octadecane	C18H38	611.44	438.15	55.66
71	N-Nonadecane	C19H40	634.32	454.86	57.89
73	N-Eicosane	C20H42	657.20	471.57	60.11
74	n-HENEICOSANE	C21H44	680.08	488.29	62.34
75	n-DOCOSANE	C22H46	702.96	505.00	64.57
76	n-TRICOSANE	C23H48	725.84	521.71	66.79
77	n-Tetracosane	C24H50	748.72	538.42	69.02
78	n-PENTACOSANE	C25H52	771.60	555.13	71.24
79	n-HEXACOSANE	C26H54	794.48	571.84	73.47
81	n-Octacosane	C28H58	840.24	605.25	77.92
2081	n-TRICONTANE	C30H62	886.00	638.67	82.37
2082	n-Dotriacontane	C32H66	931.76	672.08	86.83

Table D. 28 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Cyclic Hydrocarbons				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
269	Cyclopentene	C5H8	333.11	232.16	27.58
270	Cyclohexene	C6H10	360.26	251.46	29.98
287	3MthCyclopentene	C6H10	351.32	245.88	29.50
286	1-MthCyclPentene	C6H10	360.97	253.04	30.47
288	4MthCyclopenten	C6H10	351.32	245.88	29.50
273	Cycloheptene	C7H12	387.41	270.76	32.38
274	Cyclooctene	C8H14	414.56	290.06	34.78
101	Cyclopropane	C3H6	279.65	193.18	22.49
810	ADAMANTANE	C10H16	448.22	313.25	37.46
102	Cyclobutane	C4H8	306.80	212.50	24.89
104	Cyclopentane	C5H10	333.95	231.81	27.29
137	Cyclohexane	C6H12	361.10	251.12	29.69
105	MthCyclopentane	C6H12	352.16	245.56	29.21
146	Cs-1,4-2C1-CycC6	C8H16	397.52	278.58	33.52
142	Cs-1,2-2C1-CycC6	C8H16	397.52	278.58	33.52
141	1,1-2C1-CycC6	C8H16	402.43	278.81	32.68
145	Ts-1,3-2C1-CycC6	C8H16	397.52	278.58	33.52
144	Cs-1,3-2C1-CycC6	C8H16	397.52	278.58	33.52

Table D. 29 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

147	Ts-1,4-2C1-CycC6	C8H16	397.52	278.58	33.52
143	Ts-1,2-2C1-CycC6	C8H16	397.52	278.58	33.52
138	MthCyclohexane	C7H14	379.31	264.86	31.61
159	Cycloheptane	C7H14	388.25	270.43	32.09
140	Ethylcyclohexane	C8H16	402.19	281.64	33.83
154	Trans-Decalin	C10H18	458.96	320.80	38.37
149	N-PropylCyc-C6	C9H18	425.07	298.41	36.06
109	Cs-1,2-2C1-CycC5	C7H14	370.37	259.28	31.12
110	Ts-1,2-2C1-CycC5	C7H14	370.37	259.28	31.12
112	Ts-1,3-2C1-CycC5	C7H14	370.37	259.28	31.12
107	Eth-Cyclopentane	C7H14	375.04	262.34	31.43
114	N-PropCycPentane	C8H16	397.92	279.11	33.66
108	1,1-DiMthCycC5	C7H14	375.28	259.49	30.28
111	Cs-1,3-2C1-CycC5	C7H14	370.37	259.28	31.12
152	N-ButylCycHexane	C10H20	447.95	315.17	38.28
160	Cyclooctane	C8H16	415.40	289.74	34.48
153	Cis-Decalin	C10H18	458.96	320.80	38.37
115	Isopropylcyclopentane	C8H16	397.48	277.93	33.27
150	Isopropyl-CycC6	C9H18	424.63	297.23	35.67
116	1-C1-1-C2-CycC5	C8H16	398.16	276.31	32.51
122	Butylcyclpentane	C9H18	420.80	295.88	35.89
155	1,1-Bicyclohexyl	C12H22	513.26	359.39	43.16
158	N-Decylcyclo-C6	C16H32	585.23	415.63	51.64

Table D. 30 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

Aromatic Hydrocarbons					
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
307	1,4-Pentadiene	C5H8	307.36	214.05	25.38
306	1-ts3-Pentadiene	C5H8	314.84	219.28	26.01
414	2-Methyl-1-Butenyne	C5H6	300.68	212.27	25.99
305	Cs1,3-Pentadiene	C5H8	314.84	219.28	26.01
309	Isoprene	C5H8	307.24	214.19	25.46
421	1-Pentene-4-yne	C5H6	300.80	212.14	25.91
303	1,3-Butadiene	C4H6	284.48	197.24	23.16
332	1,4-CyclHexadien	C6H8	352.34	244.90	28.92
501	Benzene	C6H6	358.58	252.09	30.56
315	Cyclopentadiene	C5H6	325.19	225.59	26.52
319	Diisopropenyl	C6H10	330.00	231.12	27.77
615	Ethynylbezene	C8H6	399.44	284.36	35.54

Table D. 31 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

601	Styrene	C8H8	406.00	286.41	35.01
331	1,3-CycHexadiene	C6H8	352.34	244.90	28.92
310	1,5-Hexadiene	C6H10	330.24	230.83	27.61
312	MthCycPentadiene	C6H8	343.68	240.02	28.65
420	1-Pentene-3-yne	C5H6	319.68	227.03	28.21
502	Toluene	C7H8	386.44	272.92	33.45
521	T-Butylbenzene	C10H14	451.85	318.44	38.83
320	Dipropylene	C6H10	345.20	241.30	28.87
520	Sec-Butylbenzene	C10H14	454.64	322.01	39.74
313	1,4-Hexadiene	C6H10	337.72	236.07	28.24
314	Dipropylene	C6H10	345.20	241.30	28.87
316	DiCycPentadiene	C10H12	439.46	307.03	36.68
333	1,5-CycOctadiene	C8H12	406.64	283.51	33.71
701	Naphthalene	C10H8	474.06	320.58	35.65
504	Ethylbenzene	C8H10	409.32	289.67	35.68
820	Indan	C9H10	440.05	311.62	38.44
505	O-Xylene	C8H10	414.30	293.73	36.34
612	P-Methylstyrene	C9H10	433.86	307.22	37.90
330	DIISOCROTYL	C8H14	390.72	275.11	33.48
507	P-Xylene	C8H10	414.30	293.73	36.34
329	DIISOBUTENYL	C8H14	375.76	264.64	32.22
506	M-Xylene	C8H10	414.30	293.73	36.34
603	Methylstyrene	C9H10	433.86	307.22	37.90
613	Alpha-MthStyrene	C9H10	428.76	303.29	37.31
510	Isopropylbenzene	C9H12	431.76	305.27	37.52
724	2-Methylindene	C10H10	471.34	327.75	38.74
285	Vinylcyclohexene	C8H12	394.49	275.22	32.78
803	Indene	C9H8	447.75	300.69	32.96
706	Tetralin	C10H12	467.20	330.91	40.84
511	O-Ethyltoluene	C9H12	437.18	310.46	38.57
723	1-Methylindene	C10H10	441.60	309.17	37.12
738	Fluorene	C13H10	558.96	374.73	40.94
619	Tr-1PropenylBz	C9H10	436.36	308.39	37.86
525	O-Diethylbenzene	C10H14	460.06	327.20	40.79
618	Propenyl Bz(cis)	C9H10	436.36	308.39	37.86
602	O-Methylstyrene	C9H10	433.86	307.22	37.90
702	1-MthNaphthalene	C11H10	501.92	341.70	38.54
509	N-Propylbenzene	C9H12	432.20	306.41	37.90
526	M-Diethylbenzene	C10H14	460.06	327.20	40.79
583	Cs-2-PhnButene-2	C10H12	459.12	325.26	40.17
543	M-DiisopropylBz	C12H18	504.94	358.41	44.47
584	Ts-2-PhnButene-2	C10H12	459.12	325.26	40.17

Table D. 32 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

580	1,2-DiC1-3C2-Bz	C10H14	465.04	331.25	41.45
704	1-EthNaphthalene	C12H12	524.80	374.05	46.88
512	M-Ethyltoluene	C9H12	437.18	310.46	38.57
522	1-Mth-2-iC3-Benz	C10H14	459.62	326.07	40.40
513	P-Ethyltoluene	C9H12	437.18	310.46	38.57
514	1,2,3-Mesitylene	C9H12	442.16	314.52	39.23
614	M-Divinylbenzene	C10H10	453.42	320.71	39.45
524	1-Mth-4-iC3-Benz	C10H14	459.62	326.07	40.40
822	Gamma-Terpinene	C10H16	443.22	311.76	37.84
821	Alpha-Terpinene	C10H16	443.22	311.76	37.84
523	1-Mth-3-iC3-Benz	C10H14	459.62	326.07	40.40
703	2-MthNaphthalene	C11H10	501.92	341.70	38.54
557	CycHexylBenzene	C12H16	520.35	366.81	44.76
515	1,2,4-Mesitylene	C9H12	442.16	314.52	39.23
519	Isobutylbenzene	C10H14	454.64	322.01	39.74
424	DiPhnAcetylene	C14H10	582.28	418.26	53.46
544	P-DiisopropylBz	C12H18	504.94	358.41	44.47
518	N-Butylbenzene	C10H14	455.08	323.14	40.13
516	1,3,5-Mesitylene	C9H12	442.16	314.52	39.23
809	Acenaphthalene	C12H8	536.08	347.79	35.65
725	123-TriMthIndene	C12H14	521.64	364.24	43.46
527	1,4-DiEthBenzene	C10H14	460.06	327.20	40.79
558	Diphenyl	C12H10	527.52	359.79	40.74
576	2-Ethyl-m-Xylene	C10H14	465.04	331.25	41.45
620	p-ISOPROPENYLSTY	C11H12	476.18	337.58	41.76
585	o-PropylToluene	C10H14	460.06	327.20	40.79
577	2-Ethyl-p-Xylene	C10H14	465.04	331.25	41.45
579	4-Ethyl-o-Xylene	C10H14	465.04	331.25	41.45
586	m-Propyltoluene	C10H14	460.06	327.20	40.79
587	p-Propyltoluene	C10H14	460.06	327.20	40.79
578	4-Ethyl-m-Xylene	C10H14	465.04	331.25	41.45
575	5-Ethyl-m-Xylene	C10H14	465.04	331.25	41.45
530	Prehnitene	C10H14	470.02	335.29	42.12
709	2,6-2Mth-Naphtha	C12H12	529.78	362.76	41.43
715	2,7-2Mth-Naphtha	C12H12	529.78	362.76	41.43
719	2-ETHYLNAPHTHALENE	C12H12	524.80	358.59	40.77
621	p-tert-BUTYLSTY	C12H16	499.27	352.75	43.28
532	1,2,4,5-TetMthBz	C10H14	470.02	335.29	42.12
531	1,2,3,5-TetMthBz	C10H14	470.02	335.29	42.12
533	p-tert-BUTYL ET	C12H18	502.59	356.00	43.95
567	N-Pentylbenzene	C11H16	477.96	339.87	42.36
718	1-n-PROPYLNAPHTH	C13H14	547.68	375.46	42.99

Table D. 33 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

562	1,1-DiPhnEthane	C14H14	572.84	407.71	50.92
616	4-ISOBUTYLSTYRE	C12H16	502.06	356.30	44.19
260	1-Decene	C10H20	425.08	301.13	37.18
735	Cis-Stilbene	C14H12	577.44	395.38	45.15
568	Hexylbenzene	C12H18	500.84	356.60	44.58
563	Diphenylmethane	C13H12	550.40	392.10	49.08
564	1,2-DiPhnEthane	C14H14	573.28	408.82	51.31
804	Anthracene	C14H10	589.54	387.60	40.74
736	Trans-Stilbene	C14H12	577.44	410.83	51.27
805	Phenanthrene	C14H10	589.54	387.60	40.74
713	1-ButNaphthalene	C14H16	570.56	392.32	45.22
807	Pyrene	C16H10	651.56	413.47	40.74
261	1-Undecene	C11H22	447.96	317.87	39.41
581	23-2C1-23-2PhnC4	C18H22	658.34	466.46	57.62
549	N-Heptylbenzene	C13H20	523.72	373.33	46.81
710	1-PhnNaphthalene	C16H12	643.00	427.19	45.83
566	2,4-Diphenyl-4-M	C18H20	658.13	468.00	58.33
561	O-Terphenyl	C18H14	696.46	466.64	50.92
569	N-Octylbenzene	C14H22	546.60	390.05	49.03
565	Triphenylmethane	C19H16	713.92	510.09	64.33
714	N-C6-Naphthalene	C16H20	616.32	426.00	49.67
717	Fluoranthene	C16H10	651.56	413.47	40.74
716	1-Hexyl-Tetralin	C16H24	608.35	418.04	48.12
731	TriPhnEthylene	C20H16	741.28	530.06	66.98
806	Chrysene	C18H12	705.02	453.71	45.83
588	1,1,2TriPhenEth	C20H18	736.80	526.81	66.55
711	1-n-NonylNaphtha	C19H26	684.96	476.44	56.35
570	N-Nonylbenzene	C15H24	569.48	406.77	51.26
712	1-Decyl Naphtha	C20H28	707.84	493.23	58.57
559	P-Terphenyl	C18H14	696.46	466.64	50.92
560	M-Terphenyl	C18H14	696.46	466.64	50.92
589	TetraPhenylMetha	C25H20	875.09	594.67	66.82
554	Decylbenzene	C16H26	592.36	423.49	53.49
732	TetraPhnEthylene	C26H20	905.12	618.87	70.46
574	N-Dodecylbenzene	C18H30	638.12	456.92	57.94
571	N-Undecylbenzene	C17H28	615.24	440.21	55.71
572	Tridecylbenzene	C19H32	661.00	473.64	60.16
573	n-TETRADECYLBENZ	C20H34	683.88	490.35	62.39
2575	n-PENTADECYLBENZ	C21H36	706.76	507.07	64.62
2576	n-HEXADECYLBENZ	C22H38	729.64	523.78	66.84
2577	n-HEPTADECYLBENZ	C23H40	752.52	540.49	69.07
2578	n-OCTADECYLBENZE	C24H42	775.40	557.20	71.29

Table D. 34 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

DipID	Halocarbons Name	Formula	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1544	Allyl Chloride	C3H5Cl	302.35	213.09	25.99
1595	2-Chloropropene	C3H5Cl	302.23	213.22	26.07
1531	3-Chloropropyne	C3H3Cl	295.79	211.03	26.52
1535	T-Butyl Chloride	C4H9Cl	325.32	228.36	27.59
1583	Chloroprene	C4H5Cl	321.79	226.70	27.62
1530	Isopropyl Cl	C3H7Cl	305.23	215.20	26.27
1572	O-DiCl-Benzene	C6H4Cl2	443.40	318.38	40.66
1585	Propyl Chloride	C3H7Cl	305.67	216.35	26.66
1684	Isopropyl Iodide	C3H7I	360.94	254.94	31.26
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	370.02	264.30	33.31
1651	2-Bromopropane	C3H7Br	333.96	234.42	28.32
1691	Iodobenzene	C6H5I	456.70	325.05	40.60
1860	Fluorobenzene	C6H5F	362.83	253.80	30.41
1571	Chlorobenzene	C6H5Cl	400.99	285.32	35.61
1680	Bromobenzene	C6H5Br	429.72	304.59	37.66
1526	1,2-DiCl-Propane	C3H6Cl2	342.66	244.33	30.65
1683	Propyl Iodide	C3H7I	361.38	256.09	31.65
1576	Benzotrichloride	C7H5Cl3	495.50	355.52	45.31
1536	2,3-DICHLOROBUT	C4H8Cl2	365.10	259.94	32.49
2638	2-Bromobutane	C4H9Br	356.84	251.19	30.55
1586	1-Chlorobutane	C4H9Cl	328.55	233.09	28.88
1573	M-DiCl-Benzene	C6H4Cl2	443.40	318.38	40.66
2634	Benzotrifluoride	C7H5F3	381.02	260.65	29.71
1574	P-DiCl-Benzene	C6H4Cl2	443.40	318.38	40.66
1650	1-Bromopropane	C3H7Br	334.40	235.59	28.71
1587	2-Chlorobutane	C4H9Cl	328.11	231.95	28.50
2653	8F-2-Butene	C4F8	270.96	152.10	12.48
1678	M-Dibromobenzene	C6H4Br2	500.86	357.01	44.76
1537	1,2-DiCl-Butane	C4H8Cl2	365.54	261.05	32.88
1597	34-DiCl-1-Butene	C4H6Cl2	362.22	257.83	32.21
1577	O-Chlorotoluene	C7H7Cl	428.85	306.09	38.50
1532	123-3Cl-Propane	C3H5Cl3	380.09	273.33	35.04
1578	P-Chlorotoluene	C7H7Cl	428.85	306.09	38.50
1562	Benzyl Chloride	C7H7Cl	423.87	302.04	37.84
2661	P-Bromotoluene	C7H7Br	457.58	325.38	40.55
1508	1,4-DiCl-Butane	C4H8Cl2	365.98	262.15	33.27
1655	1-Bromobutane	C4H9Br	357.28	252.34	30.93
1599	BenzylDichloride	C7H6Cl2	460.86	329.98	41.83
2652	Perfluoropropane	C3F8	252.71	142.94	11.85
1505	2-Butylene DiCl	C4H6Cl2	363.70	258.55	32.20
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	370.14	264.18	33.23
1588	1-Chloropentane	C5H11Cl	351.43	249.82	31.11
2654	OctaF-CycButane	C4F8	270.96	152.10	12.48
1592	1,2,4-TriCl-Bz	C6H3Cl3	485.81	351.35	45.71

Table D. 35 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1579	2,4-2Cl-Toluene	C7H6Cl2	471.26	339.12	43.55
2593	1,3,5-TriCl-BZ	C6H3Cl3	485.81	351.35	45.71
1697	1-Br-Naphthalene	C10H7Br	545.20	388.96	48.87
1622	Perfluorobutane	C4F10	270.90	144.46	11.14
1857	P-Cl-Benzo-TriF	C7H4ClF3	423.43	294.32	34.75
1509	1,5-DiCl-Pentane	C5H10Cl2	388.86	278.86	35.49
1589	1-Cl-Naphthalene	C10H7Cl	516.47	354.50	40.70
1864	Perfluorobenzene	C6F6	384.08	261.88	29.63
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	465.84	327.73	39.80
1667	1-Bromoheptane	C7H15Br	425.92	302.56	37.61
1575	HexaCl-Benzene	C6Cl6	613.04	449.85	60.85
2640	Freon 123B1	C2HBrClF3	343.09	234.65	26.73
1504	Vinyl Chloride	C2H3Cl	280.95	197.03	23.75
1672	1,1-DiBr-Ethane	C2H4Br2	377.24	266.12	32.53
1580	Acetylene DiCl	C2H2Cl2	317.94	225.08	27.75
1692	Diiodomethane	CH2I2	408.76	291.45	36.57
1698	Bromoform	CHBr3	420.52	297.79	36.74
2687	Freon 13B1	CBrF3	283.22	189.16	20.51
2690	Br-3F-Ethylene	C2BrF3	301.47	199.21	21.14
1649	Tetrabromoethane	C2H2Br4	509.12	361.78	45.01
2686	Freon 12B1	CBrClF2	321.38	221.63	25.71
1503	Ethyl Chloride	C2H5Cl	282.79	199.60	24.43
2641	Br-TriCl-Methane	CBrCl3	397.70	284.78	36.11
1641	Methyl Bromide	CH3Br	288.64	202.06	24.26
2688	Freon 12B2	CBr2F2	350.11	240.78	27.76
2545	2,3-DiCl-Propene	C3H4Cl2	338.47	239.41	29.45
1673	1,2-DiBr-Ethane	C2H4Br2	377.68	267.27	32.92
2637	Dibromomethane	CH2Br2	354.80	250.52	30.69
1542	TetraCl-Ethylene	C2Cl4	399.00	288.92	37.70
1541	TriCl-Ethylene	C2HCl3	361.69	259.87	33.24
1527	111-TriCl-Ethane	C2H3Cl3	354.42	253.16	31.91
1612	Cl-2F-Ethylene	C2HClF2	276.26	186.94	20.82
1617	Ethyl Fluoride	C2H5F	240.00	161.09	17.64
2639	Br-Cl-Methane	CH2BrCl	326.07	231.27	28.64
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	317.94	225.08	27.75
1682	Ethyl Iodide	C2H5I	338.50	239.35	29.42
1522	1,1-DiCl-Ethane	C2H4Cl2	319.78	227.60	28.43
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	278.10	189.74	21.50
1525	Hexachloroethane	C2Cl6	463.48	335.54	43.76
1528	1112-4Cl-Ethane	C2H2Cl4	391.85	282.16	36.29
1590	Penta-Cl-Ethane	C2HCl5	428.84	310.02	40.29
1529	1122-4Cl-Ethane	C2H2Cl4	394.20	284.50	36.81
2693	Perfluoroethane	C2F6	234.52	140.21	12.55
1611	Freon 114B2	C2Br2F4	368.30	247.16	27.06
2692	Cl-PentaF-Ethane	C2ClF5	272.68	175.59	17.75
2655	122-3Cl-112-3FC2	C2Cl3F3	349.00	241.31	28.16
1609	12-2Cl-1122-4FC2	C2Cl2F4	310.84	208.96	22.96

Table D. 36 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

2526	1,1-DiCl-Propane	C3H6Cl2	342.66	244.33	30.65
1645	Ethyl Bromide	C2H5Br	311.52	218.83	26.48
2658	1112-4Cl-22-2FC2	C2Cl4F2	387.16	273.06	33.36
1619	111-3F-Ethane	C2H3F3	239.94	156.82	16.30
1524	1,1,2-3Cl-Ethane	C2H3Cl3	357.21	256.62	32.81
1640	1,1-DiF-Ethane	C2H4F2	239.97	159.01	16.97
2691	Genetron 1113	C2ClF3	272.74	180.11	19.09
2694	Vinyl Bromide	C2H3Br	308.20	215.54	25.81
1694	Refrigerant 123	C2HCl2F3	314.36	215.52	24.68
1523	1,2-DiCl-Ethane	C2H4Cl2	320.22	228.71	28.82
2656	1122-4Cl-12-2FC2	C2Cl4F2	387.16	273.06	33.36
2527	1,3-DiCl-Propane	C3H6Cl2	343.10	245.43	31.04

Table D. 37 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

	Acids				
DipID	**Name**	**Formula**	$T_{b,Joback}^{760mmHg}$	$T_{b,Joback}^{10mmHg}$	ΔH_{Joback}^{298}
1277	Acrylic Acid	C3H4O2	410.43	297.16	38.77
1274	Ts-Crotonic Acid	C4H6O2	434.35	313.55	40.59
1279	Oleic Acid	C18H34O2	761.11	552.93	72.78
1278	Methacrylic Acid	C4H6O2	432.00	311.20	40.07
2271	Cinnamic Acid	C9H8O2	581.87	421.42	55.03
1266	n-UNDECANOIC ACI	C11H22O2	596.79	433.91	57.24
1282	O-Toluic Acid	C8H8O2	559.81	406.63	53.50
2283	IBUPROFEN	C13H18O2	673.33	488.05	63.86
1261	Isovaleric Acid	C5H10O2	459.07	332.67	43.50
1264	1,4-CychexDicarboxAcid	C8H12O4	688.54	504.28	67.85
1283	P-Toluic Acid	C8H8O2	559.81	406.63	53.50
1257	3-MthButyricAcid	C5H10O2	459.07	332.67	43.50
1288	Isophthalic Acid	C8H6O4	705.32	518.86	70.67
2871	4CarboxAcidBzldhyde	C8H6O3	608.47	446.17	60.22
1256	N-Butyric Acid	C4H8O2	436.63	317.01	41.66
1276	Stearic Acid	C18H36O2	756.95	550.81	72.83
1285	Adipic Acid	C6H10O4	627.90	462.62	63.28
1273	Cs-Crotonic Acid	C4H6O2	440.79	319.11	41.62
4851	Diglycolic Acid	C4H6O5	604.56	446.02	61.24
1286	Maleic Acid	C4H4O4	586.30	431.39	58.78
2277	Citraconic Acid	C5H6O4	599.95	439.31	59.07
2278	Itaconic Acid	C5H6O4	601.58	442.91	60.46
2281	Glutaric Acid	C5H8O4	605.02	445.91	61.05
1271	TetradecylicAcid	C14H28O2	665.43	484.01	63.92

Table D. 38 Boiling Temperatures and Heats of Vaporization by the Joback-Reid Method (Continued)

1259	N-Nonanoic Acid	C9H18O2	551.03	400.51	52.79
1280	Linoleic Acid	C18H32O2	765.27	555.03	72.74
1260	Isobutyric Acid	C4H8O2	436.19	315.96	41.27
2268	Fumaric Acid	C4H4O4	579.86	425.90	57.76
1287	Phthalic Acid	C8H6O4	705.32	518.86	70.67
1289	TerephthalicAcid	C8H6O4	705.32	518.86	70.67
2280	Succinic Acid	C4H6O4	582.14	429.21	58.83
1270	Tridecanoic Acid	C13H26O2	642.55	467.31	61.70
1254	N-Decanoic Acid	C10H20O2	573.91	417.21	55.02
2270	Suberic Acid	C8H14O4	673.66	496.02	67.73
2255	Linolenic Acid	C18H30O2	769.43	557.13	72.70
1262	N-Hexanoic Acid	C6H12O2	482.39	350.41	46.11
4852	Levulinic Acid	C5H8O3	513.38	376.09	50.63
2275	Sebacic Acid	C10H18O4	719.42	529.43	72.18
1255	Oxalic Acid	C2H2O4	536.38	395.80	54.37
2259	PentadecylicAcid	C15H30O2	688.31	500.71	66.15
2266	NonadecanoicAcid	C19H38O2	779.83	567.51	75.05
2269	Pimelic Acid	C7H12O4	650.78	479.32	65.50
1252	Acetic Acid	C2H4O2	390.87	283.61	37.21
3268	Malonic Acid	C3H4O4	559.26	412.51	56.60
2279	2-EthButyricAcid	C6H12O2	481.95	349.37	45.73
1265	N-Octanoic Acid	C8H16O2	528.15	383.81	50.57
2258	NeopentanoicAcid	C5H10O2	456.28	329.27	42.59
2257	Azelaic Acid	C9H16O4	696.54	512.73	69.96
1281	Benzoic Acid	C7H6O2	531.95	385.92	50.62
1269	Dodecanoic Acid	C12H24O2	619.67	450.61	59.47
2261	Heptanoic Acid	C7H14O2	505.27	367.11	48.34
1258	N-Valeric Acid	C5H10O2	459.51	333.71	43.89
2265	HeptadecylicAcid	C17H34O2	734.07	534.11	70.60
2267	N-Eicosanic Acid	C20H40O2	802.71	584.21	77.28
1253	Propionic Acid	C3H6O2	413.75	300.31	39.44
5877	Ascorbic Acid	C6H8O6	772.97	573.57	80.05
1272	HexadecanoicAcid	C16H32O2	711.19	517.41	68.37

Table D. 39 Boiling Temperatures and Heats of Vaporization by the Gani Method

DipID	Alcohols Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1181	Phenol	C6H6O	450.15	331.51	45.29
1182	O-Cresol	C7H8O	472.33	346.98	47.08
1183	M-Cresol	C7H8O	472.33	346.98	47.08
1176	2,6-Xylenol	C8H10O	492.33	361.28	48.87
1111	2-Mth-2-Butanol	C5H12O	400.38	297.17	41.51
1178	3,5-Xylenol	C8H10O	492.33	361.28	48.87
1133	2-Octanol	C8H18O	474.80	353.14	49.62
2885	4-HYDROXYSTYREN	C8H8O	507.26	372.54	50.51
1197	P-t-Butylphenol	C10H14O	519.42	381.67	51.82
1172	2,4-Xylenol	C8H10O	492.33	361.28	48.87
1184	P-Cresol	C7H8O	472.33	346.98	47.08
1151	Cyclohexanol	C6H12O	435.68	325.06	46.10
1170	2,3-Xylenol	C8H10O	489.24	359.84	48.98
1187	P-Ethyl Phenol	C8H10O	489.24	359.84	48.98
2859	P-Methoxyphenol	C7H8O2	507.80	372.44	50.31
1121	2-Ethylhexanol	C8H18O	474.80	353.14	49.62
1179	PropargylAlcohol	C3H4O	382.69	284.68	40.02
1123	3-Mth-1-Butanol	C5H12O	410.19	304.47	42.54
2196	P-t-Amylphenol	C11H16O	533.75	394.00	54.18
1174	2,5-Xylenol	C8H10O	492.33	361.28	48.87
1115	2-Hexanol	C6H14O	434.07	321.98	44.90
1152	1-MthCycHexanol	C7H14O	449.13	338.68	49.58
4854	Guaiacol	C7H8O2	507.80	372.44	50.31
1107	Sec-Butanol	C4H10O	383.14	285.20	40.17
1167	Allyl Alcohol	C3H6O	363.43	271.25	38.51
1130	4-Mth-2-Pentanol	C6H14O	425.27	315.32	43.92
1177	3,4-Xylenol	C8H10O	492.33	361.28	48.87
1114	1-Hexanol	C6H14O	442.50	328.44	45.88
1106	Isobutanol	C4H10O	383.14	285.20	40.17
1125	1-Heptanol	C7H16O	463.05	344.12	48.24
1105	N-Butanol	C4H10O	393.90	292.94	41.16
1109	1-Pentanol	C5H12O	419.64	311.49	43.52
1132	1-Octanol	C8H18O	481.73	358.76	50.60
1113	T-Butylcarbinol	C5H12O	400.38	297.17	41.51
1137	1-Undecanol	C11H24O	529.29	397.86	57.69
1108	Tert-Butanol	C4H10O	371.91	277.11	39.15
1103	N-Propanol	C3H8O	364.44	272.32	38.79
1134	1-Nonanol	C9H20O	498.84	372.52	52.97
2195	P-t-Octylphenol	C14H22O	562.61	419.28	59.26
1102	Ethanol	C2H6O	330.01	248.85	36.43
1124	3-Mth-2-Butanol	C5H12O	400.27	297.20	41.55
1136	1-Decanol	C10H22O	514.63	385.52	55.33

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1140	Dodecanol	C12H26O	542.96	409.61	60.05
1104	Isopropanol	C3H8O	351.96	263.61	37.81
1110	2-Pentanol	C5H12O	410.19	304.47	42.54
1120	3-Pentanol	C5H12O	410.19	304.47	42.54
1112	2-Mth-1-Butanol	C5H12O	410.19	304.47	42.54
1154	Ts-2-Mth-CycC6OH	C7H14O	449.13	338.68	49.58
1153	Cs-2-Mth-CycC6OH	C7H14O	449.13	338.68	49.58
1156	Ts-3-Mth-CycC6OH	C7H14O	449.13	338.68	49.58
1157	Cs-4-Mth-CycC6OH	C7H14O	449.13	338.68	49.58
2197	P-Cumylphenol	C15H16O	591.65	445.14	64.73
1180	Benzyl Alcohol	C7H8O	478.80	354.82	49.34
1158	Ts-4-Mth-CycC6OH	C7H14O	449.13	338.68	49.58
1155	Cs-3-Mth-CycC6OH	C7H14O	449.13	338.68	49.58
1168	2-Phn-2-Propanol	C9H12O	500.10	371.57	52.05
1141	1-Tridecanol	C13H28O	555.78	420.85	62.41
1147	2-Eth-1-Butanol	C6H14O	434.07	321.98	44.90
1117	2-Mth-1-Pentanol	C6H14O	434.07	321.98	44.90
2115	2-Phenylethanol	C8H10O	485.03	362.35	51.58
1142	1-Tetradecanol	C14H30O	567.84	431.61	64.78
2118	1-PHN-1-PROPANOL	C9H12O	506.18	376.80	53.08
2119	1-PHN-2-PROPANOL	C9H12O	506.18	376.80	53.08
1126	2-Heptanol	C7H16O	455.44	338.12	47.26
1143	1-Pentadecanol	C15H32O	579.23	441.94	67.14
1129	Isoheptanol	C7H16O	455.44	338.12	47.26
2117	2,6-DiMth-4-C7OH	C9H20O	479.11	356.25	50.02
1144	1-Hexadecanol	C16H34O	590.02	451.89	69.50
1145	Heptadecanol	C17H36O	600.26	461.47	71.86
1199	Nonylphenol	C15H24O	583.92	442.06	65.52
1146	1-Octadecanol	C18H38O	610.02	470.72	74.22
1135	2-Nonanol	C9H20O	492.47	367.21	51.98
1149	1-Nonadecanol	C19H40O	619.33	479.66	76.59
1139	Isodecanol	C10H22O	508.74	380.49	54.35
1148	1-Eicosanol	C20H42O	628.24	488.32	78.95
2198	Dinonylphenol	C24H42O	664.08	519.28	85.75
1159	Menthol	C10H20O	484.41	354.65	47.67
1202	DiethyleneGlycol	C4H10O3	486.71	377.78	60.78
1245	1,3-Benzenediol	C6H6O2	516.51	393.70	59.62
1186	P-Hydroquinone	C6H6O2	516.51	393.70	59.62
1244	1,2-Benzenediol	C6H6O2	516.51	393.70	59.62
1219	2MTH,13PROPNDIO	C4H10O2	465.76	360.03	57.10
1212	1,3-Propanediol	C3H8O2	453.47	350.71	55.72
1235	P-t-But-Catechol	C10H14O2	568.81	434.34	66.15

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1203	Triglycol	C6H14O4	529.91	414.05	68.19
1198	Bisphenol A	C15H16O2	627.53	488.05	79.06
1238	2,3-Butanediol	C4H10O2	458.25	354.14	56.12
1211	1,2-Propanediol	C3H8O2	445.49	344.53	54.74
2219	2,4-PENTANEDIOL	C5H12O2	477.35	368.93	58.48
1215	1,4-Butynediol	C4H6O2	487.06	372.82	57.23
1214	Neopentyl Glycol	C5H12O2	477.43	368.91	58.44
1221	1,3-Butanediol	C4H10O2	465.76	360.03	57.10
1220	1,2-Butanediol	C4H10O2	465.76	360.03	57.10
1240	Ts2-C4H8-14-Diol	C4H8O2	472.97	364.79	57.43
1239	Cis-Butenediol	C4H8O2	472.97	364.79	57.43
1241	1,4-Butanediol	C4H10O2	473.00	365.76	58.09
1222	Hexylene Glycol	C6H14O2	488.39	377.44	59.82
1213	Dipropylene Gly	C6H14O3	507.19	393.95	63.54
1242	1,5-Pentanediol	C5H12O2	490.83	379.79	60.45
1243	1,6-Hexanediol	C6H14O2	507.22	392.96	62.81
1204	TetraC2H4 Glycol	C8H18O5	565.55	445.55	75.60
6886	C6H4(COOC2H4OH)2	C12H14O6	635.17	512.12	95.18
1248	123-Benzenetriol	C6H6O3	566.52	444.04	73.96
1231	Glycerol	C3H8O3	509.41	405.61	71.67
1247	Hexaglycerol	C6H14O3	546.67	436.21	77.73
1246	Pentaerythritol	C5H12O4	577.04	471.02	92.30

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

	Amines				
DipID	**Name**	**Formula**	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1742	Ethyleneimine	C2H5N	258.06	187.15	24.524
1745	Piperidine	C5H11N	376.22	263.76	31.772
2726	Propyleneimine	C3H7N	288.62	205.86	25.85
1766	Pyrrolidine	C4H9N	343.88	241.87	29.356
1719	Isopropylamine	C3H9N	301.71	216.70	27.693
1711	N-Propylamine	C3H9N	327.98	236.40	30.484
1726	Sec-Butylamine	C4H11N	340.80	242.00	30.055
1704	Ethylamine	C2H7N	286.09	209.39	28.122
1702	Dimethylamine	C2H7N	284.68	206.36	27.006
1710	Diethylamine	C4H11N	341.35	239.97	29.094
1740	Allylamine	C3H7N	326.78	235.15	30.197
1712	N-Butylamine	C4H11N	362.73	259.53	32.846

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1794	HexMthyleneimine	C6H13N	404.14	283.48	34.188
1729	Cyclohexylamine	C6H13N	403.73	285.61	35.149
1714	Isobutylamine	C4H11N	350.15	250.88	31.864
2853	Acetamide	C2H5NO	494.30	304.68	28.597
2731	N-C1-CycC6-Amine	C7H15N	433.79	307.27	37.934
1743	Diisopropylamine	C6H15N	357.07	250.94	30.399
1796	N,N-DiMthAniline	C8H11N	511.13	364.75	45.859
1792	Aniline	C6H7N	473.03	337.20	42.279
1713	N-Pentylamine	C5H13N	392.42	280.04	35.208
1733	Benzylamine	C7H9N	458.77	327.09	41.031
1737	M-Toluidine	C7H9N	492.97	351.43	44.069
3796	N-Ethylaniline	C8H11N	465.92	327.38	39.641
1878	2-Methacrylamide	C4H7NO	523.29	330.45	32.288
1736	O-Toluidine	C7H9N	492.97	351.43	44.069
2739	Diallylamine	C6H11N	400.58	279.37	33.244
2706	Hexylamine	C6H15N	418.33	298.61	37.57
2724	O-Ethylaniline	C8H11N	508.32	363.58	45.974
1707	Dipropylamine	C6H15N	402.25	281.64	33.818
1738	P-Toluidine	C7H9N	492.97	351.43	44.069
1795	N-Methylaniline	C7H9N	458.16	324.18	39.915
1718	Diisobutylamine	C8H19N	432.46	303.33	36.578
1879	Acrylamide	C3H5NO	509.94	318.99	30.672
2707	1-Aminoheptane	C7H17N	441.33	315.70	39.932
2730	DiCycHexylAmine	C12H23N	497.44	358.35	46.144
2787	P-Aminodiphenyl	C12H11N	580.09	433.09	61.537
1744	Dibutylamine	C8H19N	449.11	316.38	38.542
2708	1-Octylamine	C8H19N	462.00	331.58	42.294
2791	2,6-DiEthAniline	C10H15N	538.39	387.25	49.669
2709	1-Nonylamine	C9H21N	480.77	346.46	44.656
2710	1-Decylamine	C10H23N	497.96	360.49	47.018
3722	Diamylamine	C10H23N	487.21	346.66	43.266
3724	Undecylamine	C11H25N	513.81	373.78	49.38
2712	Dodecylamine	C12H27N	528.53	386.41	51.742
1720	Tetradecylamine	C14H31N	555.11	409.99	56.466
2752	Piperazine	C4H10N2	399.71	281.26	34.172
1752	Propylenediamine	C3H10N2	387.28	279.83	36.315
1741	Ethylenediamine	C2H8N2	377.14	275.37	36.744
2725	O-Aminoaniline	C6H8N2	548.81	400.99	53.602
2750	P-Aminoaniline	C6H8N2	548.81	400.99	53.602
2727	M-Aminoaniline	C6H8N2	548.81	400.99	53.602
1750	AEP	C6H15N3	465.65	340.19	45.462
1732	Toluene Diamine	C7H10N2	562.78	412.05	55.392
1731	hexamethyleneDiamine	C6H16N2	470.99	344.51	46.192
3750	P-Benzidine	C12H12N2	628.27	479.42	72.86

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Nitriles Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1773	Propionitrile	C3H5N	364.17	260.81	33.087
1782	Butyronitrile	C4H7N	393.67	281.22	35.449
2720	Allyl Cyanide	C4H5N	392.80	280.12	35.162
1783	Valeronitrile	C5H9N	419.44	299.72	37.811
3874	Benzyl Cyanide	C8H7N	496.01	357.28	45.996
1786	Hexanenitrile	C6H11N	442.32	316.75	40.173
1776	Succinonitrile	C4H4N2	472.69	346.38	46.674
1781	Glutaronitrile	C5H6N2	490.54	360.64	49.036
2735	14-2Cyano-2-C4H8	C6H6N2	506.93	372.82	50.74
1777	Adiponitrile	C6H8N2	506.96	374.10	51.398

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Imines Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1767	N-MthPyrrolidine	C5H11N	361.15	249.56	29.079
2797	3-Methylpyridine	C6H7N	402.55	289.33	37.04
1797	2-Methylpyridine	C6H7N	402.55	289.33	37.04
2799	4-Methylpyridine	C6H7N	402.55	289.33	37.04
1753	N,N-DiEthAniline	C10H15N	474.45	338.23	42.417

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Tert-N Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1706	Triethylamine	C6H15N	356.76	254.28	31.87
2716	Tributylamine	C12H27N	494.90	356.81	46.042
2719	Tripropylamine	C9H21N	437.29	311.42	38.956
3723	Triamylamine	C15H33N	539.79	395.21	53.128

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Nitrates Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1761	Nitroethane	C2H5NO2	387.22	281.39	37.069
1763	2-Nitropropane	C3H7NO2	393.40	284.06	36.799
1762	1-Nitropropane	C3H7NO2	413.76	300.30	39.431

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Thiols Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1802	Ethyl Mercaptan	C2H6S	292.34	212.27	27.908
1820	Dimethyl Sulfide	C2H6S	310.48	219.53	26.981
1843	Thiacyclopentane	C4H8S	380.75	264.55	31.212
1803	1-Propanethiol	C3H8S	333.08	238.56	30.27
1805	Isobut Mercaptan	C4H10S	354.73	252.74	31.65
6860	Ethylenedithiol	C2H6S2	385.11	278.70	36.316
1811	Cyclohexanethiol	C6H12S	422.48	300.97	37.676
1828	DiMth Disulfide	C2H6S2	385.11	278.70	36.316
1841	Butanethiol	C4H10S	367.04	261.24	32.632
1814	Methylproylsulf	C4H10S	367.04	261.24	32.632
2816	ETHYLtBUTYL SUL	C6H14S	412.35	286.15	33.664
1818	Diethyl Sulfide	C4H10S	378.63	262.85	30.95
1812	Benzyl Mercaptan	C7H8S	461.47	327.96	40.817
1838	T-OctylMercaptan	C8H18S	449.36	320.11	40.07
1827	1-Pentanethiol	C5H12S	396.15	281.44	34.994
2815	METHnBUTYL SULFD	C5H12S	407.26	284.71	34.067
1824	DiethylDisulfide	C4H10S2	451.98	315.64	37.676
1807	N-Hexylmercaptan	C6H14S	421.63	299.79	37.356
6857	Dimercaptoethyl	C4H10OS2	451.96	329.39	43.73
1839	1-Heptanethiol	C7H16S	444.27	316.72	39.718
1829	DiProp Disulfide	C6H14S2	489.59	345.82	42.4
1809	1-Octanethiol	C8H18S	464.66	332.47	42.08
1808	N-Nonanethiol	C9H20S	483.20	347.26	44.442
1826	1-Decanethiol	C10H22S	500.19	361.20	46.804
2838	tertDodecanThiol	C12H26S	519.48	377.06	49.518
1825	1-Undecanethiol	C11H24S	515.88	374.43	49.166
1837	Dodecylthiol	C12H26S	530.45	387.01	51.528

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Aldehydes Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1037	Methacrolein	C4H6O	346.65	247.76	31.271
1002	Acetaldehyde	C2H4O	269.68	199.46	27.58
1003	Propionaldehyde	C3H6O	314.71	228.31	29.942
1041	Benzaldehyde	C7H6O	451.87	322.34	40.489
1034	Acrolein	C3H4O	313.43	227.03	29.655

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1005	N-Butyraldehyde	C4H8O	351.59	252.60	32.304
1036	Trans-2-Butenal	C4H6O	351.53	251.10	31.646
1007	Valeraldehyde	C5H10O	382.82	273.91	34.666
1006	Isobutyraldehyde	C4H8O	338.28	243.56	31.322
1009	1-Hexanal	C6H12O	409.90	293.08	37.028
1040	P-Tolualdehyde	C8H8O	473.87	337.62	42.279
1016	2-Methylhexanal	C7H14O	425.01	303.92	38.408
1017	3-Methylhexanal	C7H14O	425.01	303.92	38.408
1008	1-Heptanal	C7H14O	433.81	310.63	39.39
1013	2-Ethylhexanal	C8H16O	447.31	320.64	40.77
1010	1-Octanal	C8H16O	455.22	326.89	41.752
1011	1-Nonanal	C9H18O	474.59	342.08	44.114
1020	1-Decanal	C10H20O	492.29	356.37	46.476
1021	1-Undecanal	C11H22O	508.57	369.88	48.838
1025	Dodecanal	C12H24O	523.65	382.72	51.2
1026	1-Tridecanal	C13H26O	537.70	394.94	53.562
1014	1,2-Ethanedione	C2H2O2	355.87	261.80	35.66
1044	1,4BenzDicarboxAldehy	C8H6O2	518.99	377.84	50.022

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	**Epoxides Name**	**Formula**	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1440	ISOBUTYLENE OXID	C4H8O	266.90	192.80	25.004
1478	Furan	C4H4O	261.90	191.27	25.535
1443	1,3-Propylene Ox	C3H6O	254.25	185.40	24.652
1479	Tetrahydrofuran	C4H8O	302.43	215.91	27.176
1477	2,5-Dihydrofuran	C4H6O	342.92	233.67	26.41
1471	1,2-Epoxybutane	C4H8O	285.34	204.59	26.032
1408	1-Methoxypropane	C4H10O	328.41	230.38	27.79
1442	1,2-Propylene Ox	C3H6O	232.37	171.68	23.67
1411	2-Methoxypropane	C4H10O	313.44	220.58	26.808
1421	1,4-Dioxane	C4H8O2	332.74	237.11	29.704
2422	1,3-DIOXANE	C4H8O2	332.74	237.11	29.704
1426	2-Methoxybutane	C5H12O	350.53	244.67	29.17
1422	Trioxane	C3H6O3	323.72	233.21	30.032
1413	1-Methoxybutane	C5H12O	363.09	253.28	30.152
1461	Methoxybenzene	C7H8O	438.00	304.51	35.975
1448	1-Ethoxybutane	C6H14O	371.91	261.31	31.638
1429	1-MethoxyPentane	C6H14O	371.91	261.31	31.638
6885	Ethyl-3-Ethoxypr	C7H14O3	444.80	324.10	43.003

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Ether Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1401	Dimethyl Ether	C2H6O	234.03	171.41	23.066
1407	MethylEthylEther	C3H8O	250.31	183.10	24.552
1470	VinylMethylEther	C3H6O	285.15	202.47	25.141
1405	MTBE	C5H12O	337.30	235.62	28.142
1445	VinylEthyl Ether	C4H8O	297.94	212.38	26.627
1402	Diethyl Ether	C4H10O	299.32	213.74	26.914
1431	Methylal	C3H8O2	345.75	241.89	28.994
1428	T-But EthylEther	C6H14O	347.27	244.21	29.628
1427	TAME	C6H14O	370.61	257.83	30.504
1410	Mth Isobut Ether	C5H12O	350.53	244.67	29.17
1430	Eth-t-Pent-Ether	C7H16O	379.12	265.73	31.99
1403	DiisopropylEther	C6H14O	341.45	241.92	29.884
1415	Eth Propyl Ether	C5H12O	338.82	239.16	29.276
1455	Dimethyl Acetal	C4H10O2	330.07	235.52	29.604
1446	Dipropyl Ether	C6H14O	371.91	261.31	31.638
1447	Butyl VinylEther	C6H12O	370.94	260.12	31.351
1462	EthylPhenylEther	C8H10O	444.16	311.27	37.461
1406	Di-sec-But Ether	C8H18O	402.33	283.61	34.608
1432	Acetal	C6H14O2	383.19	271.04	33.346
1460	BenzylEthylEther	C9H12O	451.52	320.35	39.703
1050	Paraldehyde	C6H12O3	370.72	267.95	34.802
1404	Di-n-Butyl Ether	C8H18O	425.37	299.30	36.362
1420	Anethole	C10H12O	507.06	352.13	41.494
1456	DimethylCarbitol	C6H14O3	446.73	315.74	38.77
1463	Dibenzyl Ether	C14H14O	546.42	397.70	52.612
1425	Di-n-PentylEther	C10H22O	467.70	331.73	41.086
1458	Diethyl Carbitol	C8H18O3	458.37	328.49	41.742
1412	Dihexyl Ether	C12H26O	502.75	360.35	45.81
1454	Triglyme	C8H18O4	498.17	358.81	46.184
1459	Dibutyl Carbitol	C12H26O3	525.91	383.90	51.19
1424	Di-n-Octyl Ether	C16H34O	558.74	409.61	55.258
1457	Tetraglyme	C10H22O5	518.93	381.46	51.846
1418	Dinonyl Ether	C18H38O	581.87	431.25	59.982
2432	ETHYLAL	C5H12O2	364.49	258.40	31.966
2405	DIISOBUTYL ETHER	C8H18O	406.56	285.19	34.398
2456	Ethyl Glyme	C6H14O2	393.94	278.76	34.328
2417	ETHYLHEXYL ETHER	C8H18O	425.37	299.30	36.362
2415	ETHYLISOPROPETH	C5H12O	318.27	227.00	28.504

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Formates Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1301	Methyl Formate	C2H4O2	285.10	208.83	28.107
1311	Vinyl Formate	C3H4O2	325.96	234.70	30.182
1302	Ethyl Formate	C3H6O2	327.17	235.95	30.469
2306	t-Butyl Formate	C5H10O2	369.60	263.81	33.183
1303	Propyl Formate	C4H8O2	362.04	259.15	32.831
2305	sec-ButylFormate	C5H10O2	380.96	271.93	34.211
2311	CYCLOHEXL FORMAT	C7H12O2	433.99	312.38	40.138
1304	N-Butyl Formate	C5H10O2	391.82	279.70	35.193
1305	Isobutyl Formate	C5H10O2	380.96	271.93	34.211
2350	Benzyl Formate	C8H8O2	477.43	341.93	43.378
2307	n-Hexyl Formate	C7H14O2	440.86	315.43	39.917
1306	N-Pentyl Formate	C6H12O2	417.81	298.31	37.555
2308	n-Heptyl Formate	C8H16O2	461.58	331.33	42.279
1308	N-Octyl Formate	C9H18O2	480.38	346.23	44.641
1309	n-Nonyl Formate	C10H20O2	497.60	360.28	47.003
1310	n-Decyl Formate	C11H22O2	513.49	373.57	49.365

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Esters Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1351	Mth Methacrylate	C5H8O2	374.08	268.25	34.138
1312	Methyl Acetate	C3H6O2	308.52	226.05	30.447
1331	Vinyl Propionate	C5H8O2	368.45	265.65	34.285
1321	Vinyl Acetate	C4H6O2	345.34	249.82	32.522
1352	Eth MthAcrylate	C6H10O2	394.30	282.56	35.901
1322	MethylPropionate	C4H8O2	346.44	251.01	32.809
1341	Methyl Acrylate	C4H6O2	341.45	248.65	32.94
1313	Ethyl Acetate	C4H8O2	335.90	244.20	32.21
1319	IsopropylAcetate	C5H10O2	366.78	264.58	34.189
1332	Methyl Butyrate	C5H10O2	369.43	266.78	34.572
1342	Ethyl Acrylate	C5H8O2	374.15	270.81	35.302
1318	Allyl Acetate	C5H8O2	377.46	271.64	34.884
1314	N-Propyl Acetate	C5H10O2	378.40	272.75	35.171
1323	Ethyl Propionate	C5H10O2	369.43	266.78	34.572
1360	I-But I-Butyrate	C8H16O2	433.25	313.23	40.711
1320	Sec-ButylAcetate	C6H12O2	395.92	284.83	36.551

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1336	PropylI-Butyrate	C7H14O2	418.76	302.71	39.331
1353	N-C3-Mthacrylate	C7H12O2	406.43	292.10	37.386
1333	Ethyl Butyrate	C6H12O2	398.22	286.86	36.934
1347	EthylIsovalerate	C7H14O2	414.18	298.14	38.314
1315	N-Butyl Acetate	C6H12O2	406.04	292.22	37.533
1390	Methyl Benzoate	C8H8O2	468.70	337.38	43.356
1388	ISOBUTYL MTHACR	C8H14O2	438.55	315.88	40.66
1343	1-PropylAcrylate	C6H10O2	397.37	285.79	36.647
1316	Isobutyl Acetate	C6H12O2	395.92	284.83	36.551
1344	N-Butyl Acrylate	C7H12O2	415.96	299.28	38.414
1357	Pentyl Acetate	C7H14O2	430.38	309.98	39.895
1327	N-PropN-Butyrate	C7H14O2	423.46	305.08	39.296
1324	N-PropPropionate	C6H12O2	398.22	286.86	36.934
1291	Acetic Anhydride	C4H6O3	403.50	292.91	38.481
1389	N-ButMthacrylate	C8H14O2	446.80	322.29	41.642
1359	Benzyl Acetate	C9H10O2	475.25	345.57	45.598
1326	N-But Propionate	C7H14O2	423.46	305.08	39.296
1391	Ethyl Benzoate	C9H10O2	484.96	351.81	46.136
1897	CH3OC3H600CH3	C6H12O3	432.59	311.61	40.117
1392	DiethylCarbonate	C5H10O3	391.71	284.16	37.262
1385	N-But N-Butyrate	C8H16O2	445.91	321.86	41.658
1317	IsopentylAcetate	C7H14O2	421.43	303.20	38.913
1363	N-Hexyl Acetate	C8H16O2	449.84	326.08	42.675
1387	Ethylene Acetate	C6H10O4	451.66	333.91	46.118
1393	Diethyl Oxalate	C6H10O4	439.00	324.73	44.92
1365	Butyl Benzoate	C11H14O2	517.38	378.68	50.86
1361	I-C5 I-Valerate	C10H20O2	470.65	340.67	44.418
1367	Heptyl Acetate	C9H18O2	469.70	341.47	45.037
1346	N-Butyl Valerate	C9H18O2	466.15	337.47	44.02
1358	2-C2-C6 Acetate	C10H20O2	483.05	350.52	45.999
1394	Diethyl Malonate	C7H12O4	463.56	344.51	48.299
1292	Propionyl Oxide	C6H10O3	450.62	325.25	42.092
1364	Benzyl Benzoate	C14H12O2	560.31	417.40	58.925
1381	2Mth p-Phthalate	C10H10O4	542.81	401.92	55.756
1368	n-Octyl Acetate	C10H20O2	487.81	355.92	47.399
1377	DiMthI-Phthalate	C10H10O4	539.86	401.84	56.592
1896	Ethylene DiAcr	C8H10O4	484.37	361.13	51.104
1386	2-Ethylhexyl Acr	C11H20O2	497.72	363.42	48.492
1395	Methyl Decanoate	C11H22O2	501.44	365.91	48.744
1369	n-Nonyl Acetate	C11H22O2	504.44	369.55	49.761
1370	n-Decyl Acetate	C12H24O2	519.82	382.48	52.123
1345	N-ButylNonanoate	C13H26O2	531.53	391.42	53.468
1375	DiProp Phthalate	C14H18O4	587.56	445.00	66.04
1376	Diisobutyl Phtha	C16H22O4	600.30	456.79	68.8
1396	IsopropMyristate	C17H34O2	578.83	434.86	62.951

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1383	Butyl Stearate	C22H44O2	629.62	483.07	74.726
1362	Methyl Oleate	C19H36O2	601.83	454.72	66.982
1355	Diisooctyl Phtha	C24H38O4	667.76	524.08	87.696
1382	DioctylTerephtha	C24H38O4	673.17	529.92	89.66
1384	DIBUTYL SEBACATE	C18H34O4	608.49	468.41	73.264
1371	Diisodecyl Phtha	C28H46O4	694.64	552.42	97.144
1354	DioctylPhthalate	C24H38O4	667.76	524.08	87.696
2375	DiethylPhthalate	C12H14O4	560.63	418.22	59.282
2388	Dipropyl Maleate	C10H16O4	517.80	388.03	55.744
2381	Diallyl Maleate	C10H12O4	511.18	379.67	53.136
2370	Glyceryl Triacet	C9H14O6	529.70	403.22	60.807
2382	Dibutyl Maleate	C12H20O4	545.73	411.88	60.468
2376	DibutylPhthalate	C16H22O4	607.79	464.23	70.764
2353	CetylMthacrylate	C20H38O2	611.92	465.41	69.986
2379	Dihexyl Adipate	C18H34O4	608.49	468.41	73.264
2321	T-Butyl Acetate	C6H12O2	382.20	276.38	35.941
2332	Methl.I-butyrate	C5H10O2	363.28	263.64	34.607
2354	AllylMthacrylate	C7H10O2	423.69	304.55	38.993
2364	CYCLOHEXL ACETAT	C8H14O2	443.26	323.06	42.896
2337	EthylIsobutyrate	C6H12O2	392.90	284.16	36.969
2384	IsobutylAcrylate	C7H12O2	417.99	301.70	39.044
2380	1,1-Diacetoxy C2	C6H10O4	438.80	326.57	45.972
2392	n-PropylBenzoate	C10H12O2	501.81	365.61	48.498
2387	Dimethyl Maleate	C6H8O4	447.00	331.69	46.296
2377	DiMth Phthalate	C10H10O4	542.81	401.92	55.756
2386	Diethyl Maleate	C8H12O4	485.45	361.58	51.02
2385	Mth Dodecanoate	C13H26O2	531.53	391.42	53.468
3379	Dioctyl Adipate	C22H42O4	637.33	497.71	81.8
5886	Mth Acetoacetate	C5H8O3	421.12	305.88	40.244
5884	Ethoxy Acetate	C6H12O3	424.83	307.78	40.223
5887	EthAcetoAcetate	C6H10O3	443.83	322.77	42.606
5885	Carbitol Acetate	C8H16O4	481.35	352.94	47.637

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	**Ketones Name**	**Formula**	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1096	Methyl Isopropen	C5H8O	371.80	260.23	31.225
1079	Cyclopentanone	C5H8O	387.62	269.92	32.006
1051	Acetone	C3H6O	305.37	218.23	27.534

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1052	MEK	C4H8O	343.82	243.14	29.896
1065	Mesityl Oxide	C6H10O	401.75	284.93	35.281
1066	T-But Mth Ketone	C6H12O	383.24	269.29	32.61
1060	2-Pentanone	C5H10O	376.17	264.93	32.258
1061	Mth iC3 Ketone	C5H10O	364.41	256.72	31.276
1053	Diethyl Ketone	C5H10O	385.58	268.26	31.744
1059	3-Hexanone	C6H12O	412.32	287.27	34.106
1099	Diketene	C4H4O2	333.23	240.84	31.277
1055	Sec-ButMthKetone	C6H12O	393.87	277.06	33.638
1054	MIBK	C6H12O	393.87	277.06	33.638
1095	EthIsopropKetone	C6H12O	402.52	280.00	33.124
1063	2-Heptanone	C7H14O	428.65	302.44	36.982
1064	5-Mth-2-Hexanone	C7H14O	419.62	295.57	36
1058	4-Heptanone	C7H14O	435.97	304.78	36.468
1057	3-Heptanone	C7H14O	435.97	304.78	36.468
1076	2,4-Pentanedione	C5H8O2	426.38	303.53	37.93
1068	DiisobutylKetone	C9H18O	461.86	324.36	39.228
1097	2-CycC6 CycC6one	C12H20O	515.88	373.26	48.612
1083	2-Octanone	C8H16O	450.58	319.03	39.344
1073	Dibutyl Ketone	C9H18O	476.36	336.32	41.192
1062	2-Hexanone	C6H12O	404.09	284.52	34.62
1077	Isophorone	C9H14O	461.59	332.87	42.98
1090	Acetophenone	C8H8O	467.27	329.99	40.443
1080	Cyclohexanone	C6H10O	414.11	288.95	34.422
1074	2-Nonanone	C9H18O	470.37	334.53	41.706

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Alcohol-Ethers Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
2862	2-Butoxyethanol	C6H14O2	458.33	342.10	48.569
4857	butyl carbitol	C8H18O3	507.25	382.47	55.983
2898	2-Chloroethanol	C2H5ClO	400.60	300.37	43.225
2864	Carbitol	C6H14O3	473.03	355.06	51.259
3854	Methyl propasol	C4H10O2	421.97	313.18	43.739
2860	2-Methoxyethanol	C3H8O2	406.63	302.18	42.359
2854	DiacetoneAlcohol	C6H12O2	471.94	350.47	49.027
2861	2-Ethoxyethanol	C4H10O2	413.78	308.84	43.845
2889	HydroxyAcetone	C3H6O2	424.99	315.23	43.951
3856	1tButoxy2Propnol	C7H16O2	455.48	339.38	47.939

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

3858	PROPGLYC2tBUTYL	C7H16O2	452.15	337.90	48.149
4855	2-Propoxyethanol	C5H12O2	437.27	326.14	46.207
4849	Acetovanillone	C9H10O3	569.92	424.31	59.795
5883	Ethyl Lactate	C5H10O3	448.85	340.07	50.521
6883	2-HydroxyEth Acr	C5H8O3	459.80	349.14	52.233
2863	Methyl Carbitol	C5H12O3	453.50	339.97	48.897
3855	Dowanol DPM	C7H16O3	502.75	377.39	54.497
3857	TriPropGlymEthlE	C10H22O4	555.80	423.83	64.273

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Hydrocarbons Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
404	DiMth-Acetylene	C4H6	300.18	205.25	23.37
202	Propylene	C3H6	200.86	150.43	21.575
412	2-Pentyne	C5H8	400.91	271.99	30.456
207	2-Methylpropene	C4H8	255.46	182.91	23.191
204	1-Butene	C4H8	261.46	187.66	23.937
205	Cis-2-Butene	C4H8	263.02	187.62	23.566
402	Propyne	C3H4	241.32	175.34	23.09
406	3-Hexyne	C6H10	372.51	252.14	28.094
206	Trans-2-Butene	C4H8	263.02	187.62	23.566
407	2-Hexyne	C6H10	372.51	252.14	28.094
231	33-2Mth-1-Butene	C6H12	317.93	222.40	26.651
230	23-2Mth-1-Butene	C6H12	328.22	228.12	26.933
229	2-Ethyl-1-Butene	C6H12	342.18	237.40	27.915
8	I-Pentane	C5H12	292.98	207.49	25.604
14	2,2-DiMth-Butane	C6H14	319.19	223.74	26.938
232	23-2Mth-2-Butene	C6H12	346.35	239.61	27.994
213	3-Mth-1-Butene	C5H10	291.55	206.10	25.317
212	2-Mth-1-Butene	C5H10	303.38	212.53	25.553
211	Trans-2-Pentene	C5H10	309.39	216.41	25.928
210	Cis-2-Pentene	C5H10	309.39	216.41	25.928
223	4-Mth-1-Pentene	C6H12	332.44	232.08	27.679
221	2-Mth-1-Pentene	C6H12	342.18	237.40	27.915
248	2-t-Butylpropene	C7H14	350.49	242.31	28.267
227	Cs-4-Mth-2-C5H10	C6H12	333.54	231.66	27.308
224	2-Mth-2-Pentene	C6H12	344.12	242.60	29.609
403	1-Butyne	C4H6	292.28	206.78	25.452
15	2,3-DiMth-Butane	C6H14	319.03	223.77	26.984

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

214	2-Mth-2-Butene	C5H10	305.73	217.75	27.247
228	Ts-4-Mth-2-C5H10	C6H12	333.54	231.66	27.308
225	Cs-3-Mth-2-C5H10	C6H12	344.12	242.60	29.609
218	Trans-2-Hexene	C6H12	347.15	240.77	28.29
2226	3-METH-Tr-2Pente	C6H12	344.12	242.60	29.609
222	3-Mth-1-Pentene	C6H12	332.44	232.08	27.679
257	2-Diisobutylene	C8H16	383.48	268.70	32.323
256	1-Diisobutylene	C8H16	381.88	263.56	30.629
217	Cis-2-Hexene	C6H12	347.15	240.77	28.29
2414	1-Heptyne	C7H12	396.12	275.40	32.538
13	3-Methylpentane	C6H14	333.61	233.37	27.966
219	Cis-3-Hexene	C6H12	347.15	240.77	28.29
12	2-Methylpentane	C6H14	333.61	233.37	27.966
220	Trans-3-Hexene	C6H12	347.15	240.77	28.29
405	1-Pentyne	C5H8	333.04	232.71	27.814
209	1-Pentene	C5H10	308.15	216.72	26.299
11	N-Hexane	C6H14	347.22	242.49	28.948
235	Cis-2-Heptene	C7H14	379.02	262.26	30.652
249	Cis-3-Heptene	C7H14	379.02	262.26	30.652
216	1-Hexene	C6H12	346.12	241.23	28.661
239	3-Eth-1-Pentene	C7H14	366.50	254.64	30.041
226	4-Mth-1-Hexene	C7H14	366.50	254.64	30.041
240	3-Mth-1-Hexene	C7H14	366.50	254.64	30.041
419	3-Mth-1-Butyne	C5H8	318.42	223.09	26.832
233	2-Eth-1-Pentene	C7H14	374.77	259.23	30.277
238	2-Mth-1-Hexene	C7H14	374.77	259.23	30.277
416	1-Octyne	C8H14	421.60	293.81	34.9
289	2,3Dimeth Hexene	C8H16	392.59	271.40	31.657
234	1-Heptene	C7H14	378.14	262.80	31.023
413	1-Hexyne	C6H10	367.00	255.23	30.176
237	Trans-3-Heptene	C7H14	379.02	262.26	30.652
236	Trans-2-Heptene	C7H14	379.02	262.26	30.652
251	Trans-2-Octene	C8H16	406.58	281.68	33.014
279	Trans-4-Octene	C8H16	406.58	281.68	33.014
277	Trans-3-Octene	C8H16	406.58	281.68	33.014
2252	2Methl-1-Heptene	C8H16	402.87	278.91	32.639
250	1-Octene	C8H16	405.81	282.27	33.385
258	2-Ethyl-1-Hexene	C8H16	402.87	278.91	32.639
280	3-Octene	C8H16	406.58	281.68	33.014
278	4-Octene	C8H16	406.58	281.68	33.014
276	2-Octene	C8H16	406.58	281.68	33.014
259	1-Nonene	C9H18	430.18	300.13	35.747
262	1-Dodecene	C12H24	489.56	346.83	42.833
263	1-Tridecene	C13H26	506.05	360.65	45.195
264	1-Tetradecene	C14H28	521.31	373.79	47.557

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

265	1-Pentadecene	C15H30	535.52	386.30	49.919
266	1-Hexadecene	C16H32	548.79	398.27	52.281
267	1-Octadecene	C18H36	573.01	420.74	57.005
281	1-Heptadecene	C17H34	561.26	409.73	54.643
284	1-Eicosene	C20H40	594.66	441.52	61.729
283	1-Nonadecene	C19H38	584.12	431.32	59.367
3	Propane	C3H8	203.08	152.18	21.862
4	I-Butane	C4H10	242.22	176.13	23.242
9	Neopentane	C5H12	275.25	196.15	24.576
5	N-Butane	C4H10	263.12	189.14	24.224
7	pentane	C5H12	309.46	218.07	26.586
44	Hexamethylethane	C8H18	363.14	252.02	29.652
25	223-TriMthButane	C7H16	342.27	238.49	28.318
24	3,3-DiMthPentane	C7H16	355.34	247.33	29.3
51	2,2,3,3-4Mth-C5	C9H20	392.77	272.43	32.014
21	2,2-DiMthPentane	C7H16	355.34	247.33	29.3
42	2,3,3-TriMth-C5	C8H18	374.85	260.33	30.68
22	2,3-DiMthPentane	C7H16	355.20	247.39	29.346
40	2,2,3-TriMth-C5	C8H18	374.85	260.33	30.68
23	2,4-DiMthPentane	C7H16	355.20	247.39	29.346
41	2,2,4-TriMth-C5	C8H18	374.85	260.33	30.68
39	3-Mth-3-Eth-C5	C8H18	386.04	268.27	31.662
20	3-Ethylpentane	C7H16	367.49	255.86	30.328
52	2,2,3,4-4Mth-C5	C9H20	392.66	272.50	32.06
54	2334TetrMethPent	C9H20	392.66	272.50	32.06
53	2,2,4,4-4Mth-C5	C9H20	392.77	272.43	32.014
43	2,3,4-TriMth-C5	C8H18	374.73	260.39	30.726
36	3,3-DiMth-Hexane	C8H18	386.04	268.27	31.662
19	3-Methylhexane	C7H16	367.49	255.86	30.328
18	2-Methylhexane	C7H16	367.49	255.86	30.328
38	2-Mth-3-Eth-C5	C8H18	385.92	268.33	31.708
190	2,2-2C1-3-C2-C5	C9H20	402.94	280.00	33.042
32	2,2-DiMth-Hexane	C8H18	386.04	268.27	31.662
37	3,4-DiMth-Hexane	C8H18	385.92	268.33	31.708
50	3,3-DiEthPentane	C9H20	412.73	287.26	34.024
34	2,4-DiMth-Hexane	C8H18	385.92	268.33	31.708
33	2,3-DiMth-Hexane	C8H18	385.92	268.33	31.708
17	N-Heptane	C7H16	379.07	263.99	31.31
49	244TriMethHexane	C9H20	402.94	280.00	33.042
192	2,4-2C1-3-C2-C5	C9H20	402.84	280.07	33.088
47	2,2,5-TriMth-C6	C9H20	402.94	280.00	33.042
35	2,5-DiMth-Hexane	C8H18	385.92	268.33	31.708
31	3-Ethylhexane	C8H18	396.54	275.99	32.69
30	4-Methylheptane	C8H18	396.54	275.99	32.69
29	3-Methylheptane	C8H18	396.54	275.99	32.69

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

28	2-Methylheptane	C8H18	396.54	275.99	32.69
96	2,2-DiMthHeptane	C9H20	412.73	287.26	34.024
176	2,6-DiMthHeptane	C9H20	412.63	287.33	34.07
27	N-Octane	C8H18	406.63	283.40	33.672
94	3-Ethylheptane	C9H20	421.97	294.37	35.052
92	3-Methyloctane	C9H20	421.97	294.37	35.052
93	4-Methyloctane	C9H20	421.97	294.37	35.052
91	2-Methyloctane	C9H20	421.97	294.37	35.052
72	2,2-DiMthOctane	C10H22	436.33	304.75	36.386
2095	2,3Dimethloctane	C10H22	436.24	304.82	36.432
2096	2,4Dimethloctane	C10H22	436.24	304.82	36.432
2098	2,6DimethlOctane	C10H22	436.24	304.82	36.432
2097	2,5Dimethloctane	C10H22	436.24	304.82	36.432
2099	2,7DimethlOctane	C10H22	436.24	304.82	36.432
46	N-Nonane	C9H20	430.90	301.21	36.034
88	5-Methylnonane	C10H22	444.58	311.36	37.414
85	3-Methylnonane	C10H22	444.58	311.36	37.414
87	4-Methylnonane	C10H22	444.58	311.36	37.414
86	2-Methylnonane	C10H22	444.58	311.36	37.414
56	N-Decane	C10H22	452.60	317.74	38.396
63	N-Undecane	C11H24	472.21	333.21	40.758
64	N-Dodecane	C12H26	490.10	347.78	43.12
65	N-Tridecane	C13H28	506.55	361.56	45.482
66	N-Tetradecane	C14H30	521.78	374.66	47.844
67	N-Pentadecane	C15H32	535.95	387.15	50.206
68	N-Hexadecane	C16H34	549.20	399.08	52.568
69	N-Heptadecane	C17H36	561.64	410.51	54.93
70	N-Octadecane	C18H38	573.37	421.49	57.292
71	N-Nonadecane	C19H40	584.46	432.05	59.654
73	N-Eicosane	C20H42	594.99	442.22	62.016
74	n-HENEICOSANE	C21H44	604.99	452.04	64.378
75	n-DOCOSANE	C22H46	614.53	461.52	66.74
76	n-TRICOSANE	C23H48	623.64	470.69	69.102
77	n-Tetracosane	C24H50	632.37	479.57	71.464
78	n-PENTACOSANE	C25H52	640.73	488.18	73.826
79	n-HEXACOSANE	C26H54	648.77	496.53	76.188
81	n-Octacosane	C28H58	663.96	512.53	80.912
2081	n-TRICONTANE	C30H62	678.09	527.65	85.636
2082	n-Dotriacontane	C32H66	691.31	542.01	90.36

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Cyclic Hydrocarbons Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
269	Cyclopentene	C5H8	312.34	221.92	27.599
270	Cyclohexene	C6H10	349.61	246.31	30.015
287	3MthCyclopentene	C6H10	336.17	238.97	29.758
286	1-MthCyclPentene	C6H10	346.61	245.82	30.436
288	4MthCyclopenten	C6H10	336.17	238.97	29.758
273	Cycloheptene	C7H12	381.13	267.81	32.431
274	Cyclooctene	C8H14	408.42	287.22	34.847
101	Cyclopropane	C3H6	208.03	155.41	22.124
810	ADAMANTANE	C10H16	423.63	303.25	38.424
102	Cyclobutane	C4H8	266.82	191.75	24.54
104	Cyclopentane	C5H10	312.42	220.43	26.956
137	Cyclohexane	C6H12	349.68	244.76	29.372
105	MthCyclopentane	C6H12	336.24	237.49	29.115
146	Cs-1,4-2C1-CycC6	C8H16	387.96	274.25	33.69
142	Cs-1,2-2C1-CycC6	C8H16	387.96	274.25	33.69
141	1,1-2C1-CycC6	C8H16	388.07	277.38	35.015
145	Ts-1,3-2C1-CycC6	C8H16	387.96	274.25	33.69
144	Cs-1,3-2C1-CycC6	C8H16	387.96	274.25	33.69
147	Ts-1,4-2C1-CycC6	C8H16	387.96	274.25	33.69
143	Ts-1,2-2C1-CycC6	C8H16	387.96	274.25	33.69
138	MthCyclohexane	C7H14	369.71	259.96	31.531
159	Cycloheptane	C7H14	381.18	266.23	31.788
140	Ethylcyclohexane	C8H16	398.47	279.96	33.893
154	Trans-Decalin	C10H18	439.41	311.97	38.73
149	N-PropylCyc-C6	C9H18	423.68	298.20	36.255
109	Cs-1,2-2C1-CycC5	C7H14	357.57	253.29	31.274
110	Ts-1,2-2C1-CycC5	C7H14	357.57	253.29	31.274
112	Ts-1,3-2C1-CycC5	C7H14	357.57	253.29	31.274
107	Eth-Cyclopentane	C7H14	369.71	259.83	31.477
114	N-PropCycPentane	C8H16	398.47	279.83	33.839
108	1,1-DiMthCycC5	C7H14	357.70	256.40	32.599
111	Cs-1,3-2C1-CycC5	C7H14	357.57	253.29	31.274
152	N-ButylCycHexane	C10H20	446.11	315.06	38.617
160	Cyclooctane	C8H16	408.47	285.64	34.204
153	Cis-Decalin	C10H18	439.41	311.97	38.73
115	ISOPROPYLCYCLOPENTANE	C8H16	387.96	272.23	32.857
150	Isopropyl-CycC6	C9H18	414.41	291.22	35.273
116	1-C1-1-C2-CycC5	C8H16	388.07	277.26	34.961
122	Butylcyclpentane	C9H18	423.68	298.07	36.201
155	1,1-Bicyclohexyl	C12H22	479.19	343.24	43.562
158	N-Decylcyclo-C6	C16H32	545.18	397.41	52.789

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Aromatic Hydrocarbons Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
307	1,4-Pentadiene	C5H8	306.82	215.36	26.012
306	1-ts3-Pentadiene	C5H8	308.07	215.04	25.641
414	2-Methyl-1-Butenyne	C5H6	327.63	227.44	26.781
305	Cs1,3-Pentadiene	C5H8	308.07	215.04	25.641
309	Isoprene	C5H8	302.03	211.15	25.266
421	1-Pentene-4-yne	C5H6	331.87	231.41	27.527
303	1,3-Butadiene	C4H6	259.80	186.16	23.65
332	1,4-CyclHexadien	C6H8	349.55	240.72	27.84
501	Benzene	C6H6	351.27	249.38	30.956
315	Cyclopentadiene	C5H6	312.27	216.52	25.424
319	Diisopropenyl	C6H10	337.00	232.20	26.882
615	Ethynylbezene	C8H6	440.72	305.89	35.999
601	Styrene	C8H8	426.39	295.04	34.484
331	1,3-CycHexadiene	C6H8	349.55	240.72	27.84
310	1,5-Hexadiene	C6H10	345.02	239.96	28.374
312	MthCycPentadiene	C6H8	346.55	242.42	29.051
420	1-Pentene-3-yne	C5H6	338.39	228.82	25.445
502	Toluene	C7H8	386.12	271.04	32.746
521	T-Butylbenzene	C10H14	454.18	316.22	37.485
320	Dipropylene	C6H10	347.09	239.00	27.632
520	Sec-Butylbenzene	C10H14	451.15	318.85	39.147
313	1,4-Hexadiene	C6H10	346.06	239.50	28.003
314	Dipropylene	C6H10	347.09	239.00	27.632
316	DiCycPentadiene	C10H12	423.54	299.67	36.892
333	1,5-CycOctadiene	C8H12	408.37	281.63	32.672
701	Naphthalene	C10H8	484.16	348.65	44.854
504	Ethylbenzene	C8H10	411.37	288.19	34.651
820	Indan	C9H10	438.23	305.04	36.138
505	O-Xylene	C8H10	415.88	290.10	34.536
612	P-Methylstyrene	C9H10	451.14	311.60	36.274
330	DIISOCROTYL	C8H14	401.97	284.36	34.994
507	P-Xylene	C8H10	415.88	290.10	34.536
329	DIISOBUTENYL	C8H14	399.04	274.33	31.606
506	M-Xylene	C8H10	415.88	290.10	34.536
603	Methylstyrene	C9H10	451.14	311.60	36.274
613	Alpha-MthStyrene	C9H10	446.16	308.76	36.1
510	Isopropylbenzene	C9H12	429.29	302.28	36.785
724	2-Methylindene	C10H10	474.37	332.51	40.032
285	Vinylcyclohexene	C8H12	397.57	276.88	32.84
803	Indene	C9H8	465.41	330.06	40.864
706	Tetralin	C10H12	459.20	321.38	38.554
511	O-Ethyltoluene	C9H12	437.89	305.65	36.441
723	1-Methylindene	C10H10	443.75	313.49	38.453
738	Fluorene	C13H10	543.10	390.52	50.048

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

619	Tr-1PropenylBz	C9H10	449.17	311.19	36.475
525	O-Diethylbenzene	C10H14	457.76	320.15	38.346
618	Propenyl Bz(cis)	C9H10	449.17	311.19	36.475
602	O-Methylstyrene	C9H10	451.14	311.60	36.274
702	1-MthNaphthalene	C11H10	503.09	362.36	46.644
509	N-Propylbenzene	C9H12	435.12	305.72	37.013
526	M-Diethylbenzene	C10H14	457.76	320.15	38.346
583	Cs-2-PhnButene-2	C10H12	467.43	329.38	40.156
543	M-DiisopropylBz	C12H18	485.62	344.34	42.614
584	Ts-2-PhnButene-2	C10H12	467.43	329.38	40.156
580	1,2-DiC1-3C2-Bz	C10H14	461.36	321.62	38.231
704	1-EthNaphthalene	C12H12	517.72	362.80	43.653
512	M-Ethyltoluene	C9H12	437.89	305.65	36.441
522	1-Mth-2-iC3-Benz	C10H14	453.71	318.73	38.575
513	P-Ethyltoluene	C9H12	437.89	305.65	36.441
514	1,2,3-Mesitylene	C9H12	441.85	307.28	36.326
614	M-Divinylbenzene	C10H10	481.20	330.54	38.012
524	1-Mth-4-iC3-Benz	C10H14	453.71	318.73	38.575
822	Gamma-Terpinene	C10H16	442.28	315.84	39.777
821	Alpha-Terpinene	C10H16	442.28	315.84	39.777
523	1-Mth-3-iC3-Benz	C10H14	453.71	318.73	38.575
703	2-MthNaphthalene	C11H10	503.09	362.36	46.644
557	CycHexylBenzene	C12H16	490.13	350.37	44.241
515	1,2,4-Mesitylene	C9H12	441.85	307.28	36.326
519	Isobutylbenzene	C10H14	448.53	315.72	38.393
424	DiPhnAcetylene	C14H10	554.95	394.64	49.188
544	P-DiisopropylBz	C12H18	485.62	344.34	42.614
518	N-Butylbenzene	C10H14	456.40	322.01	39.375
516	1,3,5-Mesitylene	C9H12	441.85	307.28	36.326
809	Acenaphthalene	C12H8	538.43	390.76	51.3
725	123-TriMthIndene	C12H14	506.31	360.34	45.002
527	1,4-DiEthBenzene	C10H14	457.76	320.15	38.346
558	Diphenyl	C12H10	516.94	377.14	50.214
576	2-Ethyl-m-Xylene	C10H14	461.36	321.62	38.231
620	p-ISOPROPENYLSTY	C11H12	496.49	342.15	39.628
585	o-PropylToluene	C10H14	458.89	321.85	38.803
577	2-Ethyl-p-Xylene	C10H14	461.36	321.62	38.231
579	4-Ethyl-o-Xylene	C10H14	461.36	321.62	38.231
586	m-Propyltoluene	C10H14	458.89	321.85	38.803
587	p-Propyltoluene	C10H14	458.89	321.85	38.803
578	4-Ethyl-m-Xylene	C10H14	461.36	321.62	38.231
575	5-Ethyl-m-Xylene	C10H14	461.36	321.62	38.231
530	Prehnitene	C10H14	464.90	323.03	38.116
709	2,6-2Mth-Naphtha	C12H12	520.41	375.24	48.434
715	2,7-2Mth-Naphtha	C12H12	520.41	375.24	48.434
719	2-ETHYLNAPHTHALENE	C12H12	517.72	374.08	48.549
621	p-tert-BUTYLSTY	C12H16	502.78	348.82	41.013

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

532	1,2,4,5-TetMthBz	C10H14	464.90	323.03	38.116
531	1,2,3,5-TetMthBz	C10H14	464.90	323.03	38.116
533	p-tert-BUTYL ET	C12H18	503.29	349.81	41.3
567	N-Pentylbenzene	C11H16	475.66	337.27	41.737
718	1-n-PROPYLNAPHTH	C13H14	541.04	391.56	51.031
562	1,1-DiPhnEthane	C14H14	532.73	384.37	49.694
616	4-ISOBUTYLSTYRE	C12H16	508.78	354.37	42.041
260	1-Decene	C10H20	451.94	316.71	38.109
735	Cis-Stilbene	C14H12	544.95	396.04	52.188
568	Hexylbenzene	C12H18	493.27	351.65	44.099
563	Diphenylmethane	C13H12	522.12	374.21	47.56
564	1,2-DiPhnEthane	C14H14	527.18	381.70	49.802
804	Anthracene	C14H10	564.01	419.14	58.752
736	Trans-Stilbene	C14H12	544.95	389.99	49.384
805	Phenanthrene	C14H10	564.01	419.14	58.752
713	1-ButNaphthalene	C14H16	545.65	398.64	53.273
807	Pyrene	C16H10	602.25	455.47	67.29
261	1-Undecene	C11H22	471.62	332.22	40.471
581	23-2C1-23-2PhnC4	C18H22	575.12	418.78	55.47
549	N-Heptylbenzene	C13H20	509.48	365.26	46.461
710	1-PhnNaphthalene	C16H12	586.75	441.33	64.112
566	2,4-Diphenyl-4-M	C18H20	581.96	424.41	56.447
561	O-Terphenyl	C18H14	607.21	461.86	69.472
569	N-Octylbenzene	C14H22	524.50	378.21	48.823
565	Triphenylmethane	C19H16	606.24	448.32	61.969
714	N-C6-Naphthalene	C16H20	570.22	421.14	57.997
717	Fluoranthene	C16H10	602.25	455.47	67.29
716	1-Hexyl-Tetralin	C16H24	564.58	413.57	55.675
731	TriPhnEthylene	C20H16	618.42	462.37	65.974
806	Chrysene	C18H12	621.29	475.02	72.65
588	1,1,2TriPhenEth	C20H18	615.73	457.92	64.331
711	1-n-NonylNaphtha	C19H26	602.30	451.76	65.083
570	N-Nonylbenzene	C15H24	538.48	390.55	51.185
712	1-Decyl Naphtha	C20H28	611.96	461.27	67.445
559	P-Terphenyl	C18H14	607.21	461.86	69.472
560	M-Terphenyl	C18H14	607.21	461.86	69.472
589	TetraPhenylMetha	C25H20	660.92	517.68	86.004
554	Decylbenzene	C16H26	551.58	402.35	53.547
732	TetraPhnEthylene	C26H20	673.41	524.28	85.238
574	N-Dodecylbenzene	C18H30	575.49	424.53	58.271
571	N-Undecylbenzene	C17H28	563.88	413.66	55.909
572	Tridecylbenzene	C19H32	586.47	434.98	60.633
573	n-TETRADECYLBENZ	C20H34	603.39	448.88	63.115
2575	n-PENTADECYLBENZ	C21H36	613.00	458.46	65.477
2576	n-HEXADECYLBENZ	C22H38	622.18	467.73	67.839
2577	n-HEPTADECYLBENZ	C23H40	630.97	476.70	70.201
2578	n-OCTADECYLBENZE	C24H42	639.39	485.39	72.563

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	Halocarbons Name	Formula	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1544	Allyl Chloride	C3H5Cl	318.27	226.69	28.369
1595	2-Chloropropene	C3H5Cl	302.01	217.27	27.879
1531	3-Chloropropyne	C3H3Cl	342.02	242.21	29.884
1535	T-Butyl Chloride	C4H9Cl	323.75	224.75	26.462
1583	Chloroprene	C4H5Cl	339.91	241.32	29.954
1530	Isopropyl Cl	C3H7Cl	306.17	213.60	25.438
1572	O-DiCl-Benzene	C6H4Cl2	448.51	317.98	39.342
1585	Propyl Chloride	C3H7Cl	319.52	227.99	28.656
1684	Isopropyl Iodide	C3H7I	367.76	257.37	30.871
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	409.88	296.79	38.729
1651	2-Bromopropane	C3H7Br	330.19	230.73	27.578
1691	Iodobenzene	C6H5I	469.30	330.02	40.038
1860	Fluorobenzene	C6H5F	351.80	250.14	31.17
1571	Chlorobenzene	C6H5Cl	405.62	286.55	35.149
1680	Bromobenzene	C6H5Br	447.28	310.98	36.745
1526	1,2-DiCl-Propane	C3H6Cl2	384.02	268.74	32.232
1683	Propyl Iodide	C3H7I	379.33	265.49	31.853
1576	Benzotrichloride	C7H5Cl3	487.29	344.69	42.408
1536	2,3-DICHLOROBUT	C4H8Cl2	402.52	275.34	31.376
2638	2-Bromobutane	C4H9Br	364.59	253.46	29.94
1586	1-Chlorobutane	C4H9Cl	355.61	251.71	31.018
1573	M-DiCl-Benzene	C6H4Cl2	448.51	317.98	39.342
2634	Benzotrifluoride	C7H5F3	413.44	280.60	31.444
1574	P-DiCl-Benzene	C6H4Cl2	448.51	317.98	39.342
1650	1-Bromopropane	C3H7Br	344.02	239.95	28.56
1587	2-Chlorobutane	C4H9Cl	344.48	238.20	27.8
2653	8F-2-Butene	C4F8	325.76	245.23	35.714
1678	M-Dibromobenzene	C6H4Br2	512.34	357.35	42.534
1537	1,2-DiCl-Butane	C4H8Cl2	410.96	287.84	34.594
1597	34-DiCl-1-Butene	C4H6Cl2	410.16	286.73	34.307
1577	O-Chlorotoluene	C7H7Cl	432.84	304.41	36.939
1532	123-3Cl-Propane	C3H5Cl3	440.26	313.09	39.026
1578	P-Chlorotoluene	C7H7Cl	432.84	304.41	36.939
1562	Benzyl Chloride	C7H7Cl	454.35	320.57	39.203
2661	P-Bromotoluene	C7H7Br	469.75	326.46	38.535
1508	1,4-DiCl-Butane	C4H8Cl2	419.05	299.53	37.812
1655	1-Bromobutane	C4H9Br	376.34	261.67	30.922
1599	BenzylDichloride	C7H6Cl2	474.68	336.41	41.584
2652	Perfluoropropane	C3F8	236.90	165.73	19.863
1505	2-Butylene DiCl	C4H6Cl2	401.54	286.37	35.948
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	419.01	298.00	37.154
1588	1-Chloropentane	C5H11Cl	386.28	272.67	33.38

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

2654	OctaF-CycButane	C4F8	182.79	143.51	24.048
1592	1,2,4-TriCl-Bz	C6H3Cl3	483.94	345.61	43.535
1579	2,4-2Cl-Toluene	C7H6Cl2	470.85	333.42	41.132
2593	1,3,5-TriCl-BZ	C6H3Cl3	483.94	345.61	43.535
1697	1-Br-Naphthalene	C10H7Br	539.80	378.85	45.747
1622	Perfluorobutane	C4F10	272.77	188.99	22.156
1857	P-Cl-Benzo-TriF	C7H4ClF3	454.88	311.65	35.637
1509	1,5-DiCl-Pentane	C5H10Cl2	441.97	316.57	40.174
1589	1-Cl-Naphthalene	C10H7Cl	514.32	373.35	49.047
1864	Perfluorobenzene	C6F6	354.43	253.92	32.24
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	489.31	339.25	39.83
1667	1-Bromoheptane	C7H15Br	450.69	315.84	38.008
1575	HexaCl-Benzene	C6Cl6	563.72	413.98	56.114
2640	Freon 123B1	C2HBrClF3	386.64	260.67	28.809
1504	Vinyl Chloride	C2H3Cl	262.75	186.59	23.176
1672	1,1-DiBr-Ethane	C2H4Br2	391.49	271.55	31.914
1580	Acetylene DiCl	C2H2Cl2	344.24	235.25	26.752
1692	Diiodomethane	CH2I2	431.30	304.09	37.12
1698	Bromoform	CHBr3	438.58	305.50	36.25
2687	Freon 13B1	CBrF3	280.08	194.38	22.871
2690	Br-3F-Ethylene	C2BrF3	304.39	228.31	32.889
1649	Tetrabromoethane	C2H2Br4	504.46	357.84	44.328
2686	Freon 12B1	CBrClF2	330.67	238.52	30.817
1503	Ethyl Chloride	C2H5Cl	275.66	200.12	26.294
2641	Br-TriCl-Methane	CBrCl3	404.25	282.65	33.835
1641	Methyl Bromide	CH3Br	258.27	185.79	23.836
2688	Freon 12B2	CBr2F2	363.09	254.06	30.465
2545	2,3-DiCl-Propene	C3H4Cl2	369.32	258.44	30.994
1673	1,2-DiBr-Ethane	C2H4Br2	401.83	279.08	32.896
2637	Dibromomethane	CH2Br2	373.57	259.33	30.534
1542	TetraCl-Ethylene	C2Cl4	449.42	333.86	46.746
1541	TriCl-Ethylene	C2HCl3	401.79	297.58	41.311
1527	111-TriCl-Ethane	C2H3Cl3	347.23	243.87	29.499
1612	Cl-2F-Ethylene	C2HClF2	244.38	176.98	23.107
1617	Ethyl Fluoride	C2H5F	148.02	123.05	26.26
2639	Br-Cl-Methane	CH2BrCl	352.54	249.25	30.63
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	344.24	235.25	26.752
1682	Ethyl Iodide	C2H5I	347.52	244.00	29.491
1522	1,1-DiCl-Ethane	C2H4Cl2	321.39	228.98	28.675
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	210.83	155.25	21.204
1525	Hexachloroethane	C2Cl6	452.61	320.41	39.498
1528	1112-4Cl-Ethane	C2H2Cl4	412.94	292.93	36.293
1590	Penta-Cl-Ethane	C2HCl5	437.57	310.91	38.674
1529	1122-4Cl-Ethane	C2H2Cl4	421.34	300.79	37.85
2693	Perfluoroethane	C2F6	193.37	138.49	17.57

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1611	Freon 114B2	C2Br2F4	383.21	269.64	32.758
2692	Cl-PentaF-Ethane	C2ClF5	237.97	167.19	20.239
2655	122-3Cl-112-3FC2	C2Cl3F3	320.75	227.99	28.387
1609	12-2Cl-1122-4FC2	C2Cl2F4	274.57	191.80	22.908
2526	1,1-DiCl-Propane	C3H6Cl2	357.18	252.54	31.037
1645	Ethyl Bromide	C2H5Br	305.61	215.22	26.198
2658	1112-4Cl-22-2FC2	C2Cl4F2	382.39	265.32	31.203
1619	111-3F-Ethane	C2H3F3	159.02	121.49	18.535
1524	1,1,2-3Cl-Ethane	C2H3Cl3	394.54	281.71	35.469
1640	1,1-DiF-Ethane	C2H4F2	82.98	71.95	19.481
2691	Genetron 1113	C2ClF3	259.93	202.83	33.241
2694	Vinyl Bromide	C2H3Br	304.27	213.85	25.911
1694	Refrigerant 123	C2HCl2F3	337.62	234.67	27.71
1523	1,2-DiCl-Ethane	C2H4Cl2	363.67	260.56	33.088
2656	1122-4Cl-12-2FC2	C2Cl4F2	358.39	259.51	33.866
2527	1,3-DiCl-Propane	C3H6Cl2	393.23	281.00	35.45

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

DipID	**Acids Name**	**Formula**	$T_{b,Gani}^{760mmHg}$	$T_{b,Gani}^{10mmHg}$	ΔH_{Gani}^{298}
1277	Acrylic Acid	C3H4O2	414.91	294.14	36.385
1274	Ts-Crotonic Acid	C4H6O2	423.15	300.13	37.17
1279	Oleic Acid	C18H34O2	626.81	476.34	71.444
1278	Methacrylic Acid	C4H6O2	423.24	300.07	37.124
2271	Cinnamic Acid	C9H8O2	538.60	390.82	51.285
1266	n-UNDECANOIC ACI	C11H22O2	553.76	407.53	55.568
1282	O-Toluic Acid	C8H8O2	526.43	379.61	49.009
2283	IBUPROFEN	C13H18O2	586.09	430.75	58.518
1261	Isovaleric Acid	C5H10O2	452.14	322.31	40.414
1264	1,4-CychexDicarboxAcid	C8H12O4	573.68	432.56	63.31
1283	P-Toluic Acid	C8H8O2	526.43	379.61	49.009
1257	3-MthButyricAcid	C5H10O2	452.14	322.31	40.414
1288	Isophthalic Acid	C8H6O4	597.78	446.42	63.482
2871	4CarboxAcidBzldhyde	C8H6O3	562.16	414.37	2.871
1256	N-Butyric Acid	C4H8O2	438.97	312.45	1.256
1276	Stearic Acid	C18H36O2	626.82	477.39	1.276

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

1285	Adipic Acid	C6H10O4	558.23	415.60	1.285
1273	Cs-Crotonic Acid	C4H6O2	438.93	310.90	1.273
4851	Diglycolic Acid	C4H6O5	542.43	403.15	4.851
1286	Maleic Acid	C4H4O4	532.04	391.16	1.286
2277	Citraconic Acid	C5H6O4	531.09	390.89	2.277
2278	Itaconic Acid	C5H6O4	543.67	401.29	2.278
2281	Glutaric Acid	C5H8O4	545.57	404.28	2.281
1271	TetradecylicAcid	C14H28O2	588.31	439.67	1.271
1259	N-Nonanoic Acid	C9H18O2	526.99	383.77	1.259
1280	Linoleic Acid	C18H32O2	626.79	475.27	1.28
1260	Isobutyric Acid	C4H8O2	430.39	305.84	1.26
2268	Fumaric Acid	C4H4O4	522.18	383.47	2.268
1287	Phthalic Acid	C8H6O4	597.78	446.42	1.287
1289	TerephthalicAcid	C8H6O4	597.78	446.42	1.289
2280	Succinic Acid	C4H6O4	532.07	392.44	2.28
1270	Tridecanoic Acid	C13H26O2	577.43	429.37	1.27
1254	N-Decanoic Acid	C10H20O2	540.81	395.92	1.254
2270	Suberic Acid	C8H14O4	581.41	436.90	2.27
2255	Linolenic Acid	C18H30O2	626.78	474.18	2.255
1262	N-Hexanoic Acid	C6H12O2	478.83	343.49	1.262
4852	Levulinic Acid	C5H8O3	494.54	358.80	4.852
2275	Sebacic Acid	C10H18O4	602.23	456.65	2.275
1255	Oxalic Acid	C2H2O4	502.07	367.00	1.255
2259	PentadecylicAcid	C15H30O2	598.64	449.59	2.259
2266	NonadecanoicAcid	C19H38O2	635.42	486.07	2.266
2269	Pimelic Acid	C7H12O4	570.15	426.46	2.269
1252	Acetic Acid	C2H4O2	389.42	276.44	1.252
3268	Malonic Acid	C3H4O4	517.62	380.04	3.268
2279	2-EthButyricAcid	C6H12O2	471.79	337.69	2.279
1265	N-Octanoic Acid	C8H16O2	512.16	371.03	1.265
2258	NeopentanoicAcid	C5H10O2	444.19	315.91	2.258
2257	Azelaic Acid	C9H16O4	592.09	446.96	2.257
1281	Benzoic Acid	C7H6O2	509.64	367.01	1.281
1269	Dodecanoic Acid	C12H24O2	565.94	418.67	1.269
2261	Heptanoic Acid	C7H14O2	496.17	357.64	2.261
1258	N-Valeric Acid	C5H10O2	459.87	328.48	1.258
2265	HeptadecylicAcid	C17H34O2	617.85	468.43	2.265

Table D.3 Boiling Temperatures and Heats of Vaporization by the Gani Method (Continued)

2267	N-Eicosanic Acid	C20H40O2	643.66	494.49	2.267
1253	Propionic Acid	C3H6O2	415.69	295.21	1.253
5877	Ascorbic Acid	C6H8O6	611.69	469.01	5.877
1272	HexadecanoicAcid	C16H32O2	608.47	459.17	1.272

APPENDIX E.

VAPOR PRESSURES CALCUATED BY THE METHODS

GIVEN IN CHAPTER IV

Table E. 1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations

Alcohols

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1181	Phenol	C6H6O	379.3825	4.8132
1182	O-Cresol	C7H8O	735.7483	13.0035
1183	M-Cresol	C7H8O	483.8041	6.1873
1176	2,6-Xylenol	C8H10O	897.0898	21.0740
1111	2-Mth-2-Butanol	C5H12O	1727.9080	13.2565
1178	3,5-Xylenol	C8H10O	925.4799	12.2380
1133	2-Octanol	C8H18O	1898.3891	19.9384
2885	4-HYDROXYSTYREN	C8H8O	773.2575	7.6719
1197	P-t-Butylphenol	C10H14O	619.9656	7.7228
1172	2,4-Xylenol	C8H10O	519.0843	8.9505
1184	P-Cresol	C7H8O	697.0422	8.2126
1151	Cyclohexanol	C6H12O	927.7405	6.3862
1170	2,3-Xylenol	C8H10O	638.2564	9.9999
1187	P-Ethyl Phenol	C8H10O	507.7102	6.9647
2859	P-Methoxyphenol	C7H8O2	316.1799	2.3318
1121	2-Ethylhexanol	C8H18O	971.7686	8.9787

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1179	PropargylAlcohol	C3H4O	299.9520	2.7377
1123	3-Mth-1-Butanol	C5H12O	601.7349	3.5138
2196	P-t-Amylphenol	C11H16O	469.0062	6.8102
1174	2,5-Xylenol	C8H10O	760.0188	13.9863
1115	2-Hexanol	C6H14O	1177.7313	10.9074
1152	1-MthCycHexanol	C7H14O	1139.5280	20.9310
4854	Guaiacol	C7H8O2	1519.7930	30.9306
1107	Sec-Butanol	C4H10O	1295.0786	8.2968
1167	Allyl Alcohol	C3H6O	313.2739	1.9477
1130	4-Mth-2-Pentanol	C6H14O	968.2150	11.5354
1177	3,4-Xylenol	C8H10O	590.1724	7.3933
1114	1-Hexanol	C6H14O	464.3676	3.2963
1106	Isobutanol	C4H10O	738.6674	3.4031
1125	1-Heptanol	C7H16O	499.1763	3.7407
1105	N-Butanol	C4H10O	363.7037	1.9647
1109	1-Pentanol	C5H12O	786.1116	5.3341
1132	1-Octanol	C8H18O	600.3388	5.0178
1113	T-Butylcarbinol	C5H12O	759.9998	4.8891
1137	1-Undecanol	C11H24O	961.3723	9.8504
1108	Tert-Butanol	C4H10O	748.4791	3.8578
1103	N-Propanol	C3H8O	369.5088	1.9025
1134	1-Nonanol	C9H20O	464.4353	4.2035
2195	P-t-Octylphenol	C14H22O	870.5594	12.7557
1102	Ethanol	C2H6O	216.5101	1.1096
1124	3-Mth-2-Butanol	C5H12O	592.7389	3.7668
1136	1-Decanol	C10H22O	1167.5826	11.4119
1140	Dodecanol	C12H26O	843.0487	9.2106
1104	Isopropanol	C3H8O	439.3369	2.4974
1110	2-Pentanol	C5H12O	750.8192	5.4698
1120	3-Pentanol	C5H12O	1704.6066	14.9951
1112	2-Mth-1-Butanol	C5H12O	672.3698	3.9735
1154	Ts-2-Mth-CycC6OH	C7H14O	813.7036	9.9966
1153	Cs-2-Mth-CycC6OH	C7H14O	568.0893	7.8814
1156	Ts-3-Mth-CycC6OH	C7H14O	844.0956	6.5717
1157	Cs-4-Mth-CycC6OH	C7H14O	792.8478	6.9214
2197	P-Cumylphenol	C15H16O	774.9449	9.2856
1180	Benzyl Alcohol	C7H8O	688.4663	5.5585
1158	Ts-4-Mth-CycC6OH	C7H14O	695.8938	5.3592
1155	Cs-3-Mth-CycC6OH	C7H14O	668.6995	4.9061
1168	2-Phn-2-Propanol	C9H12O	1313.1428	17.7188
1141	1-Tridecanol	C13H28O	601.4971	6.9507
1147	2-Eth-1-Butanol	C6H14O	816.9131	6.8484
1117	2-Mth-1-Pentanol	C6H14O	474.2520	3.9333

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

2115	2-Phenylethanol	C8H10O	588.4741	6.2340
1142	1-Tetradecanol	C14H30O	432.9330	5.2206
2118	1-PHN-1-PROPANOL	C9H12O	834.2228	11.3879
2119	1-PHN-2-PROPANOL	C9H12O	853.1945	11.2394
1126	2-Heptanol	C7H16O	642.2243	7.4333
1143	1-Pentadecanol	C15H32O	929.6040	10.7794
1129	Isoheptanol	C7H16O	680.8939	5.2078
2117	2,6-DiMth-4-C7OH	C9H20O	1692.6825	19.5585
1144	1-Hexadecanol	C16H34O	709.9339	8.5913
1145	Heptadecanol	C17H36O	597.9416	7.1899
1199	Nonylphenol	C15H24O	991.0353	11.7717
1146	1-Octadecanol	C18H38O	956.0995	11.9278
1135	2-Nonanol	C9H20O	778.6377	10.7389
1149	1-Nonadecanol	C19H40O	1072.5938	13.8406
1139	Isodecanol	C10H22O	1516.5084	13.5307
1148	1-Eicosanol	C20H42O	1316.8228	16.4358
2198	Dinonylphenol	C24H42O	388.3410	3.1646
1159	Menthol	C10H20O	590.2297	4.4338
1202	DiethyleneGlycol	C4H10O3	143.5074	0.8533
1245	1,3-Benzenediol	C6H6O2	137.8084	1.3030
1186	P-Hydroquinone	C6H6O2	121.5123	1.3255
1244	1,2-Benzenediol	C6H6O2	311.6030	8.4273
1219	2MTH,13PROPNDIO	C4H10O2	229.8765	1.5136
1212	1,3-Propanediol	C3H8O2	191.9340	1.3133
1235	P-t-But-Catechol	C10H14O2	775.4739	13.4494
1203	Triglycol	C6H14O4	197.9660	2.0099
1198	Bisphenol A	C15H16O2	1291.3329	7.2406
1238	2,3-Butanediol	C4H10O2	431.7014	3.7367
1211	1,2-Propanediol	C3H8O2	347.0268	2.5347
2219	2,4-PENTANEDIOL	C5H12O2	552.5324	5.5032
1215	1,4-Butynediol	C4H6O2	249.2242	0.0550
1214	Neopentyl Glycol	C5H12O2	436.1154	2.2753
1221	1,3-Butanediol	C4H10O2	219.0167	1.4967
1220	1,2-Butanediol	C4H10O2	407.9263	3.4535
1240	Ts2-C4H8-14-Diol	C4H8O2	150.6771	0.3713
1239	Cis-Butenediol	C4H8O2	280.1254	1.3173
1241	1,4-Butanediol	C4H10O2	176.9968	0.7368
1222	Hexylene Glycol	C6H14O2	957.5519	7.5599
1213	Dipropylene Gly	C6H14O3	679.1575	9.4018
1242	1,5-Pentanediol	C5H12O2	234.0153	1.1641
1243	1,6-Hexanediol	C6H14O2	276.4443	1.9665
1204	TetraC2H4 Glycol	C8H18O5	761.8080	6.9314
6886	C6H4(COOC2H4OH)2	C12H14O6	567.1702	1.4165

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1248	123-Benzenetriol	C6H6O3	325.7461	7.7851
1231	Glycerol	C3H8O3	105.3951	0.5606
1247	Hexaglycerol	C6H14O3	433.3901	2.7226
1246	Pentaerythritol	C5H12O4	67.4703	0.0435

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Amines

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1742	Ethyleneimine	C2H5N	51.8098	0.2893
1745	Piperidine	C5H11N	579.0961	9.0869
2726	Propyleneimine	C3H7N	152.0850	2.0680
1766	Pyrrolidine	C4H9N	395.6201	4.3674
1719	Isopropylamine	C3H9N	1338.9696	10.5508
1711	N-Propylamine	C3H9N	782.2030	10.0006
1726	Sec-Butylamine	C4H11N	759.9951	8.9544
1704	Ethylamine	C2H7N	767.6827	8.2788
1702	Dimethylamine	C2H7N	397.0235	3.8299
1710	Diethylamine	C4H11N	742.5857	9.9692
1740	Allylamine	C3H7N	604.2076	6.1122
1712	N-Butylamine	C4H11N	795.5949	10.4642
1794	HexMthyleneimine	C6H13N	354.0679	3.9598
1729	Cyclohexylamine	C6H13N	713.0353	9.9975
1714	Isobutylamine	C4H11N	783.9255	10.1763
2853	Acetamide	C2H5NO	608.1382	1.0125
2731	N-C1-CycC6-Amine	C7H15N	496.4399	10.7623
1743	Diisopropylamine	C6H15N	1942.2124	24.1996
1796	N,N-DiMthAniline	C8H11N	1567.6741	30.4510
1792	Aniline	C6H7N	625.5934	5.3940
1713	N-Pentylamine	C5H13N	760.0030	10.4879
1733	Benzylamine	C7H9N	797.6318	7.7287
1737	M-Toluidine	C7H9N	1116.4484	10.0000
3796	N-Ethylaniline	C8H11N	302.6296	1.8809
1878	2-Methacrylamide	C4H7NO	1630.2727	10.0000
1736	O-Toluidine	C7H9N	539.5540	5.8710
2739	Diallylamine	C6H11N	632.5811	6.0794
2706	Hexylamine	C6H15N	755.6971	10.4393
2724	O-Ethylaniline	C8H11N	932.6753	10.8935

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1707	Dipropylamine	C6H15N	806.2825	11.4864
1738	P-Toluidine	C7H9N	759.9234	7.5547
1795	N-Methylaniline	C7H9N	245.7235	2.0323
1718	Diisobutylamine	C8H19N	923.8741	13.3602
1879	Acrylamide	C3H5NO	759.9049	1.6237
2707	1-Aminoheptane	C7H17N	727.2955	10.7512
2730	DiCycHexylAmine	C12H23N	690.6108	10.1439
2787	P-Aminodiphenyl	C12H11N	404.1311	3.7102
1744	Dibutylamine	C8H19N	776.5848	10.3854
2708	1-Octylamine	C8H19N	603.4086	8.1307
2791	2,6-DiEthAniline	C10H15N	2190.6971	24.0538
2709	1-Nonylamine	C9H21N	752.9518	10.1197
2710	1-Decylamine	C10H23N	785.8816	9.9162
3722	Diamylamine	C10H23N	757.2077	7.0489
3724	Undecylamine	C11H25N	801.2156	10.3073
2712	Dodecylamine	C12H27N	600.0420	7.3541
1720	Tetradecylamine	C14H31N	525.1484	6.0743
2752	Piperazine	C4H10N2	217.8713	1.9368
1752	Propylenediamine	C3H10N2	567.6542	4.0265
1741	Ethylenediamine	C2H8N2	274.9076	2.1627
2725	O-Aminoaniline	C6H8N2	665.5238	5.1979
2750	P-Aminoaniline	C6H8N2	529.6171	3.5065
2727	M-Aminoaniline	C6H8N2	298.4160	2.3034
1750	AEP	C6H15N3	162.5675	2.4377
1732	Toluene Diamine	C7H10N2	512.8492	3.6710
1731	hexamethyleneDiamine	C6H16N2	463.3890	6.7057
3750	P-Benzidine	C12H12N2	291.4344	1.3792

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Nitriles

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1773	Propionitrile	C3H5N	703.9412	8.2144
1782	Butyronitrile	C4H7N	812.6426	10.0279
2720	Allyl Cyanide	C4H5N	760.4159	8.7412
1783	Valeronitrile	C5H9N	886.0842	11.9580
3874	Benzyl Cyanide	C8H7N	649.4194	6.6518
1786	Hexanenitrile	C6H11N	798.0446	11.0629
1776	Succinonitrile	C4H4N2	156.2453	0.4842
1781	Glutaronitrile	C5H6N2	114.1966	0.7932
2735	14-2Cyano-2-C4H8	C6H6N2	329.5373	1.5015
1777	Adiponitrile	C6H8N2	204.6524	1.1202

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Imines

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1767	N-MthPyrrolidine	C5H11N	357.0342	12.6605
2797	3-Methylpyridine	C6H7N	760.0021	10.0000
1797	2-Methylpyridine	C6H7N	967.2774	15.6986
2799	4-Methylpyridine	C6H7N	518.8541	6.7970
1753	N,N-DiEthAniline	C10H15N	376.6716	3.9141

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Tert-N

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1706	Triethylamine	C6H15N	398.9156	8.0292
2716	Tributylamine	C12H27N	754.5198	10.0001
2719	Tripropylamine	C9H21N	483.0636	5.0096
3723	Triamylamine	C15H33N	1847.5847	26.6016

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Nitrates

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1761	Nitroethane	C2H5NO2	605.3636	6.2626
1763	2-Nitropropane	C3H7NO2	757.1501	9.4704
1762	1-Nitropropane	C3H7NO2	753.0570	9.6718

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Thiols

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1802	Ethyl Mercaptan	C2H6S	930.9385	10.8383
1820	Dimethyl Sulfide	C2H6S	603.5652	7.8716

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1843	Thiacyclopentane	C4H8S	388.9994	4.4215
1803	1-Propanethiol	C3H8S	863.1835	10.1490
1805	Isobut Mercaptan	C4H10S	748.3576	9.1384
6860	Ethylenedithiol	C2H6S2	429.8307	3.5555
1811	Cyclohexanethiol	C6H12S	702.6478	9.0841
1828	DiMth Disulfide	C2H6S2	1112.0971	17.7206
1841	Butanethiol	C4H10S	759.7153	9.2447
1814	Methylproylsulf	C4H10S	807.6456	9.9999
2816	ETHYLtBUTYL SUL	C6H14S	819.1331	9.5149
1818	Diethyl Sulfide	C4H10S	660.7493	7.8189
1812	Benzyl Mercaptan	C7H8S	695.5329	6.8655
1838	T-OctylMercaptan	C8H18S	1217.6812	24.1055
1827	1-Pentanethiol	C5H12S	705.9070	8.2664
2815	METHnBUTYL SULFD	C5H12S	450.8229	6.3285
1824	DiethylDisulfide	C4H10S2	788.3582	9.9999
1807	N-Hexylmercaptan	C6H14S	658.4566	7.8393
6857	Dimercaptoethyl	C4H10OS2	374.5664	3.0862
1839	1-Heptanethiol	C7H16S	666.6209	7.4466
1829	DiProp Disulfide	C6H14S2	759.9630	10.7953
1809	1-Octanethiol	C8H18S	621.4300	6.9878
1808	N-Nonanethiol	C9H20S	462.0229	4.6397
1826	1-Decanethiol	C10H22S	530.2250	5.3936
2838	tertDodecanThiol	C12H26S	993.2907	11.8135
1825	1-Undecanethiol	C11H24S	771.4576	7.3108
1837	Dodecylthiol	C12H26S	398.0495	4.3969

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Aldehydes

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1037	Methacrolein	C4H6O	825.8543	11.4554
1002	Acetaldehyde	C2H4O	679.1135	5.9224
1003	Propionaldehyde	C3H6O	625.2989	6.7821
1041	Benzaldehyde	C7H6O	605.6127	6.8766
1034	Acrolein	C3H4O	400.7943	4.2950
1005	N-Butyraldehyde	C4H8O	819.6004	10.0093
1036	Trans-2-Butenal	C4H6O	285.6745	1.8062
1007	Valeraldehyde	C5H10O	1012.9108	12.3251

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1006	Isobutyraldehyde	C4H8O	752.0938	7.4274
1009	1-Hexanal	C6H12O	681.5860	8.0573
1040	P-Tolualdehyde	C8H8O	674.1107	6.2906
1016	2-Methylhexanal	C7H14O	759.7251	8.6085
1017	3-Methylhexanal	C7H14O	680.4257	9.0345
1008	1-Heptanal	C7H14O	597.7103	7.7316
1013	2-Ethylhexanal	C8H16O	806.7556	9.2785
1010	1-Octanal	C8H16O	687.9994	7.9270
1011	1-Nonanal	C9H18O	1061.8931	11.6265
1020	1-Decanal	C10H20O	844.3883	9.6410
1021	1-Undecanal	C11H22O	970.3743	10.1138
1025	Dodecanal	C12H24O	611.8557	6.8366
1026	1-Tridecanal	C13H26O	497.3398	5.3527
1014	1,2-Ethanedione	C2H2O2	1820.5798	27.7013
1044	1,4BenzDicarboxAldehy	C8H6O2	757.1023	6.2428

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Epoxides

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1440	ISOBUTYLENE OXID	C4H8O	248.9436	4.2572
1478	Furan	C4H4O	755.1815	15.0021
1443	1,3-Propylene Ox	C3H6O	142.9563	2.4876
1479	Tetrahydrofuran	C4H8O	409.5174	5.8974
1477	2,5-Dihydrofuran	C4H6O	832.3096	8.7851
1471	1,2-Epoxybutane	C4H8O	229.6862	4.0547
1408	1-Methoxypropane	C4H10O	730.9455	8.9031
1442	1,2-Propylene Ox	C3H6O	144.8793	2.0903
1411	2-Methoxypropane	C4H10O	759.8250	8.8065
1421	1,4-Dioxane	C4H8O2	262.1027	5.3870
2422	1,3-DIOXANE	C4H8O2	240.9481	4.0394
1426	2-Methoxybutane	C5H12O	807.8864	10.1631
1422	Trioxane	C3H6O3	146.9621	2.0954
1413	1-Methoxybutane	C5H12O	777.7762	10.0000
1461	Methoxybenzene	C7H8O	575.4327	5.7304
1448	1-Ethoxybutane	C6H14O	510.8809	7.1446
1429	1-MethoxyPentane	C6H14O	644.6720	8.2626
6885	Ethyl-3-Ethoxypr	C7H14O3	745.6096	9.7429

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

	Ether			
DipID	**Name**	**Formula**	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1401	Dimethyl Ether	C2H6O	608.2714	5.0562
1407	MethylEthylEther	C3H8O	657.6255	5.8261
1470	VinylMethylEther	C3H6O	712.8367	6.8837
1405	MTBE	C5H12O	671.4340	6.3065
1445	VinylEthyl Ether	C4H8O	668.1191	8.1490
1402	Diethyl Ether	C4H10O	706.9263	9.1643
1431	Methylal	C3H8O2	874.6470	10.6527
1428	T-But EthylEther	C6H14O	805.2800	9.4909
1427	TAME	C6H14O	580.1413	5.8432
1410	Mth Isobut Ether	C5H12O	820.6028	10.4892
1430	Eth-t-Pent-Ether	C7H16O	823.9849	10.9817
1403	DiisopropylEther	C6H14O	962.8419	9.2981
1415	Eth Propyl Ether	C5H12O	810.0692	11.2823
1455	Dimethyl Acetal	C4H10O2	418.7191	3.9692
1446	Dipropyl Ether	C6H14O	847.7391	12.8258
1447	Butyl VinylEther	C6H12O	761.4307	8.9732
1462	EthylPhenylEther	C8H10O	761.2095	7.9596
1406	Di-sec-But Ether	C8H18O	948.1209	9.0822
1432	Acetal	C6H14O2	1498.4257	25.5797
1460	BenzylEthylEther	C9H12O	631.2993	7.8919
1050	Paraldehyde	C6H12O3	757.4072	4.1263
1404	Di-n-Butyl Ether	C8H18O	799.6013	10.9206
1420	Anethole	C10H12O	566.9870	4.6930
1456	DimethylCarbitol	C6H14O3	467.3325	4.5834
1463	Dibenzyl Ether	C14H14O	773.2215	5.3226
1425	Di-n-PentylEther	C10H22O	797.9475	11.4841
1458	Diethyl Carbitol	C8H18O3	760.0035	10.0000
1412	Dihexyl Ether	C12H26O	739.1566	7.2308
1454	Triglyme	C8H18O4	722.6082	6.1172
1459	Dibutyl Carbitol	C12H26O3	747.0062	12.5048
1424	Di-n-Octyl Ether	C16H34O	864.1917	7.6267
1457	Tetraglyme	C10H22O5	595.5812	5.3893
1418	Dinonyl Ether	C18H38O	1163.7827	9.8843
2432	ETHYLAL	C5H12O2	934.1202	16.6490
2405	DIISOBUTYL ETHER	C8H18O	980.9786	14.1229
2456	Ethyl Glyme	C6H14O2	781.3216	9.1330
2417	ETHYLHEXYL ETHER	C8H18O	728.0069	8.4796
2415	ETHYLISOPROPETH	C5H12O	866.5700	6.1884

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Formates

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1301	Methyl Formate	C2H4O2	418.5811	3.2696
1311	Vinyl Formate	C3H4O2	760.1149	7.6718
1302	Ethyl Formate	C3H6O2	585.0913	6.7551
2306	t-Butyl Formate	C5H10O2	850.8477	11.3884
1303	Propyl Formate	C4H8O2	820.3351	9.3344
2305	sec-ButylFormate	C5H10O2	881.2155	12.0394
2311	CYCLOHEXL FORMAT	C7H12O2	984.7236	12.7874
1304	N-Butyl Formate	C5H10O2	1470.7211	18.9597
1305	Isobutyl Formate	C5H10O2	755.7983	9.9999
2350	Benzyl Formate	C8H8O2	669.1164	7.1254
2307	n-Hexyl Formate	C7H14O2	683.3417	7.8335
1306	N-Pentyl Formate	C6H12O2	690.8311	8.7594
2308	n-Heptyl Formate	C8H16O2	542.4387	7.7698
1308	N-Octyl Formate	C9H18O2	682.5713	11.1834
1309	n-Nonyl Formate	C10H20O2	831.9269	10.6033
1310	n-Decyl Formate	C11H22O2	713.0007	8.5799

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Esters

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1351	Mth Methacrylate	C5H8O2	596.0927	7.1044
1312	Methyl Acetate	C3H6O2	504.4695	4.7516
1331	Vinyl Propionate	C5H8O2	673.3318	8.3491
1321	Vinyl Acetate	C4H6O2	760.0019	9.4701
1352	Eth MthAcrylate	C6H10O2	795.5761	12.5542
1322	MethylPropionate	C4H8O2	657.2451	7.2425
1341	Methyl Acrylate	C4H6O2	753.2286	7.4456
1313	Ethyl Acetate	C4H8O2	532.7089	5.5271
1319	IsopropylAcetate	C5H10O2	961.6047	14.0434
1332	Methyl Butyrate	C5H10O2	631.3160	7.2502
1342	Ethyl Acrylate	C5H8O2	695.6869	7.8968
1318	Allyl Acetate	C5H8O2	637.9627	9.6376
1314	N-Propyl Acetate	C5H10O2	806.5127	10.0000
1323	Ethyl Propionate	C5H10O2	831.4927	9.9325

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1360	I-But I-Butyrate	C8H16O2	943.9897	13.3033
1320	Sec-ButylAcetate	C6H12O2	963.9660	14.3609
1336	PropylI-Butyrate	C7H14O2	915.9993	10.4382
1353	N-C3-Mthacrylate	C7H12O2	638.1500	11.7264
1333	Ethyl Butyrate	C6H12O2	781.5888	12.5192
1347	EthylIsovalerate	C7H14O2	853.0758	12.0401
1315	N-Butyl Acetate	C6H12O2	893.3264	11.6114
1390	Methyl Benzoate	C8H8O2	651.8014	7.5630
1388	ISOBUTYL MTHACR	C8H14O2	696.2679	10.3032
1343	1-PropylAcrylate	C6H10O2	760.0051	9.2566
1316	Isobutyl Acetate	C6H12O2	838.2777	11.4322
1344	N-Butyl Acrylate	C7H12O2	626.5299	14.6624
1357	Pentyl Acetate	C7H14O2	683.0919	9.3284
1327	N-PropN-Butyrate	C7H14O2	815.3485	12.1183
1324	N-PropPropionate	C6H12O2	699.9335	9.5367
1291	Acetic Anhydride	C4H6O3	495.9589	5.2717
1389	N-ButMthacrylate	C8H14O2	853.9117	10.6782
1359	Benzyl Acetate	C9H10O2	651.5862	7.1734
1326	N-But Propionate	C7H14O2	742.5966	9.3796
1391	Ethyl Benzoate	C9H10O2	726.0710	9.4147
1897	CH3OC3H600CH3	C6H12O3	754.5399	9.2326
1392	DiethylCarbonate	C5H10O3	630.5963	8.5720
1385	N-But N-Butyrate	C8H16O2	561.3339	8.6098
1317	IsopentylAcetate	C7H14O2	719.2041	10.4750
1363	N-Hexyl Acetate	C8H16O2	716.2330	8.3248
1387	Ethylene Acetate	C6H10O4	681.8103	3.8796
1393	Diethyl Oxalate	C6H10O4	681.3852	7.1614
1365	Butyl Benzoate	C11H14O2	760.0285	8.9797
1361	I-C5 I-Valerate	C10H20O2	767.8705	13.7531
1367	Heptyl Acetate	C9H18O2	722.4925	8.0619
1346	N-Butyl Valerate	C9H18O2	787.5841	10.0000
1358	2-C2-C6 Acetate	C10H20O2	992.9871	14.9942
1394	Diethyl Malonate	C7H12O4	631.1663	6.8223
1292	Propionyl Oxide	C6H10O3	790.9110	11.1739
1364	Benzyl Benzoate	C14H12O2	441.7167	4.1338
1381	2Mth p-Phthalate	C10H10O4	626.0287	9.5318
1368	n-Octyl Acetate	C10H20O2	354.6635	4.0032
1377	DiMthI-Phthalate	C10H10O4	429.1110	6.3696
1896	Ethylene DiAcr	C8H10O4	456.5929	4.2476
1386	2-Ethylhexyl Acr	C11H20O2	893.5894	12.0613
1395	Methyl Decanoate	C11H22O2	679.8920	7.5674
1369	n-Nonyl Acetate	C11H22O2	526.2172	5.7358

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1370	n-Decyl Acetate	C12H24O2	1550.3555	16.4779
1345	N-ButylNonanoate	C13H26O2	1428.5859	33.3459
1375	DiProp Phthalate	C14H18O4	1078.3589	13.3182
1376	Diisobutyl Phtha	C16H22O4	1138.4698	12.9549
1396	IsopropMyristate	C17H34O2	872.5392	9.4236
1383	Butyl Stearate	C22H44O2	1579.1430	24.6413
1362	Methyl Oleate	C19H36O2	460.2715	4.0850
1355	Diisooctyl Phtha	C24H38O4	886.1240	10.0000
1382	DioctylTerephtha	C24H38O4	1981.9393	24.0108
1384	DIBUTYL SEBACATE	C18H34O4	1180.8324	11.0383
1371	Diisodecyl Phtha	C28H46O4	983.2372	18.2180
1354	DioctylPhthalate	C24H38O4	2145.2292	29.2595
2375	DiethylPhthalate	C12H14O4	899.6818	9.5762
2388	Dipropyl Maleate	C10H16O4	863.9436	7.4952
2381	Diallyl Maleate	C10H12O4	537.0909	4.5382
2370	Glyceryl Triacet	C9H14O6	1657.4895	18.0168
2382	Dibutyl Maleate	C12H20O4	601.0138	4.7764
2376	DibutylPhthalate	C16H22O4	712.8928	8.5990
2353	CetylMthacrylate	C20H38O2	670.0157	8.4994
2379	Dihexyl Adipate	C18H34O4	870.1864	9.1052
2321	T-Butyl Acetate	C6H12O2	746.6652	7.9608
2332	Methl.I-butyrate	C5H10O2	683.5160	7.3635
2354	AllylMthacrylate	C7H10O2	900.1905	10.3425
2364	CYCLOHEXL ACETAT	C8H14O2	842.0870	9.9181
2337	EthylIsobutyrate	C6H12O2	951.7756	13.6105
2384	IsobutylAcrylate	C7H12O2	838.6574	10.1812
2380	1,1-Diacetoxy C2	C6H10O4	739.3426	7.3738
2392	n-PropylBenzoate	C10H12O2	947.2163	11.9837
2387	Dimethyl Maleate	C6H8O4	306.7875	1.9424
2377	DiMth Phthalate	C10H10O4	717.8355	7.8606
2386	Diethyl Maleate	C8H12O4	598.9342	6.6696
2385	Mth Dodecanoate	C13H26O2	594.2717	6.5036
3379	Dioctyl Adipate	C22H42O4	594.1622	13.6408
5886	Mth Acetoacetate	C5H8O3	429.1979	3.4175
5884	Ethoxy Acetate	C6H12O3	665.1730	7.2695
5887	EthAcetoAcetate	C6H10O3	596.1435	6.9150
5885	Carbitol Acetate	C8H16O4	973.7985	13.8336

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Ketones

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1096	Methyl Isopropen	C5H8O	783.2336	10.0001
1079	Cyclopentanone	C5H8O	347.9179	4.9899
1051	Acetone	C3H6O	502.2766	4.5958
1052	MEK	C4H8O	646.8102	7.2972
1065	Mesityl Oxide	C6H10O	757.0087	9.2383
1066	T-But Mth Ketone	C6H12O	838.5106	10.0598
1060	2-Pentanone	C5H10O	718.2472	8.7139
1061	Mth iC3 Ketone	C5H10O	714.6010	9.2981
1053	Diethyl Ketone	C5H10O	610.5369	8.5848
1059	3-Hexanone	C6H12O	712.1173	9.7605
1099	Diketene	C4H4O2	96.3344	0.9668
1055	Sec-ButMthKetone	C6H12O	791.1229	10.7280
1054	MIBK	C6H12O	835.3850	10.9516
1095	EthIsopropKetone	C6H12O	788.9529	10.3986
1063	2-Heptanone	C7H14O	759.9984	9.3168
1064	5-Mth-2-Hexanone	C7H14O	1356.1050	15.7899
1058	4-Heptanone	C7H14O	996.2183	15.2148
1057	3-Heptanone	C7H14O	702.5812	8.7348
1076	2,4-Pentanedione	C5H8O2	1125.2705	34.9283
1068	DiisobutylKetone	C9H18O	947.9960	14.3011
1097	2-CycC6 CycC6one	C12H20O	772.8765	7.2424
1083	2-Octanone	C8H16O	741.8580	9.2323
1073	Dibutyl Ketone	C9H18O	768.1190	10.5118
1062	2-Hexanone	C6H12O	418.8468	5.1548
1077	Isophorone	C9H14O	286.6216	4.6690
1090	Acetophenone	C8H8O	595.6356	6.3394
1080	Cyclohexanone	C6H10O	372.8452	5.3068
1074	2-Nonanone	C9H18O	769.3292	9.4366

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Alcohol-Ethers

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
2862	2-Butoxyethanol	C6H14O2	858.7310	13.1335
4857	butyl carbitol	C8H18O3	692.4033	10.2538

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

2898	2-Chloroethanol	C2H5ClO	459.5587	5.6205
2864	Carbitol	C6H14O3	541.3824	7.0654
3854	Methyl propasol	C4H10O2	841.0105	14.4267
2860	2-Methoxyethanol	C3H8O2	529.9271	5.9723
2854	DiacetoneAlcohol	C6H12O2	985.3386	18.9087
2861	2-Ethoxyethanol	C4H10O2	698.9091	10.1698
2889	HydroxyAcetone	C3H6O2	455.7211	6.5536
3856	1tButoxy2Propnol	C7H16O2	2418.5205	32.8208
3858	PROPGLYC2tBUTYL	C7H16O2	1497.7020	12.1846
4855	2-Propoxyethanol	C5H12O2	916.5856	14.9145
4849	Acetovanillone	C9H10O3	800.3432	7.9712
5883	Ethyl Lactate	C5H10O3	1159.1771	27.9479
6883	2-HydroxyEth Acr	C5H8O3	243.7069	1.3409
2863	Methyl Carbitol	C5H12O3	445.5158	5.1983
3855	Dowanol DPM	C7H16O3	1684.4285	37.8809
3857	TriPropGlymEthlE	C10H22O4	1776.7274	25.6315

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Hydrocarbons

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
404	DiMth-Acetylene	C4H6	607.5677	0.0258
202	Propylene	C3H6	1231.4234	13.2902
412	2-Pentyne	C5H8	2427.9885	10.0000
207	2-Methylpropene	C4H8	1055.7643	11.6843
204	1-Butene	C4H8	1026.9512	12.7631
205	Cis-2-Butene	C4H8	821.2498	7.8872
402	Propyne	C3H4	668.6299	4.0674
406	3-Hexyne	C6H10	759.9944	0.5833
206	Trans-2-Butene	C4H8	934.5026	10.2699
407	2-Hexyne	C6H10	690.4276	0.3552
231	33-2Mth-1-Butene	C6H12	859.6331	9.1244
230	23-2Mth-1-Butene	C6H12	774.8280	8.8331
229	2-Ethyl-1-Butene	C6H12	747.3426	8.5395
8	I-Pentane	C5H12	733.9949	8.6726
14	2,2-DiMth-Butane	C6H14	680.3703	6.6940
232	23-2Mth-2-Butene	C6H12	330.7387	1.0262
213	3-Mth-1-Butene	C5H10	968.3635	12.4893

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

212	2-Mth-1-Butene	C5H10	633.2131	7.1457
211	Trans-2-Pentene	C5H10	897.0879	10.1756
210	Cis-2-Pentene	C5H10	781.5372	8.6128
223	4-Mth-1-Pentene	C6H12	749.4823	9.9970
221	2-Mth-1-Pentene	C6H12	861.7846	10.3618
248	2-t-Butylpropene	C7H14	752.5577	7.1975
227	Cs-4-Mth-2-C5H10	C6H12	902.8562	10.9724
224	2-Mth-2-Pentene	C6H12	825.2726	10.0001
403	1-Butyne	C4H6	830.6689	7.6183
15	2,3-DiMth-Butane	C6H14	623.9769	6.5510
214	2-Mth-2-Butene	C5H10	759.9941	8.7376
228	Ts-4-Mth-2-C5H10	C6H12	846.5142	9.6862
225	Cs-3-Mth-2-C5H10	C6H12	801.8668	10.1379
218	Trans-2-Hexene	C6H12	802.6495	9.3777
2226	3-METH-Tr-2Pente	C6H12	740.0230	8.3985
222	3-Mth-1-Pentene	C6H12	808.9505	10.8405
257	2-Diisobutylene	C8H16	812.4791	8.7828
256	1-Diisobutylene	C8H16	800.8231	9.1283
217	Cis-2-Hexene	C6H12	764.5519	9.1713
2414	1-Heptyne	C7H12	759.9484	9.6414
13	3-Methylpentane	C6H14	663.8231	7.5551
219	Cis-3-Hexene	C6H12	806.9205	9.9972
12	2-Methylpentane	C6H14	746.9674	9.0837
220	Trans-3-Hexene	C6H12	823.4061	9.8028
405	1-Pentyne	C5H8	842.9821	10.1849
209	1-Pentene	C5H10	911.6530	12.1103
11	N-Hexane	C6H14	1024.8846	12.1036
235	Cis-2-Heptene	C7H14	729.7923	9.3989
249	Cis-3-Heptene	C7H14	1365.3156	17.5074
216	1-Hexene	C6H12	767.5248	9.9992
239	3-Eth-1-Pentene	C7H14	752.0133	9.0596
226	4-Mth-1-Hexene	C7H14	747.8386	8.7414
240	3-Mth-1-Hexene	C7H14	720.7978	8.7326
419	3-Mth-1-Butyne	C5H8	954.8206	10.8326
233	2-Eth-1-Pentene	C7H14	757.5961	9.0487
238	2-Mth-1-Hexene	C7H14	846.3980	10.5882
416	1-Octyne	C8H14	714.8123	8.7210
289	2,3Dimeth Hexene	C8H16	789.6642	9.3980
234	1-Heptene	C7H14	577.1908	7.4173
413	1-Hexyne	C6H10	679.4357	8.3177
237	Trans-3-Heptene	C7H14	758.5732	9.6216
236	Trans-2-Heptene	C7H14	685.8878	8.5877

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

251	Trans-2-Octene	C8H16	760.0032	10.0307
279	Trans-4-Octene	C8H16	794.2108	10.4768
277	Trans-3-Octene	C8H16	728.4150	9.6573
2252	2Methl-1-Heptene	C8H16	759.4868	10.0994
250	1-Octene	C8H16	453.6965	5.6119
258	2-Ethyl-1-Hexene	C8H16	760.2424	9.8990
280	3-Octene	C8H16	749.0210	10.2292
278	4-Octene	C8H16	804.3161	11.0877
276	2-Octene	C8H16	407.1464	5.3673
259	1-Nonene	C9H18	589.0396	6.9144
262	1-Dodecene	C12H24	630.7736	7.1162
263	1-Tridecene	C13H26	616.5793	6.6768
264	1-Tetradecene	C14H28	388.4424	4.0118
265	1-Pentadecene	C15H30	516.9958	5.3921
266	1-Hexadecene	C16H32	615.7238	5.9235
267	1-Octadecene	C18H36	408.4984	3.8895
281	1-Heptadecene	C17H34	1136.7161	11.1284
284	1-Eicosene	C20H40	458.3920	4.3148
283	1-Nonadecene	C19H38	640.5431	5.8178
3	Propane	C3H8	1131.7273	12.6043
4	I-Butane	C4H10	655.3328	7.2740
9	Neopentane	C5H12	1029.7005	11.6994
5	N-Butane	C4H10	850.6204	10.5458
7	pentane	C5H12	734.4954	9.0697
44	Hexamethylethane	C8H18	460.1847	3.0698
25	223-TriMthButane	C7H16	534.4064	4.7543
24	3,3-DiMthPentane	C7H16	615.3210	6.1739
51	2,2,3,3-4Mth-C5	C9H20	375.2879	2.4823
21	2,2-DiMthPentane	C7H16	722.2252	7.6909
42	2,3,3-TriMth-C5	C8H18	442.2808	3.8537
22	2,3-DiMthPentane	C7H16	533.8519	5.5676
40	2,2,3-TriMth-C5	C8H18	527.0495	4.7715
23	2,4-DiMthPentane	C7H16	750.1684	9.0979
41	2,2,4-TriMth-C5	C8H18	685.4305	7.6866
39	3-Mth-3-Eth-C5	C8H18	515.6974	5.0163
20	3-Ethylpentane	C7H16	674.3348	7.6424
52	2,2,3,4-4Mth-C5	C9H20	471.0216	4.1675
54	2334TetrMethPent	C9H20	299.9481	2.2492
53	2,2,4,4-4Mth-C5	C9H20	571.0857	5.2598
43	2,3,4-TriMth-C5	C8H18	495.9595	4.9397
36	3,3-DiMth-Hexane	C8H18	697.6636	7.0997

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

19	3-Methylhexane	C7H16	668.8719	7.8128
18	2-Methylhexane	C7H16	659.2998	7.8715
38	2-Mth-3-Eth-C5	C8H18	670.1110	7.3481
190	2,2-2C1-3-C2-C5	C9H20	553.0560	5.3252
32	2,2-DiMth-Hexane	C8H18	570.3196	6.1803
37	3,4-DiMth-Hexane	C8H18	405.3580	4.2553
50	3,3-DiEthPentane	C9H20	510.9171	5.1902
34	2,4-DiMth-Hexane	C8H18	1300.2766	15.4457
33	2,3-DiMth-Hexane	C8H18	648.5684	6.8891
17	N-Heptane	C7H16	656.3727	7.7442
49	244TriMethHexane	C9H20	646.0166	6.8146
192	2,4-2C1-3-C2-C5	C9H20	505.2693	5.4114
47	2,2,5-TriMth-C6	C9H20	497.6881	5.4614
35	2,5-DiMth-Hexane	C8H18	649.1674	7.6568
31	3-Ethylhexane	C8H18	511.1262	6.0508
30	4-Methylheptane	C8H18	499.6218	5.8809
29	3-Methylheptane	C8H18	548.7411	6.4086
28	2-Methylheptane	C8H18	505.7413	5.9862
96	2,2-DiMthHeptane	C9H20	724.4702	8.1090
176	2,6-DiMthHeptane	C9H20	410.7451	4.6438
27	N-Octane	C8H18	676.6324	7.8353
94	3-Ethylheptane	C9H20	666.6343	7.8588
92	3-Methyloctane	C9H20	627.4451	7.0691
93	4-Methyloctane	C9H20	707.7993	8.2864
91	2-Methyloctane	C9H20	668.9920	7.4880
72	2,2-DiMthOctane	C10H22	659.6780	7.0461
2095	2,3Dimethloctane	C10H22	829.3550	8.9425
2096	2,4Dimethloctane	C10H22	709.4397	8.2983
2098	2,6DimethlOctane	C10H22	669.7236	7.5771
2097	2,5Dimethloctane	C10H22	670.5900	7.7886
2099	2,7DimethlOctane	C10H22	765.0920	8.6812
46	N-Nonane	C9H20	404.0285	4.5476
88	5-Methylnonane	C10H22	683.2181	7.8002
85	3-Methylnonane	C10H22	811.2348	9.0570
87	4-Methylnonane	C10H22	658.9941	7.7843
86	2-Methylnonane	C10H22	697.1477	7.4817
56	N-Decane	C10H22	1071.3877	11.5073
63	N-Undecane	C11H24	514.7980	5.6897
64	N-Dodecane	C12H26	359.9219	3.6804
65	N-Tridecane	C13H28	564.8405	5.8046
66	N-Tetradecane	C14H30	315.2982	3.2362

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

67	N-Pentadecane	C15H32	1041.8382	9.9986
68	N-Hexadecane	C16H34	776.0493	7.5052
69	N-Heptadecane	C17H36	485.3382	4.5049
70	N-Octadecane	C18H38	644.2641	6.0615
71	N-Nonadecane	C19H40	998.5017	9.2376
73	N-Eicosane	C20H42	1128.3235	10.5863
74	n-HENEICOSANE	C21H44	692.6115	6.4592
75	n-DOCOSANE	C22H46	472.1538	4.4416
76	n-TRICOSANE	C23H48	1044.0604	9.3641
77	n-Tetracosane	C24H50	342.8265	3.0982
78	n-PENTACOSANE	C25H52	449.2870	3.9834
79	n-HEXACOSANE	C26H54	1155.7357	10.0280
81	n-Octacosane	C28H58	891.5500	7.7026
2081	n-TRICONTANE	C30H62	406.1738	3.8535
2082	n-Dotriacontane	C32H66	1607.2720	15.3668

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Cyclic Hydrocarbons

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
269	Cyclopentene	C5H8	973.7588	18.7960
270	Cyclohexene	C6H10	603.0007	9.3933
287	3MthCyclopentene	C6H10	961.1219	14.8033
286	1-MthCyclPentene	C6H10	852.5491	15.9111
288	4MthCyclopenten	C6H10	950.2232	14.3779
273	Cycloheptene	C7H12	664.5501	9.2948
274	Cyclooctene	C8H14	650.3757	8.2507
101	Cyclopropane	C3H6	1349.3914	32.1394
810	ADAMANTANE	C10H16	532.6425	10.3253
102	Cyclobutane	C4H8	880.9984	16.5673
104	Cyclopentane	C5H10	829.2352	13.1493
137	Cyclohexane	C6H12	836.0522	12.4756
105	MthCyclopentane	C6H12	893.8896	11.9928
146	Cs-1,4-2C1-CycC6	C8H16	761.1272	8.0582
142	Cs-1,2-2C1-CycC6	C8H16	688.1755	6.6938
141	1,1-2C1-CycC6	C8H16	640.9889	8.5278
145	Ts-1,3-2C1-CycC6	C8H16	751.6857	7.8981

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

144	Cs-1,3-2C1-CycC6	C8H16	862.7883	9.9997
147	Ts-1,4-2C1-CycC6	C8H16	845.4970	10.1873
143	Ts-1,2-2C1-CycC6	C8H16	759.9700	8.6517
138	MthCyclohexane	C7H14	836.2727	10.8161
159	Cycloheptane	C7H14	677.0102	8.1091
140	Ethylcyclohexane	C8H16	725.2460	8.9044
154	Trans-Decalin	C10H18	605.4789	7.9855
149	N-PropylCyc-C6	C9H18	719.2128	8.5874
109	Cs-1,2-2C1-CycC5	C7H14	571.7835	5.6224
110	Ts-1,2-2C1-CycC5	C7H14	779.3018	8.8221
112	Ts-1,3-2C1-CycC5	C7H14	507.4874	5.7802
107	Eth-Cyclopentane	C7H14	1002.4943	12.4031
114	N-PropCycPentane	C8H16	502.9459	6.1916
108	1,1-DiMthCycC5	C7H14	759.9828	10.5304
111	Cs-1,3-2C1-CycC5	C7H14	1179.7090	13.8086
152	N-ButylCycHexane	C10H20	636.9340	7.3123
160	Cyclooctane	C8H16	521.4002	5.5217
153	Cis-Decalin	C10H18	826.6137	9.2767
115	ISOPROPYLCYCLOPENTANE	C8H16	657.4547	7.9531
150	Isopropyl-CycC6	C9H18	729.0634	8.0151
116	1-C1-1-C2-CycC5	C8H16	562.8820	7.2069
122	Butylcyclpentane	C9H18	648.4338	7.4851
155	1,1-Bicyclohexyl	C12H22	735.6135	8.0705
158	N-Decylcyclo-C6	C16H32	839.2755	7.8573

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Aromatic Hydrocarbons

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
307	1,4-Pentadiene	C5H8	958.8345	12.1440
306	1-ts3-Pentadiene	C5H8	604.4079	5.5646
414	2-Methyl-1-Butenyne	C5H6	959.8347	14.7761
305	Cs1,3-Pentadiene	C5H8	591.7636	4.9973
309	Isoprene	C5H8	759.9990	7.5267
421	1-Pentene-4-yne	C5H6	740.7030	10.0000
303	1,3-Butadiene	C4H6	888.0259	9.1084
332	1,4-CyclHexadien	C6H8	610.0277	7.9579
501	Benzene	C6H6	804.2842	8.8347

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

315	Cyclopentadiene	C5H6	985.0170	30.4380
319	Diisopropenyl	C6H10	654.4381	5.9943
615	Ethynylbezene	C8H6	890.1238	13.2432
601	Styrene	C8H8	879.7513	9.5025
331	1,3-CycHexadiene	C6H8	756.4759	13.3633
310	1,5-Hexadiene	C6H10	831.2557	12.1639
312	MthCycPentadiene	C6H8	874.9728	19.5290
420	1-Pentene-3-yne	C5H6	782.9210	0.1626
502	Toluene	C7H8	804.7977	10.4921
521	T-Butylbenzene	C10H14	1455.4748	17.3999
320	Dipropylene	C6H10	518.8790	4.3458
520	Sec-Butylbenzene	C10H14	1010.2926	12.3638
313	1,4-Hexadiene	C6H10	819.3019	10.0000
314	Dipropylene	C6H10	645.7502	5.0918
316	DiCycPentadiene	C10H12	688.0658	13.9368
333	1,5-CycOctadiene	C8H12	514.9813	5.6324
701	Naphthalene	C10H8	625.5208	7.7156
504	Ethylbenzene	C8H10	772.8860	10.0057
820	Indan	C9H10	690.0600	11.8978
505	O-Xylene	C8H10	677.5784	8.3875
612	P-Methylstyrene	C9H10	1380.3127	15.8535
330	DIISOCROTYL	C8H14	564.5855	4.8458
507	P-Xylene	C8H10	858.0224	11.9004
329	DIISOBUTENYL	C8H14	807.9579	9.9980
506	M-Xylene	C8H10	837.5559	11.2996
603	Methylstyrene	C9H10	785.8297	9.0338
613	Alpha-MthStyrene	C9H10	797.5851	9.4383
510	Isopropylbenzene	C9H12	962.8383	11.1441
724	2-Methylindene	C10H10	530.0843	7.9880
285	Vinylcyclohexene	C8H12	1359.3993	19.1690
803	Indene	C9H8	832.6707	12.7439
706	Tetralin	C10H12	405.8197	5.9738
511	O-Ethyltoluene	C9H12	701.2372	8.9065
723	1-Methylindene	C10H10	457.5695	7.9268
738	Fluorene	C13H10	623.6860	8.2681
619	Tr-1PropenylBz	C9H10	628.6481	6.1606
525	O-Diethylbenzene	C10H14	754.4239	9.9452
618	Propenyl Bz(cis)	C9H10	583.6127	6.4119
602	O-Methylstyrene	C9H10	767.2960	8.5795
702	1-MthNaphthalene	C11H10	555.8267	6.5908
509	N-Propylbenzene	C9H12	655.6837	8.7789
526	M-Diethylbenzene	C10H14	770.1156	10.6523

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

583	Cs-2-PhnButene-2	C10H12	720.5870	8.2569
543	M-DiisopropylBz	C12H18	763.3336	9.6562
584	Ts-2-PhnButene-2	C10H12	1219.3645	18.2137
580	1,2-DiC1-3C2-Bz	C10H14	688.5006	8.3157
704	1-EthNaphthalene	C12H12	513.7655	5.6436
512	M-Ethyltoluene	C9H12	776.6356	10.6358
522	1-Mth-2-iC3-Benz	C10H14	759.9919	9.9969
513	P-Ethyltoluene	C9H12	565.5406	7.8496
514	1,2,3-Mesitylene	C9H12	619.8547	7.4766
614	M-Divinylbenzene	C10H10	866.2601	10.0007
524	1-Mth-4-iC3-Benz	C10H14	479.4723	6.0565
822	Gamma-Terpinene	C10H16	618.1963	7.3693
821	Alpha-Terpinene	C10H16	791.5578	11.2393
523	1-Mth-3-iC3-Benz	C10H14	757.1901	10.0181
703	2-MthNaphthalene	C11H10	642.9430	7.8692
557	CycHexylBenzene	C12H16	519.7394	4.8745
515	1,2,4-Mesitylene	C9H12	760.5056	10.0006
519	Isobutylbenzene	C10H14	760.0025	10.4758
424	DiPhnAcetylene	C14H10	595.7862	2.8792
544	P-DiisopropylBz	C12H18	664.8764	7.0962
518	N-Butylbenzene	C10H14	702.7133	8.7676
516	1,3,5-Mesitylene	C9H12	900.0192	12.1835
809	Acenaphthalene	C12H8	680.5994	8.8482
725	123-TriMthIndene	C12H14	742.9599	12.2061
527	1,4-DiEthBenzene	C10H14	1010.7626	13.2709
558	Diphenyl	C12H10	619.3468	6.0870
576	2-Ethyl-m-Xylene	C10H14	977.8636	12.8961
620	p-ISOPROPENYLSTY	C11H12	548.8525	6.2435
585	o-PropylToluene	C10H14	714.1674	9.8018
577	2-Ethyl-p-Xylene	C10H14	818.4125	11.0735
579	4-Ethyl-o-Xylene	C10H14	995.5815	13.0698
586	m-Propyltoluene	C10H14	771.8371	10.5656
587	p-Propyltoluene	C10H14	750.9934	10.2201
578	4-Ethyl-m-Xylene	C10H14	786.0144	10.5661
575	5-Ethyl-m-Xylene	C10H14	488.3658	6.8114
530	Prehnitene	C10H14	598.2853	6.3737
709	2,6-2Mth-Naphtha	C12H12	591.0912	7.2951
715	2,7-2Mth-Naphtha	C12H12	602.0537	7.3979
719	2-ETHYLNAPHTHALENE	C12H12	829.6059	10.9030
621	p-tert-BUTYLSTY	C12H16	653.7241	7.8594
532	1,2,4,5-TetMthBz	C10H14	749.0524	9.3398
531	1,2,3,5-TetMthBz	C10H14	760.0009	9.1216

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

533	p-tert-BUTYL ET	C12H18	1428.2517	18.4882
567	N-Pentylbenzene	C11H16	647.2463	7.8148
718	1-n-PROPYLNAPHTH	C13H14	758.8964	10.6263
562	1,1-DiPhnEthane	C14H14	640.2264	6.9618
616	4-ISOBUTYLSTYRE	C12H16	455.5150	4.0296
260	1-Decene	C10H20	690.2736	7.9061
735	Cis-Stilbene	C14H12	785.3440	9.2834
568	Hexylbenzene	C12H18	651.3975	7.7909
563	Diphenylmethane	C13H12	698.3722	7.2331
564	1,2-DiPhnEthane	C14H14	745.4986	8.1852
804	Anthracene	C14H10	316.1275	3.4485
736	Trans-Stilbene	C14H12	436.8410	3.1783
805	Phenanthrene	C14H10	404.6580	4.1913
713	1-ButNaphthalene	C14H16	397.7337	4.4848
807	Pyrene	C16H10	308.1261	3.5622
261	1-Undecene	C11H22	936.7807	10.6778
581	23-2C1-23-2PhnC4	C18H22	505.1788	6.3989
549	N-Heptylbenzene	C13H20	767.3948	9.0377
710	1-PhnNaphthalene	C16H12	726.8178	8.1028
566	2,4-Diphenyl-4-M	C18H20	1102.6027	11.4195
561	O-Terphenyl	C18H14	1557.0781	22.5204
569	N-Octylbenzene	C14H22	733.9638	8.3289
565	Triphenylmethane	C19H16	808.8399	9.4079
714	N-C6-Naphthalene	C16H20	1107.3799	11.0191
717	Fluoranthene	C16H10	743.7451	11.4914
716	1-Hexyl-Tetralin	C16H24	830.5285	9.9354
731	TriPhnEthylene	C20H16	536.8384	5.3741
806	Chrysene	C18H12	211.6945	1.3104
588	1,1,2TriPhenEth	C20H18	1144.4242	16.6262
711	1-n-NonylNaphtha	C19H26	589.7673	7.3938
570	N-Nonylbenzene	C15H24	839.2340	9.2201
712	1-Decyl Naphtha	C20H28	561.5893	6.9920
559	P-Terphenyl	C18H14	455.6945	2.9548
560	M-Terphenyl	C18H14	604.6826	5.2874
589	TetraPhenylMetha	C25H20	324.4443	2.7646
554	Decylbenzene	C16H26	392.4241	4.1816
732	TetraPhnEthylene	C26H20	238.4488	1.6984
574	N-Dodecylbenzene	C18H30	324.0752	3.2518
571	N-Undecylbenzene	C17H28	795.6837	8.0850
572	Tridecylbenzene	C19H32	1029.4329	9.8589
573	n-TETRADECYLBENZ	C20H34	469.4934	4.8544
2575	n-PENTADECYLBENZ	C21H36	420.7652	4.0453

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

2576	n-HEXADECYLBENZ	C22H38	440.8441	4.1604
2577	n-HEPTADECYLBENZ	C23H40	773.1987	7.8231
2578	n-OCTADECYLBENZE	C24H42	919.5096	9.4604

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Halocarbons

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1544	Allyl Chloride	C3H5Cl	679.4352	9.9404
1595	2-Chloropropene	C3H5Cl	663.0829	7.2808
1531	3-Chloropropyne	C3H3Cl	608.7866	9.4039
1535	T-Butyl Chloride	C4H9Cl	599.4624	3.4634
1583	Chloroprene	C4H5Cl	620.0575	6.3543
1530	Isopropyl Cl	C3H7Cl	476.6115	2.8125
1572	O-DiCl-Benzene	C6H4Cl2	638.5272	6.7549
1585	Propyl Chloride	C3H7Cl	713.7214	9.8779
1684	Isopropyl Iodide	C3H7I	759.8543	10.7743
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	553.6116	6.0345
1651	2-Bromopropane	C3H7Br	167.8620	0.3400
1691	Iodobenzene	C6H5I	865.2461	12.2633
1860	Fluorobenzene	C6H5F	681.7489	7.5271
1571	Chlorobenzene	C6H5Cl	738.6123	8.6705
1680	Bromobenzene	C6H5Br	456.3026	3.1132
1526	1,2-DiCl-Propane	C3H6Cl2	655.3073	7.8609
1683	Propyl Iodide	C3H7I	696.9716	9.6574
1576	Benzotrichloride	C7H5Cl3	762.6823	10.4528
1536	2,3-DICHLOROBUT	C4H8Cl2	343.2495	1.8211
2638	2-Bromobutane	C4H9Br	177.4903	0.4282
1586	1-Chlorobutane	C4H9Cl	704.6969	9.7802
1573	M-DiCl-Benzene	C6H4Cl2	797.7618	10.0865
2634	Benzotrifluoride	C7H5F3	811.0073	9.5878
1574	P-DiCl-Benzene	C6H4Cl2	755.5030	8.7133
1650	1-Bromopropane	C3H7Br	150.2270	0.3226
1587	2-Chlorobutane	C4H9Cl	491.9766	3.8539
2653	8F-2-Butene	C4F8	8.3100	0.0175
1678	M-Dibromobenzene	C6H4Br2	322.3242	1.6692
1537	1,2-DiCl-Butane	C4H8Cl2	761.5084	10.0000
1597	34-DiCl-1-Butene	C4H6Cl2	691.4334	6.3410

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1577	O-Chlorotoluene	C7H7Cl	768.7368	9.2799
1532	123-3Cl-Propane	C3H5Cl3	582.4955	7.6392
1578	P-Chlorotoluene	C7H7Cl	575.6053	6.0159
1562	Benzyl Chloride	C7H7Cl	704.6389	8.5896
2661	P-Bromotoluene	C7H7Br	464.7251	3.8219
1508	1,4-DiCl-Butane	C4H8Cl2	409.4598	5.0113
1655	1-Bromobutane	C4H9Br	207.0663	0.5877
1599	BenzylDichloride	C7H6Cl2	604.5765	8.2556
2652	Perfluoropropane	C3F8	0.1352	0.0000
1505	2-Butylene DiCl	C4H6Cl2	293.6018	4.7657
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	489.8972	5.9089
1588	1-Chloropentane	C5H11Cl	625.5583	9.5756
2654	OctaF-CycButane	C4F8	227.9498	0.0000
1592	1,2,4-TriCl-Bz	C6H3Cl3	760.0012	9.9992
1579	2,4-2Cl-Toluene	C7H6Cl2	709.4373	7.7626
2593	1,3,5-TriCl-BZ	C6H3Cl3	813.2165	11.3391
1697	1-Br-Naphthalene	C10H7Br	349.3968	2.4848
1622	Perfluorobutane	C4F10	1.4232	0.0000
1857	P-Cl-Benzo-TriF	C7H4ClF3	887.5934	12.1893
1509	1,5-DiCl-Pentane	C5H10Cl2	358.8766	3.9851
1589	1-Cl-Naphthalene	C10H7Cl	486.8052	5.3549
1864	Perfluorobenzene	C6F6	761.0612	9.9997
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	942.0363	12.0907
1667	1-Bromoheptane	C7H15Br	335.7381	1.5695
1575	HexaCl-Benzene	C6Cl6	586.2817	2.2862
2640	Freon 123B1	C2HBrClF3	196.4693	0.4626
1504	Vinyl Chloride	C2H3Cl	823.7280	17.0300
1672	1,1-DiBr-Ethane	C2H4Br2	54.5378	0.0231
1580	Acetylene DiCl	C2H2Cl2	399.7729	4.4387
1692	Diiodomethane	CH2I2	531.2279	4.1447
1698	Bromoform	CHBr3	36.6630	0.0112
2687	Freon 13B1	CBrF3	151.9823	0.1460
2690	Br-3F-Ethylene	C2BrF3	379.8800	0.1724
1649	Tetrabromoethane	C2H2Br4	18.3249	0.0033
2686	Freon 12B1	CBrClF2	995.2864	1.1074
1503	Ethyl Chloride	C2H5Cl	818.3536	11.3066
2641	Br-TriCl-Methane	CBrCl3	520.8681	3.0986
1641	Methyl Bromide	CH3Br	69.7260	0.0227
2688	Freon 12B2	CBr2F2	339.2251	0.0563
2545	2,3-DiCl-Propene	C3H4Cl2	548.3751	6.4640
1673	1,2-DiBr-Ethane	C2H4Br2	44.1695	0.0420
2637	Dibromomethane	CH2Br2	29.3937	0.0057

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1542	TetraCl-Ethylene	C2Cl4	569.0867	4.5077
1541	TriCl-Ethylene	C2HCl3	760.0075	11.0188
1527	111-TriCl-Ethane	C2H3Cl3	759.9970	6.4260
1612	Cl-2F-Ethylene	C2HClF2	760.3573	2.5211
1617	Ethyl Fluoride	C2H5F	75.2473	0.1764
2639	Br-Cl-Methane	CH2BrCl	248.8699	0.9924
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	822.1025	11.5131
1682	Ethyl Iodide	C2H5I	769.4922	10.0001
1522	1,1-DiCl-Ethane	C2H4Cl2	760.0097	7.3176
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	0.2014	0.0001
1525	Hexachloroethane	C2Cl6	713.6206	4.5409
1528	1112-4Cl-Ethane	C2H2Cl4	846.2796	10.0684
1590	Penta-Cl-Ethane	C2HCl5	817.1674	10.0003
1529	1122-4Cl-Ethane	C2H2Cl4	873.4027	10.2675
2693	Perfluoroethane	C2F6	0.0000	0.0000
1611	Freon 114B2	C2Br2F4	515.4675	0.0131
2692	Cl-PentaF-Ethane	C2ClF5	0.0000	0.0000
2655	122-3Cl-112-3FC2	C2Cl3F3	60.7468	0.5727
1609	12-2Cl-1122-4FC2	C2Cl2F4	0.0000	0.0000
2526	1,1-DiCl-Propane	C3H6Cl2	702.7908	7.2178
1645	Ethyl Bromide	C2H5Br	113.4155	0.1250
2658	1112-4Cl-22-2FC2	C2Cl4F2	199.2947	1.2243
1619	111-3F-Ethane	C2H3F3	1.8964	0.0001
1524	1,1,2-3Cl-Ethane	C2H3Cl3	912.3795	13.4772
1640	1,1-DiF-Ethane	C2H4F2	16.3316	0.0000
2691	Genetron 1113	C2ClF3	879.9907	1.6504
2694	Vinyl Bromide	C2H3Br	261.3966	0.7443
1694	Refrigerant 123	C2HCl2F3	747.9749	9.9993
1523	1,2-DiCl-Ethane	C2H4Cl2	596.2978	9.9998
2656	1122-4Cl-12-2FC2	C2Cl4F2	760.0028	9.9999
2527	1,3-DiCl-Propane	C3H6Cl2	578.1505	8.4454

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

Acids

DipID	Name	Formula	$P_{Calc}^{760mmHg}$	P_{Calc}^{10mmHg}
1277	Acrylic Acid	C3H4O2	528.5677	9.9997

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

1274	Ts-Crotonic Acid	C4H6O2	229.1848	2.8521
1279	Oleic Acid	C18H34O2	706.1128	7.5748
1278	Methacrylic Acid	C4H6O2	686.8739	12.4345
2271	Cinnamic Acid	C9H8O2	363.9654	1.5581
1266	n-UNDECANOIC ACI	C11H22O2	565.5110	6.1485
1282	O-Toluic Acid	C8H8O2	739.8604	8.6290
2283	IBUPROFEN	C13H18O2	1227.0038	13.5374
1261	Isovaleric Acid	C5H10O2	759.9997	9.8107
1264	1,4-CychexDicarboxAcid	C8H12O4	114.2315	0.4268
1283	P-Toluic Acid	C8H8O2	462.5542	4.2829
1257	3-MthButyricAcid	C5H10O2	638.9172	9.4388
1288	Isophthalic Acid	C8H6O4	12.0525	0.0173
2871	4CarboxAcidBzldhyde	C8H6O3	14.5852	0.0227
1256	N-Butyric Acid	C4H8O2	605.9547	7.8757
1276	Stearic Acid	C18H36O2	1142.5510	14.1905
1285	Adipic Acid	C6H10O4	273.7500	2.2405
1273	Cs-Crotonic Acid	C4H6O2	474.5300	5.8448
4851	Diglycolic Acid	C4H6O5	257.9058	1.2085
1286	Maleic Acid	C4H4O4	230.2499	1.7004
2277	Citraconic Acid	C5H6O4	80.1288	0.5735
2278	Itaconic Acid	C5H6O4	206.9128	1.3909
2281	Glutaric Acid	C5H8O4	255.4796	1.6652
1271	TetradecylicAcid	C14H28O2	559.1364	6.0620
1259	N-Nonanoic Acid	C9H18O2	1302.8647	14.0676
1280	Linoleic Acid	C18H32O2	847.2806	10.1467
1260	Isobutyric Acid	C4H8O2	397.6140	5.7898
2268	Fumaric Acid	C4H4O4	297.1542	2.8176
1287	Phthalic Acid	C8H6O4	1456.6905	16.1828
1289	TerephthalicAcid	C8H6O4	2.7956	0.0009
2280	Succinic Acid	C4H6O4	159.5624	0.8625
1270	Tridecanoic Acid	C13H26O2	406.0359	4.4244
1254	N-Decanoic Acid	C10H20O2	435.6582	4.1197
2270	Suberic Acid	C8H14O4	276.6472	2.4389
2255	Linolenic Acid	C18H30O2	1139.0320	12.7056
1262	N-Hexanoic Acid	C6H12O2	852.7409	8.4596
4852	Levulinic Acid	C5H8O3	239.7943	1.7299
2275	Sebacic Acid	C10H18O4	344.7000	3.2825
1255	Oxalic Acid	C2H2O4	64.9777	0.2995
2259	PentadecylicAcid	C15H30O2	725.1632	8.7462
2266	NonadecanoicAcid	C19H38O2	1664.0070	21.0620
2269	Pimelic Acid	C7H12O4	279.6179	1.9377
1252	Acetic Acid	C2H4O2	583.0714	14.7507

Table E.1 Vapor Pressures Calculated from the Suggested Boiling Temperature Correlations (Continued)

3268	Malonic Acid	C3H4O4	124.0809	0.6489
2279	2-EthButyricAcid	C6H12O2	853.8953	12.9497
1265	N-Octanoic Acid	C8H16O2	617.4731	5.9591
2258	NeopentanoicAcid	C5H10O2	1130.5811	10.8792
2257	Azelaic Acid	C9H16O4	327.9216	2.9141
1281	Benzoic Acid	C7H6O2	585.5980	4.6847
1269	Dodecanoic Acid	C12H24O2	1502.5328	14.9473
2261	Heptanoic Acid	C7H14O2	441.4864	4.4565
1258	N-Valeric Acid	C5H10O2	876.8039	9.8182
2265	HeptadecylicAcid	C17H34O2	648.7133	7.8104
2267	N-Eicosanic Acid	C20H40O2	1209.0769	15.7447
1253	Propionic Acid	C3H6O2	606.1297	10.6439
5877	Ascorbic Acid	C6H8O6	1288.8827	2.4812
1272	HexadecanoicAcid	C16H32O2	815.1523	9.8826

Table E. 2Vapor Pressures Calculated by the Joback Method

Alcohols

DipID	Name	Formula	$P_{Joback}^{760\,mmHg}$	$P_{Joback}^{10\,mmHg}$
1181	Phenol	C6H6O	446.4594	2.3219
1182	O-Cresol	C7H8O	894.2708	7.4621
1183	M-Cresol	C7H8O	597.1293	3.4204
1176	2,6-Xylenol	C8H10O	1166.5251	14.8305
1111	2-Mth-2-Butanol	C5H12O	2836.1976	27.5957
1178	3,5-Xylenol	C8H10O	1239.7094	8.1102
1133	2-Octanol	C8H18O	2523.3862	25.0627
2885	4-HYDROXYSTYREN	C8H8O	884.8485	8.1957
1197	P-t-Butylphenol	C10H14O	1025.7119	8.0239
1172	2,4-Xylenol	C8H10O	687.6207	6.1012
1184	P-Cresol	C7H8O	860.0803	4.4400
1151	Cyclohexanol	C6H12O	1374.8030	10.1669
1170	2,3-Xylenol	C8H10O	896.3171	6.8963
1187	P-Ethyl Phenol	C8H10O	723.1207	4.7781
2859	P-Methoxyphenol	C7H8O2	339.1538	0.9231
1121	2-Ethylhexanol	C8H18O	1300.3059	11.3920
1179	PropargylAlcohol	C3H4O	235.5825	1.8848
1123	3-Mth-1-Butanol	C5H12O	838.3871	4.9015
2196	P-t-Amylphenol	C11H16O	864.7387	8.2412
1174	2,5-Xylenol	C8H10O	1011.3277	9.7178
1115	2-Hexanol	C6H14O	1531.8910	13.4397
1152	1-MthCycHexanol	C7H14O	2257.9164	43.0778
4854	Guaiacol	C7H8O2	1608.7600	14.6877
1107	Sec-Butanol	C4H10O	2001.9822	14.1383
1167	Allyl Alcohol	C3H6O	434.1657	2.6819
1130	4-Mth-2-Pentanol	C6H14O	1487.2191	18.3831
1177	3,4-Xylenol	C8H10O	800.1836	4.9004
1114	1-Hexanol	C6H14O	506.1001	3.0256
1106	Isobutanol	C4H10O	1167.5740	6.0324
1125	1-Heptanol	C7H16O	556.2495	3.4746
1105	N-Butanol	C4H10O	442.0056	2.2442
1109	1-Pentanol	C5H12O	873.5445	5.1909
1132	1-Octanol	C8H18O	706.5472	4.9989
1113	T-Butylcarbinol	C5H12O	1261.3698	10.5611
1137	1-Undecanol	C11H24O	1486.2199	14.5347
1108	Tert-Butanol	C4H10O	1456.3520	11.5731
1103	N-Propanol	C3H8O	539.8800	2.9103
1134	1-Nonanol	C9H20O	589.9197	4.6640
2195	P-t-Octylphenol	C14H22O	2530.8514	32.1662
1102	Ethanol	C2H6O	435.2310	2.7000
1124	3-Mth-2-Butanol	C5H12O	983.6682	7.7590
1136	1-Decanol	C10H22O	1626.6836	14.4706

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1140	Dodecanol	C12H26O	1455.8646	16.0588
1104	Isopropanol	C3H8O	863.6107	6.0203
1110	2-Pentanol	C5H12O	1027.4208	7.5402
1120	3-Pentanol	C5H12O	2287.3626	20.5517
1112	2-Mth-1-Butanol	C5H12O	939.1417	5.5244
1154	Ts-2-Mth-CycC6OH	C7H14O	1825.2163	21.3592
1153	Cs-2-Mth-CycC6OH	C7H14O	1237.5526	16.7029
1156	Ts-3-Mth-CycC6OH	C7H14O	1962.1860	15.5966
1157	Cs-4-Mth-CycC6OH	C7H14O	1812.9206	16.0755
2197	P-Cumylphenol	C15H16O	2838.6073	32.5491
1180	Benzyl Alcohol	C7H8O	863.4874	6.9395
1158	Ts-4-Mth-CycC6OH	C7H14O	1615.0690	12.7707
1155	Cs-3-Mth-CycC6OH	C7H14O	1579.4774	11.7126
1168	2-Phn-2-Propanol	C9H12O	2345.8488	35.5015
1141	1-Tridecanol	C13H28O	1168.1332	14.3692
1147	2-Eth-1-Butanol	C6H14O	1055.5319	8.5989
1117	2-Mth-1-Pentanol	C6H14O	614.7802	4.9103
2115	2-Phenylethanol	C8H10O	1006.2700	10.5877
1142	1-Tetradecanol	C14H30O	956.9336	12.8564
2118	1-PHN-1-PROPANOL	C9H12O	1373.8803	19.3501
2119	1-PHN-2-PROPANOL	C9H12O	1407.1342	19.1954
1126	2-Heptanol	C7H16O	819.2052	8.9673
1143	1-Pentadecanol	C15H32O	2353.1723	32.4312
1129	Isoheptanol	C7H16O	902.8714	6.3355
2117	2,6-DiMth-4-C7OH	C9H20O	3101.1049	38.7321
1144	1-Hexadecanol	C16H34O	2061.3933	30.9032
1145	Heptadecanol	C17H36O	2016.1552	31.1597
1199	Nonylphenol	C15H24O	3127.5360	30.0726
1146	1-Octadecanol	C18H38O	3729.6208	61.8593
1135	2-Nonanol	C9H20O	1094.4071	14.2630
1149	1-Nonadecanol	C19H40O	4808.3746	85.5396
1139	Isodecanol	C10H22O	2431.0991	20.5293
1148	1-Eicosanol	C20H42O	6735.1230	125.5919
2198	Dinonylphenol	C24H42O	5364.9184	69.5600
1159	Menthol	C10H20O	840.0672	5.2795
1202	DiethyleneGlycol	C4H10O3	281.7436	2.2095
1245	1,3-Benzenediol	C6H6O2	278.7806	0.9946
1186	P-Hydroquinone	C6H6O2	244.7758	1.0245
1244	1,2-Benzenediol	C6H6O2	554.5845	6.8818
1219	2MTH,13PROPNDIO	C4H10O2	516.4961	4.8982
1212	1,3-Propanediol	C3H8O2	357.8881	3.1894
1235	P-t-But-Catechol	C10H14O2	2275.7011	28.4674
1203	Triglycol	C6H14O4	469.9765	6.5563

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1198	Bisphenol A	C15H16O2	9591.3566	98.2702
1238	2,3-Butanediol	C4H10O2	1148.0769	14.0922
1211	1,2-Propanediol	C3H8O2	780.6809	8.1583
2219	2,4-PENTANEDIOL	C5H12O2	1456.0420	20.0562
1215	1,4-Butynediol	C4H6O2	497.6295	1.6974
1214	Neopentyl Glycol	C5H12O2	1214.7634	10.3615
1221	1,3-Butanediol	C4H10O2	484.1609	4.8333
1220	1,2-Butanediol	C4H10O2	868.3956	10.6200
1240	Ts2-C4H8-14-Diol	C4H8O2	340.1068	1.2994
1239	Cis-Butenediol	C4H8O2	597.9144	3.9383
1241	1,4-Butanediol	C4H10O2	355.0096	2.0088
1222	Hexylene Glycol	C6H14O2	3055.8910	38.1704
1213	Dipropylene Gly	C6H14O3	1983.2900	32.6996
1242	1,5-Pentanediol	C5H12O2	498.0799	3.2205
1243	1,6-Hexanediol	C6H14O2	613.5627	5.5778
1204	TetraC2H4 Glycol	C8H18O5	2772.9371	37.2620
6886	C6H4(COOC2H4OH)2	C12H14O6	11424.7906	121.4494
1248	123-Benzenetriol	C6H6O3	1153.2706	13.1064
1231	Glycerol	C3H8O3	463.5977	5.2453
1247	Hexaglycerol	C6H14O3	2886.0806	37.3758
1246	Pentaerythritol	C5H12O4	1955.6436	9.1283

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Amines

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1742	Ethyleneimine	C2H5N	214.6946	0.4987
1745	Piperidine	C5H11N	843.1856	7.5861
2726	Propyleneimine	C3H7N	411.8792	2.1828
1766	Pyrrolidine	C4H9N	673.5343	3.9400
1719	Isopropylamine	C3H9N	4252.4251	77.5424
1711	N-Propylamine	C3H9N	1493.4893	21.4919
1726	Sec-Butylamine	C4H11N	1739.9947	32.0483
1704	Ethylamine	C2H7N	2128.2460	34.9451
1702	Dimethylamine	C2H7N	1362.9848	11.5913
1710	Diethylamine	C4H11N	1091.5298	12.6280
1740	Allylamine	C3H7N	1159.3453	12.8132
1712	N-Butylamine	C4H11N	1193.5271	14.9972
1794	HexMthyleneimine	C6H13N	500.0812	3.2621
1729	Cyclohexylamine	C6H13N	1414.3875	19.2413

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1714	Isobutylamine	C4H11N	1478.4544	21.3155
2853	Acetamide	C2H5NO	7.7526	0.0032
2731	N-C1-CycC6-Amine	C7H15N	524.0235	2.9580
1743	Diisopropylamine	C6H15N	2531.6787	33.8410
1796	N,N-DiMthAniline	C8H11N	1405.7148	20.3299
1792	Aniline	C6H7N	433.7654	2.4829
1713	N-Pentylamine	C5H13N	991.7093	11.5729
1733	Benzylamine	C7H9N	1028.3556	8.5375
1737	M-Toluidine	C7H9N	866.3075	5.0406
3796	N-Ethylaniline	C8H11N	345.0674	1.3918
1878	2-Methacrylamide	C4H7NO	78.2588	0.1918
1736	O-Toluidine	C7H9N	423.2117	3.0412
2739	Diallylamine	C6H11N	638.8319	3.4322
2706	Hexylamine	C6H15N	919.0108	9.9441
2724	O-Ethylaniline	C8H11N	855.8727	6.9350
1707	Dipropylamine	C6H15N	874.5513	8.2788
1738	P-Toluidine	C7H9N	591.2725	3.9160
1795	N-Methylaniline	C7H9N	260.3298	1.0786
1718	Diisobutylamine	C8H19N	1302.3471	13.5662
1879	Acrylamide	C3H5NO	16.5491	0.0028
2707	1-Aminoheptane	C7H17N	865.9768	9.6234
2730	DiCycHexylAmine	C12H23N	1415.6316	16.5097
2787	P-Aminodiphenyl	C12H11N	670.7003	2.9054
1744	Dibutylamine	C8H19N	800.3535	6.3419
2708	1-Octylamine	C8H19N	734.2391	7.2365
2791	2,6-DiEthAniline	C10H15N	2794.0322	22.6882
2709	1-Nonylamine	C9H21N	962.1262	9.4189
2710	1-Decylamine	C10H23N	1080.2135	10.0212
3722	Diamylamine	C10H23N	863.9836	4.5329
3724	Undecylamine	C11H25N	1201.1621	11.6779
2712	Dodecylamine	C12H27N	1002.5301	9.5439
1720	Tetradecylamine	C14H31N	1120.9387	10.9542
2752	Piperazine	C4H10N2	463.1408	2.3137
1752	Propylenediamine	C3H10N2	1994.1820	26.9564
1741	Ethylenediamine	C2H8N2	776.4516	8.2869
2725	O-Aminoaniline	C6H8N2	528.5409	3.4124
2750	P-Aminoaniline	C6H8N2	417.8145	2.2651
2727	M-Aminoaniline	C6H8N2	234.8785	1.5308
1750	AEP	C6H15N3	1122.7925	12.7975
1732	Toluene Diamine	C7H10N2	496.4567	3.0957
1731	hexamethyleneDiamine	C6H16N2	929.2781	13.6513
3750	P-Benzidine	C12H12N2	823.1234	2.9631

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Nitriles

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1773	Propionitrile	C3H5N	759.2409	6.5524
1782	Butyronitrile	C4H7N	807.5979	6.6053
2720	Allyl Cyanide	C4H5N	727.6951	5.2138
1783	Valeronitrile	C5H9N	857.7060	7.2021
3874	Benzyl Cyanide	C8H7N	835.2294	5.8184
1786	Hexanenitrile	C6H11N	783.0895	6.6755
1776	Succinonitrile	C4H4N2	243.7513	0.5319
1781	Glutaronitrile	C5H6N2	185.1185	0.9453
2735	14-2Cyano-2-C4H8	C6H6N2	646.9260	2.2892
1777	Adiponitrile	C6H8N2	381.4222	1.5283

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Imines

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1767	N-MthPyrrolidine	C5H11N	1867.0013	28.4068
2797	3-Methylpyridine	C6H7N	1020.5864	7.8728
1797	2-Methylpyridine	C6H7N	1280.9360	12.5035
2799	4-Methylpyridine	C6H7N	697.0176	5.3508
1753	N,N-DiEthAniline	C10H15N	412.8583	2.0394

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Tert-N

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1706	Triethylamine	C6H15N	496.0988	4.5437
2716	Tributylamine	C12H27N	840.0222	4.7863
2719	Tripropylamine	C9H21N	460.8711	1.7359
3723	Triamylamine	C15H33N	2826.4607	21.5392

Table E.2 Continued

Nitrates

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1761	Nitroethane	C2H5NO2	964.1429	9.5318
1763	2-Nitropropane	C3H7NO2	1485.9516	19.9286
1762	1-Nitropropane	C3H7NO2	1104.3546	12.2660

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Thiols

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1802	Ethyl Mercaptan	C2H6S	771.9894	6.7264
1820	Dimethyl Sulfide	C2H6S	850.5523	6.9611
1843	Thiacyclopentane	C4H8S	390.6319	1.7841
1803	1-Propanethiol	C3H8S	577.3583	3.9624
1805	Isobut Mercaptan	C4H10S	555.8049	4.0003
6860	Ethylenedithiol	C2H6S2	170.4174	0.6238
1811	Cyclohexanethiol	C6H12S	539.3312	3.7077
1828	DiMth Disulfide	C2H6S2	504.2909	3.8211
1841	Butanethiol	C4H10S	450.5562	2.7487
1814	Methylproylsulf	C4H10S	478.4945	2.9888
2816	ETHYLtBUTYL SUL	C6H14S	964.3217	8.4523
1818	Diethyl Sulfide	C4H10S	630.7197	5.0888
1812	Benzyl Mercaptan	C7H8S	468.1376	2.2273
1838	T-OctylMercaptan	C8H18S	1029.1348	11.9166
1827	1-Pentanethiol	C5H12S	394.9583	2.1017
2815	METHnBUTYL SULFD	C5H12S	375.2139	2.1772
1824	DiethylDisulfide	C4H10S2	779.7918	6.4107
1807	N-Hexylmercaptan	C6H14S	369.4594	1.9118
6857	Dimercaptoethyl	C4H10OS2	175.1832	0.5202
1839	1-Heptanethiol	C7H16S	389.3975	1.7956
1829	DiProp Disulfide	C6H14S2	821.7519	7.4526
1809	1-Octanethiol	C8H18S	390.7195	1.8427
1808	N-Nonanethiol	C9H20S	320.3514	1.2969
1826	1-Decanethiol	C10H22S	411.2642	1.8188
2838	tertDodecanThiol	C12H26S	1190.1355	8.1790
1825	1-Undecanethiol	C11H24S	682.2515	2.8768
1837	Dodecylthiol	C12H26S	404.8718	2.1512

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Aldehydes

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1037	Methacrolein	C4H6O	655.8500	6.2456
1002	Acetaldehyde	C2H4O	1036.0965	10.1522
1003	Propionaldehyde	C3H6O	658.9796	5.6218
1041	Benzaldehyde	C7H6O	463.2031	3.0982
1034	Acrolein	C3H4O	410.8975	3.2650

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1005	N-Butyraldehyde	C4H8O	687.8918	5.3555
1036	Trans-2-Butenal	C4H6O	249.6338	1.0203
1007	Valeraldehyde	C5H10O	745.4265	5.0314
1006	Isobutyraldehyde	C4H8O	816.4921	6.0897
1009	1-Hexanal	C6H12O	473.7035	2.8359
1040	P-Tolualdehyde	C8H8O	558.2973	3.0396
1016	2-Methylhexanal	C7H14O	624.7217	3.8930
1017	3-Methylhexanal	C7H14O	560.5487	4.2857
1008	1-Heptanal	C7H14O	413.6851	2.7002
1013	2-Ethylhexanal	C8H16O	676.7584	4.1415
1010	1-Octanal	C8H16O	492.7973	2.7189
1011	1-Nonanal	C9H18O	819.6000	4.0031
1020	1-Decanal	C10H20O	712.5103	3.8681
1021	1-Undecanal	C11H22O	911.4862	4.5612
1025	Dodecanal	C12H24O	648.9258	3.8588
1026	1-Tridecanal	C13H26O	602.6862	3.6390
1014	1,2-Ethanedione	C2H2O2	1439.4386	15.1836
1044	1,4BenzDicarboxAldehy	C8H6O2	673.1368	3.5772

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Epoxides

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1440	ISOBUTYLENE OXID	C4H8O	463.6704	2.6443
1478	Furan	C4H4O	1037.4565	6.8198
1443	1,3-Propylene Ox	C3H6O	208.6270	0.7667
1479	Tetrahydrofuran	C4H8O	470.0386	2.2203
1477	2,5-Dihydrofuran	C4H6O	410.7607	2.8961
1471	1,2-Epoxybutane	C4H8O	305.3265	1.2600
1408	1-Methoxypropane	C4H10O	752.0407	5.5644
1442	1,2-Propylene Ox	C3H6O	323.4995	1.1572
1411	2-Methoxypropane	C4H10O	1050.5430	9.2136
1421	1,4-Dioxane	C4H8O2	189.9337	0.6829
2422	1,3-DIOXANE	C4H8O2	172.4823	0.4421
1426	2-Methoxybutane	C5H12O	851.1246	6.3889
1422	Trioxane	C3H6O3	101.6123	0.1634
1413	1-Methoxybutane	C5H12O	634.8276	4.0836
1461	Methoxybenzene	C7H8O	405.5677	1.8757
1448	1-Ethoxybutane	C6H14O	394.4566	2.5133
1429	1-MethoxyPentane	C6H14O	495.7809	2.8554
6885	Ethyl-3-Ethoxypr	C7H14O3	711.3182	4.8727

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Ether

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1401	Dimethyl Ether	C2H6O	1660.2565	19.4146
1407	MethylEthylEther	C3H8O	1128.9941	8.7848
1470	VinylMethylEther	C3H6O	1060.4843	8.1081
1405	MTBE	C5H12O	921.0609	6.9923
1445	VinylEthyl Ether	C4H8O	742.6428	5.3506
1402	Diethyl Ether	C4H10O	802.5059	6.5489
1431	Methylal	C3H8O2	808.8417	4.7408
1428	T-But EthylEther	C6H14O	968.2822	7.7146
1427	TAME	C6H14O	647.2208	4.2364
1410	Mth Isobut Ether	C5H12O	864.3649	6.6047
1430	Eth-t-Pent-Ether	C7H16O	874.0837	6.9644
1403	DiisopropylEther	C6H14O	1193.2775	12.5009
1415	Eth Propyl Ether	C5H12O	725.4442	5.0707
1455	Dimethyl Acetal	C4H10O2	365.5007	1.4146
1446	Dipropyl Ether	C6H14O	659.0910	4.5857
1447	Butyl VinylEther	C6H12O	561.7962	2.6903
1462	EthylPhenylEther	C8H10O	589.3793	2.8431
1406	Di-sec-But Ether	C8H18O	980.2046	7.4413
1432	Acetal	C6H14O2	1309.8903	9.8353
1460	BenzylEthylEther	C9H12O	657.3704	4.2024
1050	Paraldehyde	C6H12O3	871.7612	4.3093
1404	Di-n-Butyl Ether	C8H18O	569.4013	3.1291
1420	Anethole	C10H12O	455.6681	1.7315
1456	DimethylCarbitol	C6H14O3	274.7765	0.7403
1463	Dibenzyl Ether	C14H14O	1641.3143	7.6818
1425	Di-n-PentylEther	C10H22O	618.3165	3.7895
1458	Diethyl Carbitol	C8H18O3	571.1699	2.6257
1412	Dihexyl Ether	C12H26O	690.3954	2.7407
1454	Triglyme	C8H18O4	526.7241	1.2207
1459	Dibutyl Carbitol	C12H26O3	887.7778	6.7994
1424	Di-n-Octyl Ether	C16H34O	1400.3343	6.5429
1457	Tetraglyme	C10H22O5	715.4119	2.2937
1418	Dinonyl Ether	C18H38O	2579.5817	13.6678
2432	ETHYLAL	C5H12O2	719.2369	5.3994
2405	DIISOBUTYL ETHER	C8H18O	991.1265	7.2611
2456	Ethyl Glyme	C6H14O2	549.5067	2.2276
2417	ETHYLHEXYL ETHER	C8H18O	512.6850	2.3065
2415	ETHYLISOPROPETH	C5H12O	1029.9935	8.8024

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Formates

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1301	Methyl Formate	C2H4O2	1167.3055	8.9921
1311	Vinyl Formate	C3H4O2	1375.7698	9.6846
1302	Ethyl Formate	C3H6O2	1069.0460	9.2001
2306	t-Butyl Formate	C5H10O2	1553.4157	17.0876
1303	Propyl Formate	C4H8O2	1182.5132	8.4344
2305	sec-ButylFormate	C5H10O2	1348.6845	11.9526
2311	CYCLOHEXL FORMAT	C7H12O2	1473.8828	11.6951
1304	N-Butyl Formate	C5H10O2	1845.1176	13.4342
1305	Isobutyl Formate	C5H10O2	1172.5606	9.9287
2350	Benzyl Formate	C8H8O2	871.8880	5.5263
2307	n-Hexyl Formate	C7H14O2	786.1166	4.5387
1306	N-Pentyl Formate	C6H12O2	805.9659	5.3694
2308	n-Heptyl Formate	C8H16O2	634.8152	4.7223
1308	N-Octyl Formate	C9H18O2	835.1273	7.3438
1309	n-Nonyl Formate	C10H20O2	1110.1966	7.4906
1310	n-Decyl Formate	C11H22O2	1048.9585	6.8494

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Esters

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1351	Mth Methacrylate	C5H8O2	514.5833	3.4671
1312	Methyl Acetate	C3H6O2	674.4265	4.7541
1331	Vinyl Propionate	C5H8O2	731.5656	5.2933
1321	Vinyl Acetate	C4H6O2	769.0807	5.7361
1352	Eth MthAcrylate	C6H10O2	773.7027	7.4091
1322	MethylPropionate	C4H8O2	688.0088	4.7325
1341	Methyl Acrylate	C4H6O2	883.3194	6.3354
1313	Ethyl Acetate	C4H8O2	712.5732	5.1580
1319	IsopropylAcetate	C5H10O2	1091.9114	10.5244
1332	Methyl Butyrate	C5H10O2	711.3389	5.0178
1342	Ethyl Acrylate	C5H8O2	694.8651	5.0225
1318	Allyl Acetate	C5H8O2	563.6062	4.7104
1314	N-Propyl Acetate	C5H10O2	739.1735	5.0800
1323	Ethyl Propionate	C5H10O2	935.4845	6.8720
1360	I-But I-Butyrate	C8H16O2	1211.1734	12.0175
1320	Sec-ButylAcetate	C6H12O2	1004.4421	9.1223

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1336	PropylI-Butyrate	C7H14O2	1021.4655	7.5440
1353	N-C3-Mthacrylate	C7H12O2	793.4887	5.4603
1333	Ethyl Butyrate	C6H12O2	805.6617	7.6685
1347	EthylIsovalerate	C7H14O2	1014.2560	8.8713
1315	N-Butyl Acetate	C6H12O2	770.8117	5.1967
1390	Methyl Benzoate	C8H8O2	646.4985	4.4455
1388	ISOBUTYL MTHACR	C8H14O2	732.0562	7.0094
1343	1-PropylAcrylate	C6H10O2	754.7697	4.9152
1316	Isobutyl Acetate	C6H12O2	874.1140	7.1686
1344	N-Butyl Acrylate	C7H12O2	663.8927	5.4332
1357	Pentyl Acetate	C7H14O2	585.7661	4.0086
1327	N-PropN-Butyrate	C7H14O2	817.5554	6.8730
1324	N-PropPropionate	C6H12O2	722.3339	5.7190
1291	Acetic Anhydride	C4H6O3	451.0649	2.8468
1389	N-ButMthacrylate	C8H14O2	773.2462	5.6054
1359	Benzyl Acetate	C9H10O2	866.4736	5.9936
1326	N-But Propionate	C7H14O2	744.6546	5.1633
1391	Ethyl Benzoate	C9H10O2	837.8916	7.4082
1897	CH3OC3H600CH3	C6H12O3	713.6382	4.3379
1392	DiethylCarbonate	C5H10O3	646.4798	4.3113
1385	N-But N-Butyrate	C8H16O2	570.6493	4.8415
1317	IsopentylAcetate	C7H14O2	727.1031	5.9847
1363	N-Hexyl Acetate	C8H16O2	687.3672	4.5523
1387	Ethylene Acetate	C6H10O4	720.2542	1.9544
1393	Diethyl Oxalate	C6H10O4	975.9459	6.4799
1365	Butyl Benzoate	C11H14O2	1075.5882	8.8785
1361	I-C5 I-Valerate	C10H20O2	1116.0058	13.0476
1367	Heptyl Acetate	C9H18O2	731.3011	4.6309
1346	N-Butyl Valerate	C9H18O2	840.5804	5.8295
1358	2-C2-C6 Acetate	C10H20O2	1136.7198	9.8233
1394	Diethyl Malonate	C7H12O4	884.0835	6.4580
1292	Propionyl Oxide	C6H10O3	1009.0226	8.6210
1364	Benzyl Benzoate	C14H12O2	1129.1180	11.9766
1381	2Mth p-Phthalate	C10H10O4	1033.1113	11.8261
1368	n-Octyl Acetate	C10H20O2	388.4391	2.5237
1377	DiMthI-Phthalate	C10H10O4	753.8626	10.1597
1896	Ethylene DiAcr	C8H10O4	601.0804	3.5832
1386	2-Ethylhexyl Acr	C11H20O2	1154.6018	9.4980
1395	Methyl Decanoate	C11H22O2	858.4919	5.3489
1369	n-Nonyl Acetate	C11H22O2	634.0239	4.0661
1370	n-Decyl Acetate	C12H24O2	2070.3429	13.5058
1345	N-ButylNonanoate	C13H26O2	2149.5613	32.7743
1375	DiProp Phthalate	C14H18O4	3352.2332	43.1925

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1376	Diisobutyl Phtha	C16H22O4	5042.1496	74.3140
1396	IsopropMyristate	C17H34O2	2490.5150	22.5013
1383	Butyl Stearate	C22H44O2	8126.7961	130.1988
1362	Methyl Oleate	C19H36O2	1837.6133	15.0841
1355	Diisooctyl Phtha	C24H38O4	12292.2824	239.3768
1382	DioctylTerephtha	C24H38O4	24459.2019	500.5597
1384	DIBUTYL SEBACATE	C18H34O4	6413.6650	67.6859
1371	Diisodecyl Phtha	C28H46O4	16890.7142	541.6948
1354	DioctylPhthalate	C24H38O4	24016.1869	622.7167
2375	DiethylPhthalate	C12H14O4	2271.5774	22.6970
2388	Dipropyl Maleate	C10H16O4	1575.6138	10.9261
2381	Diallyl Maleate	C10H12O4	1001.0561	5.4727
2370	Glyceryl Triacet	C9H14O6	3726.5353	33.4461
2382	Dibutyl Maleate	C12H20O4	1412.7045	9.8393
2376	DibutylPhthalate	C16H22O4	2969.7655	40.4850
2353	CetylMthacrylate	C20H38O2	2756.9298	28.8530
2379	Dihexyl Adipate	C18H34O4	4545.4105	54.6005
2321	T-Butyl Acetate	C6H12O2	1029.0070	9.6195
2332	Methl.I-butyrate	C5H10O2	880.9313	7.3642
2354	AllylMthacrylate	C7H10O2	767.5244	4.7804
2364	CYCLOHEXL ACETAT	C8H14O2	1082.4501	8.5727
2337	EthylIsobutyrate	C6H12O2	1102.2737	11.1612
2384	IsobutylAcrylate	C7H12O2	899.4654	6.7227
2380	1,1-Diacetoxy C2	C6H10O4	1082.2462	8.5446
2392	n-PropylBenzoate	C10H12O2	1193.6735	10.3869
2387	Dimethyl Maleate	C6H8O4	420.8563	1.9375
2377	DiMth Phthalate	C10H10O4	1211.6993	9.9665
2386	Diethyl Maleate	C8H12O4	903.5335	7.4391
2385	Mth Dodecanoate	C13H26O2	937.9301	6.3704
3379	Dioctyl Adipate	C22H42O4	5895.6203	116.0100
5886	Mth Acetoacetate	C5H8O3	461.8793	2.2175
5884	Ethoxy Acetate	C6H12O3	559.2390	2.6716
5887	EthAcetoAcetate	C6H10O3	653.5067	4.7303
5885	Carbitol Acetate	C8H16O4	979.0963	6.4876

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Table E.2 Continued

Ketones

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1096	Methyl Isopropen	C5H8O	600.7004	4.7773

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1079	Cyclopentanone	C5H8O	372.3122	1.9447
1051	Acetone	C3H6O	581.4232	4.4304
1052	MEK	C4H8O	594.7957	4.5801
1065	Mesityl Oxide	C6H10O	611.5995	4.2167
1066	T-But Mth Ketone	C6H12O	932.7090	8.5957
1060	2-Pentanone	C5H10O	582.8466	4.2189
1061	Mth iC3 Ketone	C5H10O	720.8744	6.5575
1053	Diethyl Ketone	C5H10O	616.1495	5.0495
1059	3-Hexanone	C6H12O	662.3485	4.7893
1099	Diketene	C4H4O2	104.2526	0.2590
1055	Sec-ButMthKetone	C6H12O	735.4510	6.3670
1054	MIBK	C6H12O	778.7776	6.3193
1095	EthIsopropKetone	C6H12O	892.9364	7.0398
1063	2-Heptanone	C7H14O	581.3589	3.7087
1064	5-Mth-2-Hexanone	C7H14O	1228.2999	8.2133
1058	4-Heptanone	C7H14O	905.3193	7.1311
1057	3-Heptanone	C7H14O	636.2880	3.9337
1076	2,4-Pentanedione	C5H8O2	950.7890	20.6222
1068	DiisobutylKetone	C9H18O	1199.2426	10.9423
1097	2-CycC6 CycC6one	C12H20O	1465.2888	9.1485
1083	2-Octanone	C8H16O	586.0490	3.8070
1073	Dibutyl Ketone	C9H18O	745.5274	5.1268
1062	2-Hexanone	C6H12O	322.0388	2.1460
1077	Isophorone	C9H14O	440.5335	3.0708
1090	Acetophenone	C8H8O	532.7194	3.4362
1080	Cyclohexanone	C6H10O	398.7531	2.2735
1074	2-Nonanone	C9H18O	647.8308	4.1794

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Alcohol-Ethers

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
2862	2-Butoxyethanol	C6H14O2	943.9989	11.2859
4857	butyl carbitol	C8H18O3	941.9126	11.0788
2898	2-Chloroethanol	C2H5ClO	309.6387	2.6633
2864	Carbitol	C6H14O3	630.0823	5.9317
3854	Methyl propasol	C4H10O2	1043.2078	15.5530
2860	2-Methoxyethanol	C3H8O2	578.9170	5.3031
2854	DiacetoneAlcohol	C6H12O2	1829.9189	35.9877
2861	2-Ethoxyethanol	C4H10O2	764.1077	8.8296

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

2889	HydroxyAcetone	C3H6O2	656.9553	8.5850
3856	1tButoxy2Propnol	C7H16O2	4132.2212	58.7175
3858	PROPGLYC2tBUTYL	C7H16O2	2655.1675	33.0068
4855	2-Propoxyethanol	C5H12O2	979.8022	12.4784
4849	Acetovanillone	C9H10O3	1470.9310	9.6417
5883	Ethyl Lactate	C5H10O3	2048.2737	46.1922
6883	2-HydroxyEth Acr	C5H8O3	365.6192	1.9252
2863	Methyl Carbitol	C5H12O3	492.0110	4.0156
3855	Dowanol DPM	C7H16O3	2011.0109	34.4333
3857	TriPropGlymEthlE	C10H22O4	3483.7863	41.0829

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Hydrocarbons

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
404	DiMth-Acetylene	C4H6	759.2270	6.7414
202	Propylene	C3H6	3383.9032	68.2258
412	2-Pentyne	C5H8	1813.6153	35.7840
207	2-Methylpropene	C4H8	1622.5834	21.6518
204	1-Butene	C4H8	1643.9880	21.3330
205	Cis-2-Butene	C4H8	1395.6917	15.6540
402	Propyne	C3H4	1068.2547	9.4818
406	3-Hexyne	C6H10	578.7851	5.1130
206	Trans-2-Butene	C4H8	1568.7453	19.9531
407	2-Hexyne	C6H10	525.9195	3.8406
231	33-2Mth-1-Butene	C6H12	1225.6412	12.3813
230	23-2Mth-1-Butene	C6H12	843.0123	7.2139
229	2-Ethyl-1-Butene	C6H12	632.1936	4.5055
8	I-Pentane	C5H12	1106.4879	12.3909
14	2,2-DiMth-Butane	C6H14	1001.7892	9.9001
232	23-2Mth-2-Butene	C6H12	621.9060	4.1575
213	3-Mth-1-Butene	C5H10	1417.9971	16.5270
212	2-Mth-1-Butene	C5H10	681.2649	6.1865
211	Trans-2-Pentene	C5H10	1066.8516	9.6873
210	Cis-2-Pentene	C5H10	929.5887	8.1975
223	4-Mth-1-Pentene	C6H12	837.1074	7.6106
221	2-Mth-1-Pentene	C6H12	731.7446	5.4429
248	2-t-Butylpropene	C7H14	858.3553	6.5935
227	Cs-4-Mth-2-C5H10	C6H12	1085.3045	9.9845
224	2-Mth-2-Pentene	C6H12	771.2393	5.7105

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

403	1-Butyne	C4H6	757.3296	5.6959
15	2,3-DiMth-Butane	C6H14	928.7283	8.4663
214	2-Mth-2-Butene	C5H10	890.1240	7.9144
228	Ts-4-Mth-2-C5H10	C6H12	1020.2947	8.8037
225	Cs-3-Mth-2-C5H10	C6H12	749.5102	5.8351
218	Trans-2-Hexene	C6H12	761.0651	5.5611
2226	3-METH-Tr-2Pente	C6H12	690.8908	4.7526
222	3-Mth-1-Pentene	C6H12	903.4312	8.2539
257	2-Diisobutylene	C8H16	901.1939	6.5621
256	1-Diisobutylene	C8H16	806.6366	6.2356
217	Cis-2-Hexene	C6H12	724.5053	5.5038
2414	1-Heptyne	C7H12	363.3484	1.9850
13	3-Methylpentane	C6H14	765.7164	6.2463
219	Cis-3-Hexene	C6H12	765.4367	5.9805
12	2-Methylpentane	C6H14	860.5005	7.5376
220	Trans-3-Hexene	C6H12	780.6961	5.8376
405	1-Pentyne	C5H8	552.2385	3.9577
209	1-Pentene	C5H10	1010.6268	9.6906
11	N-Hexane	C6H14	920.6135	6.3921
235	Cis-2-Heptene	C7H14	605.6041	4.2581
249	Cis-3-Heptene	C7H14	1134.4617	7.8165
216	1-Hexene	C6H12	667.7073	4.9658
239	3-Eth-1-Pentene	C7H14	706.5395	4.7735
226	4-Mth-1-Hexene	C7H14	702.1455	4.5970
240	3-Mth-1-Hexene	C7H14	677.6134	4.5602
419	3-Mth-1-Butyne	C5H8	846.3336	7.0310
233	2-Eth-1-Pentene	C7H14	559.3882	3.4438
238	2-Mth-1-Hexene	C7H14	623.3626	4.1282
416	1-Octyne	C8H14	327.4065	1.5659
289	2,3Dimeth Hexene	C8H16	659.3680	4.2510
234	1-Heptene	C7H14	434.9939	2.6642
413	1-Hexyne	C6H10	362.6594	2.0974
237	Trans-3-Heptene	C7H14	629.6253	4.3269
236	Trans-2-Heptene	C7H14	568.6726	3.8387
251	Trans-2-Octene	C8H16	591.6216	3.8822
279	Trans-4-Octene	C8H16	619.9809	4.0077
277	Trans-3-Octene	C8H16	567.7441	3.7253
2252	2Methl-1-Heptene	C8H16	522.9173	3.4030
250	1-Octene	C8H16	317.2086	1.6804
258	2-Ethyl-1-Hexene	C8H16	521.0895	3.3489
280	3-Octene	C8H16	583.5193	3.9747
278	4-Octene	C8H16	625.7038	4.3812
276	2-Octene	C8H16	316.4428	2.0649

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

259	1-Nonene	C9H18	403.7514	1.9058
262	1-Dodecene	C12H24	511.9734	2.3697
263	1-Tridecene	C13H26	556.3378	2.5010
264	1-Tetradecene	C14H28	394.4659	1.7690
265	1-Pentadecene	C15H30	597.1185	2.8900
266	1-Hexadecene	C16H32	819.8037	3.8884
267	1-Octadecene	C18H36	722.9393	4.0104
281	1-Heptadecene	C17H34	1733.5227	9.1028
284	1-Eicosene	C20H40	1111.2258	7.1522
283	1-Nonadecene	C19H38	1317.5123	7.6321
3	Propane	C3H8	3096.5794	65.3656
4	I-Butane	C4H10	1456.3181	23.7563
9	Neopentane	C5H12	2032.2180	31.7696
5	N-Butane	C4H10	1382.4989	18.6672
7	pentane	C5H12	835.0044	7.8484
44	Hexamethylethane	C8H18	744.5422	4.9026
25	223-TriMthButane	C7H16	812.7066	6.7030
24	3,3-DiMthPentane	C7H16	743.9512	5.7864
51	2,2,3,3-4Mth-C5	C9H20	544.6718	2.9683
21	2,2-DiMthPentane	C7H16	869.4995	7.2097
42	2,3,3-TriMth-C5	C8H18	580.5430	3.8372
22	2,3-DiMthPentane	C7H16	650.1582	4.7135
40	2,2,3-TriMth-C5	C8H18	689.5106	4.7511
23	2,4-DiMthPentane	C7H16	906.7541	7.7369
41	2,2,4-TriMth-C5	C8H18	886.5065	7.6554
39	3-Mth-3-Eth-C5	C8H18	550.7184	3.5044
20	3-Ethylpentane	C7H16	654.8778	4.3893
52	2,2,3,4-4Mth-C5	C9H20	680.8891	4.6072
54	2334TetrMethPent	C9H20	439.1417	2.4974
53	2,2,4,4-4Mth-C5	C9H20	808.3271	6.2184
43	2,3,4-TriMth-C5	C8H18	655.2942	4.5272
36	3,3-DiMth-Hexane	C8H18	744.3526	4.9686
19	3-Methylhexane	C7H16	649.5310	4.5409
18	2-Methylhexane	C7H16	640.3833	4.5799
38	2-Mth-3-Eth-C5	C8H18	721.6120	4.7684
190	2,2-2C1-3-C2-C5	C9H20	665.2444	4.2950
32	2,2-DiMth-Hexane	C8H18	607.8241	4.3420
37	3,4-DiMth-Hexane	C8H18	436.7596	2.7480
50	3,3-DiEthPentane	C9H20	512.9804	3.0853
34	2,4-DiMth-Hexane	C8H18	1398.1636	10.0781
33	2,3-DiMth-Hexane	C8H18	698.7275	4.4549
17	N-Heptane	C7H16	510.2320	3.0534
49	244TriMethHexane	C9H20	773.5913	5.5132

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

192	2,4-2C1-3-C2-C5	C9H20	614.0485	4.1100
47	2,2,5-TriMth-C6	C9H20	594.4466	4.4137
35	2,5-DiMth-Hexane	C8H18	698.0680	4.9953
31	3-Ethylhexane	C8H18	451.9575	2.8125
30	4-Methylheptane	C8H18	441.7684	2.7286
29	3-Methylheptane	C8H18	484.9579	2.9749
28	2-Methylheptane	C8H18	446.9703	2.7927
96	2,2-DiMthHeptane	C9H20	727.3043	4.8467
176	2,6-DiMthHeptane	C9H20	417.4960	2.6061
27	N-Octane	C8H18	489.9970	2.5938
94	3-Ethylheptane	C9H20	568.4290	3.3080
92	3-Methyloctane	C9H20	534.8759	2.9273
93	4-Methyloctane	C9H20	603.9783	3.4632
91	2-Methyloctane	C9H20	570.1352	3.0932
72	2,2-DiMthOctane	C10H22	654.4306	3.9042
2095	2,3Dimethloctane	C10H22	835.2731	4.6772
2096	2,4Dimethloctane	C10H22	714.4085	4.4132
2098	2,6DimethlOctane	C10H22	674.4877	4.0299
2097	2,5Dimethloctane	C10H22	675.2782	4.1266
2099	2,7DimethlOctane	C10H22	770.5162	4.5907
46	N-Nonane	C9H20	288.2227	1.3873
88	5-Methylnonane	C10H22	589.2211	3.1202
85	3-Methylnonane	C10H22	697.3310	3.6327
87	4-Methylnonane	C10H22	567.0395	3.2025
86	2-Methylnonane	C10H22	599.8461	2.9342
56	N-Decane	C10H22	783.6119	3.5040
63	N-Undecane	C11H24	401.9194	1.8449
64	N-Dodecane	C12H26	305.0192	1.3144
65	N-Tridecane	C13H28	532.0529	2.4082
66	N-Tetradecane	C14H30	334.6180	1.5940
67	N-Pentadecane	C15H32	1262.9692	5.9402
68	N-Hexadecane	C16H34	1079.3238	5.4797
69	N-Heptadecane	C17H36	783.4638	4.0894
70	N-Octadecane	C18H38	1202.8028	6.8996
71	N-Nonadecane	C19H40	2171.2479	13.2740
73	N-Eicosane	C20H42	2871.1116	19.1892
74	n-HENEICOSANE	C21H44	2020.7231	14.8735
75	n-DOCOSANE	C22H46	1601.6851	12.9640
76	n-TRICOSANE	C23H48	4262.1224	34.5601
77	n-Tetracosane	C24H50	1645.7290	14.2899
78	n-PENTACOSANE	C25H52	2511.4933	23.5548
79	n-HEXACOSANE	C26H54	7721.7813	74.5040
81	n-Octacosane	C28H58	8782.7421	88.1942
2081	n-TRICONTANE	C30H62	6174.4900	63.5621
2082	n-Dotriacontane	C32H66	36177.2402	373.2124

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Cyclic Hydrocarbons

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
269	Cyclopentene	C5H8	1286.3533	12.8296
270	Cyclohexene	C6H10	696.9493	5.3543
287	3MthCyclopentene	C6H10	1113.7172	10.3369
286	1-MthCyclPentene	C6H10	1065.5523	9.7764
288	4MthCyclopenten	C6H10	1101.9013	10.0263
273	Cycloheptene	C7H12	733.4405	5.1641
274	Cyclooctene	C8H14	727.7022	4.8019
101	Cyclopropane	C3H6	3234.9788	56.6535
810	ADAMANTANE	C10H16	579.6698	5.0567
102	Cyclobutane	C4H8	1417.8332	16.3842
104	Cyclopentane	C5H10	1046.8186	9.2194
137	Cyclohexane	C6H12	929.1033	7.4530
105	MthCyclopentane	C6H12	995.7141	8.6369
146	Cs-1,4-2C1-CycC6	C8H16	774.8822	5.8978
142	Cs-1,2-2C1-CycC6	C8H16	700.8456	4.8710
141	1,1-2C1-CycC6	C8H16	985.3806	7.7367
145	Ts-1,3-2C1-CycC6	C8H16	765.2735	5.7754
144	Cs-1,3-2C1-CycC6	C8H16	878.0777	7.3631
147	Ts-1,4-2C1-CycC6	C8H16	860.4001	7.5237
143	Ts-1,2-2C1-CycC6	C8H16	773.5285	6.3667
138	MthCyclohexane	C7H14	873.5138	7.0267
159	Cycloheptane	C7H14	722.6454	4.5131
140	Ethylcyclohexane	C8H16	716.3403	4.9397
154	Trans-Decalin	C10H18	710.8337	4.7423
149	N-PropylCyc-C6	C9H18	703.1776	4.4264
109	Cs-1,2-2C1-CycC5	C7H14	589.6785	4.2378
110	Ts-1,2-2C1-CycC5	C7H14	802.9780	6.7067
112	Ts-1,3-2C1-CycC5	C7H14	522.8962	4.3933
107	Eth-Cyclopentane	C7H14	987.1775	6.7079
114	N-PropCycPentane	C8H16	466.3601	2.8679
108	1,1-DiMthCycC5	C7H14	1245.8021	10.1824
111	Cs-1,3-2C1-CycC5	C7H14	1216.0291	10.5744
152	N-ButylCycHexane	C10H20	639.3769	3.7444
160	Cyclooctane	C8H16	567.5025	3.1938
153	Cis-Decalin	C10H18	974.7922	5.3849
115	ISOPROPYLCYCLOPENTANE	C8H16	728.8940	5.0384
150	Isopropyl-CycC6	C9H18	833.4934	5.3437
116	1-C1-1-C2-CycC5	C8H16	830.4051	5.5508
122	Butylcyclpentane	C9H18	594.0262	3.2289
155	1,1-Bicyclohexyl	C12H22	1106.6615	7.1959
158	N-Decylcyclo-C6	C16H32	1530.9989	8.6778

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Aromatic Hydrocarbons

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
307	1,4-Pentadiene	C5H8	1038.5807	8.9104
306	1-ts3-Pentadiene	C5H8	706.3262	4.8474
414	2-Methyl-1-Butenyne	C5H6	612.3343	6.0875
305	Cs1,3-Pentadiene	C5H8	693.2583	4.3402
309	Isoprene	C5H8	799.4907	5.9626
421	1-Pentene-4-yne	C5H6	477.0802	3.5954
303	1,3-Butadiene	C4H6	1425.5923	14.6811
332	1,4-CyclHexadien	C6H8	593.1666	2.5977
501	Benzene	C6H6	873.1499	6.8320
315	Cyclopentadiene	C5H6	1094.0684	13.8964
319	Diisopropenyl	C6H10	519.1754	2.9970
615	Ethynylbezene	C8H6	465.9203	3.4498
601	Styrene	C8H8	645.9164	3.4351
331	1,3-CycHexadiene	C6H8	737.2399	4.6097
310	1,5-Hexadiene	C6H10	704.6107	5.5937
312	MthCycPentadiene	C6H8	741.4290	4.6021
420	1-Pentene-3-yne	C5H6	695.6127	5.7036
502	Toluene	C7H8	776.8598	6.4230
521	T-Butylbenzene	C10H14	1557.6357	12.1285
320	Dipropylene	C6H10	518.5338	2.7857
520	Sec-Butylbenzene	C10H14	1304.3449	10.4680
313	1,4-Hexadiene	C6H10	753.4522	5.4189
314	Dipropylene	C6H10	645.3234	3.2105
316	DiCycPentadiene	C10H12	657.7711	4.4888
333	1,5-CycOctadiene	C8H12	487.0348	1.9536
701	Naphthalene	C10H8	530.5226	1.2617
504	Ethylbenzene	C8H10	782.1285	5.9907
820	Indan	C9H10	728.3641	4.5201
505	O-Xylene	C8H10	631.7780	4.6037
612	P-Methylstyrene	C9H10	1053.2848	6.0236
330	DIISOCROTYL	C8H14	448.8907	1.7450
507	P-Xylene	C8H10	801.3256	6.6406
329	DIISOBUTENYL	C8H14	524.1407	3.1628
506	M-Xylene	C8H10	781.7601	6.2913
603	Methylstyrene	C9H10	599.1788	3.4701
613	Alpha-MthStyrene	C9H10	591.8592	3.7449
510	Isopropylbenzene	C9H12	1241.2758	9.7381
724	2-Methylindene	C10H10	502.3426	2.0871
285	Vinylcyclohexene	C8H12	1210.0833	7.4714
803	Indene	C9H8	624.5666	1.3170
706	Tetralin	C10H12	476.4276	2.7717

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

511	O-Ethyltoluene	C9H12	714.3919	5.2198
723	1-Methylindene	C10H10	369.2357	1.3079
738	Fluorene	C13H10	778.4644	1.3884
619	Tr-1PropenylBz	C9H10	522.8513	2.7284
525	O-Diethylbenzene	C10H14	854.0695	6.4868
618	Propenyl Bz(cis)	C9H10	486.0798	2.9250
602	O-Methylstyrene	C9H10	584.8135	3.2441
702	1-MthNaphthalene	C11H10	535.0376	1.3957
509	N-Propylbenzene	C9H12	662.8633	5.0421
526	M-Diethylbenzene	C10H14	870.9064	6.9845
583	Cs-2-PhnButene-2	C10H12	632.6840	3.8178
543	M-DiisopropylBz	C12H18	1401.2079	13.6562
584	Ts-2-PhnButene-2	C10H12	1079.0120	8.8009
580	1,2-DiC1-3C2-Bz	C10H14	741.2642	5.1622
704	1-EthNaphthalene	C12H12	586.7543	3.4018
512	M-Ethyltoluene	C9H12	791.1763	6.3450
522	1-Mth-2-iC3-Benz	C10H14	999.3388	8.7857
513	P-Ethyltoluene	C9H12	575.8783	4.6268
514	1,2,3-Mesitylene	C9H12	592.4969	4.1485
614	M-Divinylbenzene	C10H10	574.6714	3.0028
524	1-Mth-4-iC3-Benz	C10H14	626.7726	5.2941
822	Gamma-Terpinene	C10H16	563.5302	2.6846
821	Alpha-Terpinene	C10H16	724.0833	4.2375
523	1-Mth-3-iC3-Benz	C10H14	991.7114	8.7898
703	2-MthNaphthalene	C11H10	619.9696	1.5818
557	CycHexylBenzene	C12H16	949.5044	5.1177
515	1,2,4-Mesitylene	C9H12	727.6984	5.5972
519	Isobutylbenzene	C10H14	909.7372	7.6864
424	DiPhnAcetylene	C14H10	909.9703	8.7048
544	P-DiisopropylBz	C12H18	1241.1620	10.1928
518	N-Butylbenzene	C10H14	734.9013	5.0590
516	1,3,5-Mesitylene	C9H12	861.4650	6.8396
809	Acenaphthalene	C12H8	629.1799	0.4874
725	123-TriMthIndene	C12H14	1030.9520	6.5221
527	1,4-DiEthBenzene	C10H14	1144.8800	8.6265
558	Diphenyl	C12H10	731.7216	1.9498
576	2-Ethyl-m-Xylene	C10H14	1051.3193	8.0578
620	p-ISOPROPENYLSTY	C11H12	404.8993	1.9911
585	o-PropylToluene	C10H14	756.1216	5.9410
577	2-Ethyl-p-Xylene	C10H14	880.5678	7.0192
579	4-Ethyl-o-Xylene	C10H14	1070.6726	8.1730
586	m-Propyltoluene	C10H14	817.2557	6.4070
587	p-Propyltoluene	C10H14	795.2960	6.1958

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

578	4-Ethyl-m-Xylene	C10H14	845.6394	6.6850
575	5-Ethyl-m-Xylene	C10H14	524.7210	4.2856
530	Prehnitene	C10H14	613.8516	3.7458
709	2,6-2Mth-Naphtha	C12H12	660.1009	2.0782
715	2,7-2Mth-Naphtha	C12H12	673.1321	2.1293
719	2-ETHYLNAPHTHALENE	C12H12	943.6057	2.9927
621	p-tert-BUTYLSTY	C12H16	685.1551	4.8468
532	1,2,4,5-TetMthBz	C10H14	768.2762	5.6324
531	1,2,3,5-TetMthBz	C10H14	779.5252	5.4705
533	p-tert-BUTYL ET	C12H18	1556.1385	12.7520
567	N-Pentylbenzene	C11H16	718.1910	4.7582
718	1-n-PROPYLNAPHTH	C13H14	833.1261	2.9992
562	1,1-DiPhnEthane	C14H14	1280.8995	10.8805
616	4-ISOBUTYLSTYRE	C12H16	437.0906	1.9824
260	1-Decene	C10H20	485.5052	2.1938
735	Cis-Stilbene	C14H12	1236.0170	5.0445
568	Hexylbenzene	C12H18	783.6615	5.2508
563	Diphenylmethane	C13H12	1093.7807	7.6483
564	1,2-DiPhnEthane	C14H14	1527.5751	12.2801
804	Anthracene	C14H10	446.6535	0.5311
736	Trans-Stilbene	C14H12	728.6158	3.5292
805	Phenanthrene	C14H10	571.5001	0.6192
713	1-ButNaphthalene	C14H16	586.6426	1.8508
807	Pyrene	C16H10	573.6684	0.3150
261	1-Undecene	C11H22	701.2461	3.0916
581	23-2C1-23-2PhnC4	C18H22	1507.2009	19.4072
549	N-Heptylbenzene	C13H20	1014.6650	6.9135
710	1-PhnNaphthalene	C16H12	1504.0916	3.1226
566	2,4-Diphenyl-4-M	C18H20	3032.6864	28.6453
561	O-Terphenyl	C18H14	4273.8221	20.0092
569	N-Octylbenzene	C14H22	1083.6425	7.4276
565	Triphenylmethane	C19H16	2959.3419	36.7942
714	N-C6-Naphthalene	C16H20	2198.3406	7.3061
717	Fluoranthene	C16H10	1356.8622	1.2076
716	1-Hexyl-Tetralin	C16H24	1477.9452	5.8330
731	TriPhnEthylene	C20H16	2355.4352	26.0926
806	Chrysene	C18H12	675.5987	0.2856
588	1,1,2TriPhenEth	C20H18	4480.1461	73.1180
711	1-n-NonylNaphtha	C19H26	1724.9864	10.2685
570	N-Nonylbenzene	C15H24	1391.4531	9.7764
712	1-Decyl Naphtha	C20H28	1895.7055	12.3169
559	P-Terphenyl	C18H14	1539.5552	2.5750
560	M-Terphenyl	C18H14	1939.0701	4.6511

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

589	TetraPhenylMetha	C25H20	3440.0024	22.5609
554	Decylbenzene	C16H26	744.2512	5.3463
732	TetraPhnEthylene	C26H20	3310.8306	23.8511
574	N-Dodecylbenzene	C18H30	817.2835	6.2039
571	N-Undecylbenzene	C17H28	1729.8438	12.6622
572	Tridecylbenzene	C19H32	3008.5463	23.4192
573	n-TETRADECYLBENZ	C20H34	1395.1826	12.1477
2575	n-PENTADECYLBENZ	C21H36	1485.6600	12.7778
2576	n-HEXADECYLBENZ	C22H38	1814.5619	16.4469
2577	n-HEPTADECYLBENZ	C23H40	3602.4449	37.9060
2578	n-OCTADECYLBENZE	C24H42	4934.8248	56.6430

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Halocarbons

DipID	Name	Formula	$P_{Joback}^{760mmHg}$	P_{Joback}^{10mmHg}
1544	Allyl Chloride	C3H5Cl	406.1918	2.5442
1595	2-Chloropropene	C3H5Cl	897.3104	10.4899
1531	3-Chloropropyne	C3H3Cl	205.4644	1.2170
1535	T-Butyl Chloride	C4H9Cl	831.1335	7.6855
1583	Chloroprene	C4H5Cl	603.3925	4.5485
1530	Isopropyl Cl	C3H7Cl	704.1039	5.6066
1572	O-DiCl-Benzene	C6H4Cl2	582.9426	4.6623
1585	Propyl Chloride	C3H7Cl	438.3111	2.7213
1684	Isopropyl Iodide	C3H7I	674.4454	6.1869
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	276.7032	1.0495
1651	2-Bromopropane	C3H7Br	837.8496	6.9143
1691	Iodobenzene	C6H5I	693.6269	5.5403
1860	Fluorobenzene	C6H5F	853.1769	6.1936
1571	Chlorobenzene	C6H5Cl	673.6773	5.6321
1680	Bromobenzene	C6H5Br	732.6069	5.9017
1526	1,2-DiCl-Propane	C3H6Cl2	335.4232	2.0354
1683	Propyl Iodide	C3H7I	497.9976	3.9418
1576	Benzotrichloride	C7H5Cl3	899.9335	11.3333
1536	2,3-DICHLOROBUT	C4H8Cl2	300.0279	1.4704
2638	2-Bromobutane	C4H9Br	615.7126	3.5042
1586	1-Chlorobutane	C4H9Cl	356.9565	1.8624
1573	M-DiCl-Benzene	C6H4Cl2	729.9422	7.1015
2634	Benzotrifluoride	C7H5F3	1068.6556	4.4079
1574	P-DiCl-Benzene	C6H4Cl2	690.9507	6.0476

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1650	1-Bromopropane	C3H7Br	549.2182	3.5810
1587	2-Chlorobutane	C4H9Cl	524.7802	3.8748
2653	8F-2-Butene	C4F8	749.8809	0.0862
1678	M-Dibromobenzene	C6H4Br2	840.5522	8.1594
1537	1,2-DiCl-Butane	C4H8Cl2	374.2966	2.1768
1597	34-DiCl-1-Butene	C4H6Cl2	310.6810	1.0483
1577	O-Chlorotoluene	C7H7Cl	703.7047	5.7228
1532	123-3Cl-Propane	C3H5Cl3	168.3239	0.6913
1578	P-Chlorotoluene	C7H7Cl	525.9725	3.6222
1562	Benzyl Chloride	C7H7Cl	364.4158	1.7978
2661	P-Bromotoluene	C7H7Br	746.7385	6.3504
1508	1,4-DiCl-Butane	C4H8Cl2	99.5877	0.2747
1655	1-Bromobutane	C4H9Br	515.3094	2.9228
1599	BenzylDichloride	C7H6Cl2	422.3786	3.4406
2652	Perfluoropropane	C3F8	1436.5167	0.4507
1505	2-Butylene DiCl	C4H6Cl2	90.0674	0.1873
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	132.1311	0.3733
1588	1-Chloropentane	C5H11Cl	291.0408	1.5972
2654	OctaF-CycButane	C4F8	893.2039	0.0691
1592	1,2,4-TriCl-Bz	C6H3Cl3	774.4683	8.7484
1579	2,4-2Cl-Toluene	C7H6Cl2	699.6742	5.7585
2593	1,3,5-TriCl-BZ	C6H3Cl3	828.4705	9.9368
1697	1-Br-Naphthalene	C10H7Br	605.0482	3.6919
1622	Perfluorobutane	C4F10	784.7449	0.0156
1857	P-Cl-Benzo-TriF	C7H4ClF3	1022.2257	5.9524
1509	1,5-DiCl-Pentane	C5H10Cl2	91.2108	0.2267
1589	1-Cl-Naphthalene	C10H7Cl	496.2242	1.3486
1864	Perfluorobenzene	C6F6	1852.1220	10.6866
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	1108.2023	7.1220
1667	1-Bromoheptane	C7H15Br	539.6912	2.4457
1575	HexaCl-Benzene	C6Cl6	1181.4857	7.3037
2640	Freon 123B1	C2HBrClF3	1492.0281	9.9121
1504	Vinyl Chloride	C2H3Cl	1511.6489	17.4264
1672	1,1-DiBr-Ethane	C2H4Br2	659.9046	3.4431
1580	Acetylene DiCl	C2H2Cl2	440.0687	2.5283
1692	Diiodomethane	CH2I2	322.8833	1.1396
1698	Bromoform	CHBr3	746.2075	5.5199
2687	Freon 13B1	CBrF3	8874.9623	189.3835
2690	Br-3F-Ethylene	C2BrF3	2184.8608	14.4577
1649	Tetrabromoethane	C2H2Br4	623.1549	3.1809
2686	Freon 12B1	CBrClF2	4075.0667	78.1423
1503	Ethyl Chloride	C2H5Cl	692.8828	5.7231
2641	Br-TriCl-Methane	CBrCl3	1200.6562	18.4267

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1641	Methyl Bromide	CH3Br	1174.9255	11.6138
2688	Freon 12B2	CBr2F2	2742.6629	50.7949
2545	2,3-DiCl-Propene	C3H4Cl2	290.2656	0.8614
1673	1,2-DiBr-Ethane	C2H4Br2	360.7190	2.1884
2637	Dibromomethane	CH2Br2	462.2872	2.2822
1542	TetraCl-Ethylene	C2Cl4	908.1225	11.7010
1541	TriCl-Ethylene	C2HCl3	789.7469	9.1587
1527	111-TriCl-Ethane	C2H3Cl3	902.4516	10.7296
1612	Cl-2F-Ethylene	C2HClF2	1792.4897	12.6164
1617	Ethyl Fluoride	C2H5F	879.0468	3.9863
2639	Br-Cl-Methane	CH2BrCl	470.0642	2.7457
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	899.1846	6.6713
1682	Ethyl Iodide	C2H5I	619.7433	5.2636
1522	1,1-DiCl-Ethane	C2H4Cl2	529.0668	3.8037
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	1318.5799	9.1172
1525	Hexachloroethane	C2Cl6	934.8981	9.3221
1528	1112-4Cl-Ethane	C2H2Cl4	544.3231	4.5192
1590	Penta-Cl-Ethane	C2HCl5	642.6079	7.2059
1529	1122-4Cl-Ethane	C2H2Cl4	363.8211	2.3756
2693	Perfluoroethane	C2F6	4353.5880	12.3282
1611	Freon 114B2	C2Br2F4	3425.7531	31.4193
2692	Cl-PentaF-Ethane	C2ClF5	3231.7191	19.2398
2655	122-3Cl-112-3FC2	C2Cl3F3	1864.2845	19.2668
1609	12-2Cl-1122-4FC2	C2Cl2F4	2291.9936	20.0788
2526	1,1-DiCl-Propane	C3H6Cl2	417.5875	2.5767
1645	Ethyl Bromide	C2H5Br	744.6949	5.6925
2658	1112-4Cl-22-2FC2	C2Cl4F2	1478.9452	15.5904
1619	111-3F-Ethane	C2H3F3	1445.7906	5.1342
1524	1,1,2-3Cl-Ethane	C2H3Cl3	305.2602	1.7971
1640	1,1-DiF-Ethane	C2H4F2	481.2950	0.8292
2691	Genetron 1113	C2ClF3	2205.7770	12.6255
2694	Vinyl Bromide	C2H3Br	1414.7014	18.6047
1694	Refrigerant 123	C2HCl2F3	1180.4944	7.2168
1523	1,2-DiCl-Ethane	C2H4Cl2	164.9961	0.6714
2656	1122-4Cl-12-2FC2	C2Cl4F2	1602.5989	17.9971
2527	1,3-DiCl-Propane	C3H6Cl2	147.5573	0.4668

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

Table E.2 Continued

Acids

DipID	Name	Formula	$P_{Joback}^{760\,mmHg}$	$P_{Joback}^{10\,mmHg}$
1277	Acrylic Acid	C3H4O2	641.3647	3.8227

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

1274	Ts-Crotonic Acid	C4H6O2	388.3643	0.7871
1279	Oleic Acid	C18H34O2	4560.0299	48.4220
1278	Methacrylic Acid	C4H6O2	1084.3304	4.0192
2271	Cinnamic Acid	C9H8O2	903.7980	2.1832
1266	n-UNDECANOIC ACI	C11H22O2	1275.5058	7.8217
1282	O-Toluic Acid	C8H8O2	1438.8089	9.0627
2283	IBUPROFEN	C13H18O2	5115.2730	41.9451
1261	Isovaleric Acid	C5H10O2	1143.5470	5.3505
1264	1,4-CychexDicarboxAcid	C8H12O4	1105.1105	3.2460
1283	P-Toluic Acid	C8H8O2	933.4702	4.5088
1257	3-MthButyricAcid	C5H10O2	951.2100	5.2574
1288	Isophthalic Acid	C8H6O4	155.0772	0.1609
2871	4CarboxAcidBzldhyde	C8H6O3	48.3163	0.0424
1256	N-Butyric Acid	C4H8O2	758.5630	3.0759
1276	Stearic Acid	C18H36O2	6506.0821	86.8094
1285	Adipic Acid	C6H10O4	1282.1792	5.2886
1273	Cs-Crotonic Acid	C4H6O2	635.3631	2.5659
4851	Diglycolic Acid	C4H6O5	1273.8275	2.2436
1286	Maleic Acid	C4H4O4	917.0881	2.7412
2277	Citraconic Acid	C5H6O4	475.7517	1.0633
2278	Itaconic Acid	C5H6O4	843.5979	2.4095
2281	Glutaric Acid	C5H8O4	1113.3160	3.1713
1271	TetradecylicAcid	C14H28O2	1835.2381	15.6888
1259	N-Nonanoic Acid	C9H18O2	2342.4890	11.4852
1280	Linoleic Acid	C18H32O2	5605.8573	65.9483
1260	Isobutyric Acid	C4H8O2	585.9781	2.9909
2268	Fumaric Acid	C4H4O4	1309.5484	3.4273
1287	Phthalic Acid	C8H6O4	8359.5771	76.2194
1289	TerephthalicAcid	C8H6O4	59.0011	0.0148
2280	Succinic Acid	C4H6O4	659.4564	1.2866
1270	Tridecanoic Acid	C13H26O2	1152.0628	9.0721
1254	N-Decanoic Acid	C10H20O2	902.1277	4.1793
2270	Suberic Acid	C8H14O4	1711.8065	8.9516
2255	Linolenic Acid	C18H30O2	8128.7589	89.8035
1262	N-Hexanoic Acid	C6H12O2	1168.6377	3.9082
4852	Levulinic Acid	C5H8O3	406.2077	1.2071
2275	Sebacic Acid	C10H18O4	2643.5631	19.2293
1255	Oxalic Acid	C2H2O4	229.9843	0.2688
2259	PentadecylicAcid	C15H30O2	2639.9223	28.0127
2266	NonadecanoicAcid	C19H38O2	11388.0458	157.4154
2269	Pimelic Acid	C7H12O4	1541.1136	6.0937
1252	Acetic Acid	C2H4O2	778.2355	6.7759
3268	Malonic Acid	C3H4O4	466.8247	0.7492

Table E.2 Vapor Pressures Calculated by the Joback Method (Continued)

2279	2-EthButyricAcid	C6H12O2	1311.2907	7.9754
1265	N-Octanoic Acid	C8H16O2	1006.4086	3.9148
2258	NeopentanoicAcid	C5H10O2	1941.8452	7.5258
2257	Azelaic Acid	C9H16O4	2189.6243	14.0768
1281	Benzoic Acid	C7H6O2	1042.6294	3.8069
1269	Dodecanoic Acid	C12H24O2	3836.0920	24.3700
2261	Heptanoic Acid	C7H14O2	654.5425	2.4404
1258	N-Valeric Acid	C5H10O2	1130.7508	4.0693
2265	HeptadecylicAcid	C17H34O2	3217.8379	38.5606
2267	N-Eicosanic Acid	C20H40O2	9697.6296	142.3594
1253	Propionic Acid	C3H6O2	768.2091	4.4045
5877	Ascorbic Acid	C6H8O6	50868.1603	93.6105
1272	HexadecanoicAcid	C16H32O2	3459.6116	39.3850

Table E. 3 Vapor Pressures Calculated by the Gani Method

Alcohols

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1181	Phenol	C6H6O	613.8897	4.1899
1182	O-Cresol	C7H8O	1022.2656	9.3750
1183	M-Cresol	C7H8O	689.6330	4.3623
1176	2,6-Xylenol	C8H10O	1099.4265	13.2160
1111	2-Mth-2-Butanol	C5H12O	2626.2754	23.3321
1178	3,5-Xylenol	C8H10O	1160.8505	7.0859
1133	2-Octanol	C8H18O	2548.9298	25.2064
2885	4-HYDROXYSTYREN	C8H8O	979.3038	7.6765
1197	P-t-Butylphenol	C10H14O	766.4755	5.4973
1172	2,4-Xylenol	C8H10O	645.3959	5.3801
1184	P-Cresol	C7H8O	992.9203	5.7162
1151	Cyclohexanol	C6H12O	955.6767	6.3699
1170	2,3-Xylenol	C8H10O	880.4362	6.9681
1187	P-Ethyl Phenol	C8H10O	709.7881	4.8285
2859	P-Methoxyphenol	C7H8O2	561.4508	2.1314
1121	2-Ethylhexanol	C8H18O	1313.7826	11.4599
1179	PropargylAlcohol	C3H4O	771.6787	7.8992
1123	3-Mth-1-Butanol	C5H12O	971.1513	5.4979
2196	P-t-Amylphenol	C11H16O	538.9190	4.7838
1174	2,5-Xylenol	C8H10O	948.1856	8.6269
1115	2-Hexanol	C6H14O	1791.7349	15.5956
1152	1-MthCycHexanol	C7H14O	1360.1202	29.0358
4854	Guaiacol	C7H8O2	2432.1252	28.7831
1107	Sec-Butanol	C4H10O	2021.4503	13.1697
1167	Allyl Alcohol	C3H6O	554.1537	3.6592
1130	4-Mth-2-Pentanol	C6H14O	1371.3719	15.1490
1177	3,4-Xylenol	C8H10O	747.1192	4.2819
1114	1-Hexanol	C6H14O	755.8658	5.1494
1106	Isobutanol	C4H10O	1179.4938	5.5900
1125	1-Heptanol	C7H16O	753.2918	5.4539
1105	N-Butanol	C4H10O	646.2479	3.5301
1109	1-Pentanol	C5H12O	1343.8964	8.9643
1132	1-Octanol	C8H18O	843.6408	6.6863
1113	T-Butylcarbinol	C5H12O	1165.9377	8.8568
1137	1-Undecanol	C11H24O	1084.5320	10.4982
1108	Tert-Butanol	C4H10O	1107.2997	7.3848
1103	N-Propanol	C3H8O	633.6995	3.4167
1134	1-Nonanol	C9H20O	606.5423	5.1821
2195	P-t-Octylphenol	C14H22O	816.7545	8.3830
1102	Ethanol	C2H6O	311.3837	1.7930
1124	3-Mth-2-Butanol	C5H12O	845.6369	5.4522
1136	1-Decanol	C10H22O	1416.8216	13.0399

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1140	Dodecanol	C12H26O	884.6503	9.2077
1104	Isopropanol	C3H8O	629.7534	3.7949
1110	2-Pentanol	C5H12O	1180.4201	8.4226
1120	3-Pentanol	C5H12O	2604.8593	22.9066
1112	2-Mth-1-Butanol	C5H12O	1089.1856	6.1898
1154	Ts-2-Mth-CycC6OH	C7H14O	1001.1963	14.0823
1153	Cs-2-Mth-CycC6OH	C7H14O	693.4526	11.0710
1156	Ts-3-Mth-CycC6OH	C7H14O	1049.8658	9.7180
1157	Cs-4-Mth-CycC6OH	C7H14O	981.7454	10.1351
2197	P-Cumylphenol	C15H16O	581.1321	4.9616
1180	Benzyl Alcohol	C7H8O	867.5382	6.4170
1158	Ts-4-Mth-CycC6OH	C7H14O	865.2662	7.9403
1155	Cs-3-Mth-CycC6OH	C7H14O	835.1178	7.2728
1168	2-Phn-2-Propanol	C9H12O	1442.7942	19.0058
1141	1-Tridecanol	C13H28O	588.2433	6.5496
1147	2-Eth-1-Butanol	C6H14O	1230.1418	10.1039
1117	2-Mth-1-Pentanol	C6H14O	717.4495	5.7486
2115	2-Phenylethanol	C8H10O	653.4638	6.1689
1142	1-Tetradecanol	C14H30O	395.0543	4.6590
2118	1-PHN-1-PROPANOL	C9H12O	904.4240	11.1961
2119	1-PHN-2-PROPANOL	C9H12O	925.2617	11.0483
1126	2-Heptanol	C7H16O	903.4850	9.9757
1143	1-Pentadecanol	C15H32O	791.6524	9.1177
1129	Isoheptanol	C7H16O	1011.8899	7.0835
2117	2,6-DiMth-4-C7OH	C9H20O	2046.7287	21.1424
1144	1-Hexadecanol	C16H34O	565.4647	6.9329
1145	Heptadecanol	C17H36O	444.6915	5.5514
1199	Nonylphenol	C15H24O	812.2304	6.3941
1146	1-Octadecanol	C18H38O	667.4372	8.8357
1135	2-Nonanol	C9H20O	980.8388	12.5139
1149	1-Nonadecanol	C19H40O	704.6332	9.8704
1139	Isodecanol	C10H22O	1831.8508	14.9232
1148	1-Eicosanol	C20H42O	813.9736	11.2154
2198	Dinonylphenol	C24H42O	166.1306	1.1882
1159	Menthol	C10H20O	441.3210	3.0814
1202	DiethyleneGlycol	C4H10O3	200.8935	1.5296
1245	1,3-Benzenediol	C6H6O2	252.0294	1.2012
1186	P-Hydroquinone	C6H6O2	221.3373	1.2265
1244	1,2-Benzenediol	C6H6O2	510.2548	7.9281
1219	2MTH,13PROPNDIO	C4H10O2	385.3104	3.4048
1212	1,3-Propanediol	C3H8O2	368.5393	3.3214
1235	P-t-But-Catechol	C10H14O2	892.8236	10.3909
1203	Triglycol	C6H14O4	195.2812	2.3900

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1198	Bisphenol A	C15H16O2	825.3398	3.5784
1238	2,3-Butanediol	C4H10O2	687.1631	7.5762
1211	1,2-Propanediol	C3H8O2	625.3935	6.0955
2219	2,4-PENTANEDIOL	C5H12O2	808.0946	10.1761
1215	1,4-Butynediol	C4H6O2	546.8508	1.4094
1214	Neopentyl Glycol	C5H12O2	697.0193	5.4388
1221	1,3-Butanediol	C4H10O2	363.5073	3.3629
1220	1,2-Butanediol	C4H10O2	661.0673	7.5020
1240	Ts2-C4H8-14-Diol	C4H8O2	266.7730	0.9378
1239	Cis-Butenediol	C4H8O2	476.2893	2.9588
1241	1,4-Butanediol	C4H10O2	325.5995	1.8631
1222	Hexylene Glycol	C6H14O2	1329.2897	14.8520
1213	Dipropylene Gly	C6H14O3	760.1131	12.4616
1242	1,5-Pentanediol	C5H12O2	387.2960	2.5452
1243	1,6-Hexanediol	C6H14O2	401.5536	3.7270
1204	TetraC2H4 Glycol	C8H18O5	557.3331	6.1944
6886	C6H4(COOC2H4OH)2	C12H14O6	230.9018	1.3394
1248	123-Benzenetriol	C6H6O3	487.6101	7.1720
1231	Glycerol	C3H8O3	158.7470	1.5395
1247	Hexaglycerol	C6H14O3	484.9494	5.9673
1246	Pentaerythritol	C5H12O4	59.8983	0.1527

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Amines

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1742	Ethyleneimine	C2H5N	22.8873	0.0253
1745	Piperidine	C5H11N	700.5311	4.3532
2726	Propyleneimine	C3H7N	124.1847	0.3670
1766	Pyrrolidine	C4H9N	452.9522	1.6237
1719	Isopropylamine	C3H9N	1167.4593	7.8495
1711	N-Propylamine	C3H9N	979.0811	9.4311
1726	Sec-Butylamine	C4H11N	894.2654	7.8452
1704	Ethylamine	C2H7N	660.6685	6.1916
1702	Dimethylamine	C2H7N	897.2693	7.8646
1710	Diethylamine	C4H11N	1093.5771	9.4244
1740	Allylamine	C3H7N	801.6032	6.1332
1712	N-Butylamine	C4H11N	1160.7413	10.4970
1794	HexMthyleneimine	C6H13N	428.8959	1.8701
1729	Cyclohexylamine	C6H13N	733.1940	4.9403

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1714	Isobutylamine	C4H11N	996.1851	9.0011
2853	Acetamide	C2H5NO	809.6382	0.0727
2731	N-C1-CycC6-Amine	C7H15N	1062.2530	7.6810
1743	Diisopropylamine	C6H15N	1175.3802	5.2537
1796	N,N-DiMthAniline	C8H11N	2124.5822	26.7250
1792	Aniline	C6H7N	1171.9319	8.0153
1713	N-Pentylamine	C5H13N	1172.9106	10.4852
1733	Benzylamine	C7H9N	1022.9735	5.7687
1737	M-Toluidine	C7H9N	1787.7743	11.0976
3796	N-Ethylaniline	C8H11N	410.8233	1.1811
1878	2-Methacrylamide	C4H7NO	1784.7775	1.2322
1736	O-Toluidine	C7H9N	846.7721	6.4882
2739	Diallylamine	C6H11N	1161.7919	6.0019
2706	Hexylamine	C6H15N	1172.6762	10.1104
2724	O-Ethylaniline	C8H11N	1415.7051	11.0293
1707	Dipropylamine	C6H15N	1335.3212	10.5311
1738	P-Toluidine	C7H9N	1210.8673	8.3509
1795	N-Methylaniline	C7H9N	479.0021	2.1569
1718	Diisobutylamine	C8H19N	1320.0147	9.9717
1879	Acrylamide	C3H5NO	938.8069	0.0995
2707	1-Aminoheptane	C7H17N	1095.9983	9.9837
2730	DiCycHexylAmine	C12H23N	370.6972	2.2687
2787	P-Aminodiphenyl	C12H11N	392.6001	3.8873
1744	Dibutylamine	C8H19N	1209.3811	8.6028
2708	1-Octylamine	C8H19N	873.3096	7.1785
2791	2,6-DiEthAniline	C10H15N	2848.9972	18.1596
2709	1-Nonylamine	C9H21N	1028.1797	8.4996
2710	1-Decylamine	C10H23N	1006.9673	7.8850
3722	Diamylamine	C10H23N	1072.1159	5.1338
3724	Undecylamine	C11H25N	957.6235	7.7949
2712	Dodecylamine	C12H27N	670.1846	5.3227
1720	Tetradecylamine	C14H31N	509.3211	4.0157
2752	Piperazine	C4H10N2	403.7069	0.9850
1752	Propylenediamine	C3H10N2	909.8279	4.5845
1741	Ethylenediamine	C2H8N2	498.2638	2.7433
2725	O-Aminoaniline	C6H8N2	1246.5825	9.4174
2750	P-Aminoaniline	C6H8N2	1009.3150	6.4969
2727	M-Aminoaniline	C6H8N2	575.9785	4.1131
1750	AEP	C6H15N3	316.3723	1.2982
1732	Toluene Diamine	C7H10N2	830.0944	5.1852
1731	hexamethyleneDiamine	C6H16N2	703.6503	6.9844
3750	P-Benzidine	C12H12N2	257.1621	1.6852

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Nitriles

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1773	Propionitrile	C3H5N	630.2174	5.5983
1782	Butyronitrile	C4H7N	818.2485	7.1755
2720	Allyl Cyanide	C4H5N	791.8185	6.4937
1783	Valeronitrile	C5H9N	937.0132	8.6522
3874	Benzyl Cyanide	C8H7N	576.3636	3.8253
1786	Hexanenitrile	C6H11N	854.3277	8.0188
1776	Succinonitrile	C4H4N2	121.5426	0.2838
1781	Glutaronitrile	C5H6N2	89.7108	0.4928
2735	14-2Cyano-2-C4H8	C6H6N2	236.6285	0.7830
1777	Adiponitrile	C6H8N2	153.1154	0.6681

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Imines

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1767	N-MthPyrrolidine	C5H11N	1028.5857	7.1087
2797	3-Methylpyridine	C6H7N	673.8985	4.6304
1797	2-Methylpyridine	C6H7N	862.6112	7.5454
2799	4-Methylpyridine	C6H7N	459.9975	3.1468
1753	N,N-DiEthAniline	C10H15N	497.0790	2.1532

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Tert-N

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1706	Triethylamine	C6H15N	628.9548	5.4263
2716	Tributylamine	C12H27N	1031.4212	6.3001
2719	Tripropylamine	C9H21N	825.0486	3.3592
3723	Triamylamine	C15H33N	2020.0844	15.4265

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Nitrates

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1761	Nitroethane	C2H5NO2	726.7607	7.2782
1763	2-Nitropropane	C3H7NO2	745.4471	7.3150
1762	1-Nitropropane	C3H7NO2	935.9682	10.8930

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Thiols

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1802	Ethyl Mercaptan	C2H6S	426.6387	4.2720
1820	Dimethyl Sulfide	C2H6S	750.3525	6.1654
1843	Thiacyclopentane	C4H8S	523.6750	2.3444
1803	1-Propanethiol	C3H8S	617.3806	5.3230
1805	Isobut Mercaptan	C4H10S	576.8989	4.7627
6860	Ethylenedithiol	C2H6S2	276.6261	1.6574
1811	Cyclohexanethiol	C6H12S	570.0175	4.7207
1828	DiMth Disulfide	C2H6S2	763.1367	9.0625
1841	Butanethiol	C4H10S	678.5936	5.5273
1814	Methylproylsulf	C4H10S	721.1312	5.9937
2816	ETHYLtBUTYL SUL	C6H14S	1238.8874	9.9998
1818	Diethyl Sulfide	C4H10S	1096.6237	8.6777
1812	Benzyl Mercaptan	C7H8S	642.5500	3.5509
1838	T-OctylMercaptan	C8H18S	1208.0765	16.4765
1827	1-Pentanethiol	C5H12S	703.6933	5.1819
2815	METHnBUTYL SULFD	C5H12S	746.2251	5.2667
1824	DiethylDisulfide	C4H10S2	1365.1930	11.5215
1807	N-Hexylmercaptan	C6H14S	688.4514	4.9893
6857	Dimercaptoethyl	C4H10OS2	257.7785	1.2872
1839	1-Heptanethiol	C7H16S	703.7325	4.6540
1829	DiProp Disulfide	C6H14S2	1166.3228	10.5845
1809	1-Octanethiol	C8H18S	646.4714	4.3011
1808	N-Nonanethiol	C9H20S	466.1660	2.7189
1826	1-Decanethiol	C10H22S	513.2386	3.1111
2838	tertDodecanThiol	C12H26S	870.5845	6.8551
1825	1-Undecanethiol	C11H24S	711.3255	4.0274
1837	Dodecylthiol	C12H26S	350.2447	2.3738

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Aldehydes

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1037	Methacrolein	C4H6O	911.9718	9.9363
1002	Acetaldehyde	C2H4O	387.8050	3.6464
1003	Propionaldehyde	C3H6O	608.8986	6.0332
1041	Benzaldehyde	C7H6O	721.6338	5.3381
1034	Acrolein	C3H4O	408.5993	4.0866

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1005	N-Butyraldehyde	C4H8O	1007.6536	9.9209
1036	Trans-2-Butenal	C4H6O	330.3107	1.5187
1007	Valeraldehyde	C5H10O	1380.9145	12.4246
1006	Isobutyraldehyde	C4H8O	787.4844	6.3396
1009	1-Hexanal	C6H12O	957.3856	7.9375
1040	P-Tolualdehyde	C8H8O	743.6605	3.8107
1016	2-Methylhexanal	C7H14O	1007.5524	7.6335
1017	3-Methylhexanal	C7H14O	900.8546	8.0671
1008	1-Heptanal	C7H14O	834.9595	7.3243
1013	2-Ethylhexanal	C8H16O	1048.4039	7.9129
1010	1-Octanal	C8H16O	932.2933	7.1377
1011	1-Nonanal	C9H18O	1365.5153	9.8510
1020	1-Decanal	C10H20O	1029.6383	7.7822
1021	1-Undecanal	C11H22O	1114.4757	7.6611
1025	Dodecanal	C12H24O	661.5904	5.0157
1026	1-Tridecanal	C13H26O	503.1676	3.7288
1014	1,2-Ethanedione	C2H2O2	2197.4540	32.8858
1044	1,4BenzDicarboxAldehy	C8H6O2	809.3293	4.5543

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Epoxides

DipID	**Name**	**Formula**	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1440	ISOBUTYLENE OXID	C4H8O	76.6481	0.3545
1478	Furan	C4H4O	115.2327	0.5480
1443	1,3-Propylene Ox	C3H6O	35.9866	0.1236
1479	Tetrahydrofuran	C4H8O	194.7685	0.8445
1477	2,5-Dihydrofuran	C4H6O	896.2169	3.9238
1471	1,2-Epoxybutane	C4H8O	97.6742	0.3482
1408	1-Methoxypropane	C4H10O	1217.5207	11.5157
1442	1,2-Propylene Ox	C3H6O	15.2284	0.0324
1411	2-Methoxypropane	C4H10O	1062.6471	9.8437
1421	1,4-Dioxane	C4H8O2	176.8371	0.7223
2422	1,3-DIOXANE	C4H8O2	160.1326	0.4696
1426	2-Methoxybutane	C5H12O	1331.8931	11.4230
1422	Trioxane	C3H6O3	63.2191	0.1162
1413	1-Methoxybutane	C5H12O	1442.5936	12.3938
1461	Methoxybenzene	C7H8O	902.0896	4.7992
1448	1-Ethoxybutane	C6H14O	581.0279	4.0840
1429	1-MethoxyPentane	C6H14O	734.4990	4.6763
6885	Ethyl-3-Ethoxypr	C7H14O3	799.6951	7.1480

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Ether

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1401	Dimethyl Ether	C2H6O	389.8600	4.5680
1407	MethylEthylEther	C3H8O	193.2347	1.1459
1470	VinylMethylEther	C3H6O	976.9903	9.3073
1405	MTBE	C5H12O	1047.5092	8.5443
1445	VinylEthyl Ether	C4H8O	473.0221	3.4853
1402	Diethyl Ether	C4H10O	484.0369	3.6235
1431	Methylal	C3H8O2	2320.6511	23.1045
1428	T-But EthylEther	C6H14O	740.0098	5.2668
1427	TAME	C6H14O	990.9966	7.4529
1410	Mth Isobut Ether	C5H12O	1350.5846	11.7847
1430	Eth-t-Pent-Ether	C7H16O	878.3719	6.6771
1403	DiisopropylEther	C6H14O	709.6778	6.4254
1415	Eth Propyl Ether	C5H12O	782.5571	5.7085
1455	Dimethyl Acetal	C4H10O2	291.6162	1.1618
1446	Dipropyl Ether	C6H14O	960.6676	7.3944
1447	Butyl VinylEther	C6H12O	901.5788	5.2272
1462	EthylPhenylEther	C8H10O	822.2542	3.8174
1406	Di-sec-But Ether	C8H18O	932.9001	6.5756
1432	Acetal	C6H14O2	1385.2199	10.4136
1460	BenzylEthylEther	C9H12O	606.2261	3.5407
1050	Paraldehyde	C6H12O3	324.2561	1.3934
1404	Di-n-Butyl Ether	C8H18O	993.8959	6.4853
1420	Anethole	C10H12O	754.9799	2.4560
1456	DimethylCarbitol	C6H14O3	965.8407	4.9675
1463	Dibenzyl Ether	C14H14O	530.8675	1.8463
1425	Di-n-PentylEther	C10H22O	953.5045	6.7739
1458	Diethyl Carbitol	C8H18O3	723.7244	3.9523
1412	Dihexyl Ether	C12H26O	804.7008	3.7953
1454	Triglyme	C8H18O4	1070.2742	4.4490
1459	Dibutyl Carbitol	C12H26O3	619.7131	5.4855
1424	Di-n-Octyl Ether	C16H34O	730.1457	3.5376
1457	Tetraglyme	C10H22O5	398.9655	1.5127
1418	Dinonyl Ether	C18H38O	859.6025	4.3411
2432	ETHYLAL	C5H12O2	857.2077	7.0148
2405	DIISOBUTYL ETHER	C8H18O	1056.7998	7.0925
2456	Ethyl Glyme	C6H14O2	804.0102	3.8383
2417	ETHYLHEXYL ETHER	C8H18O	911.2267	4.9288
2415	ETHYLISOPROPETH	C5H12O	568.0856	4.3189

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Formates

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1301	Methyl Formate	C2H4O2	343.9652	2.6385
1311	Vinyl Formate	C3H4O2	977.3946	8.2884
1302	Ethyl Formate	C3H6O2	714.2221	6.8334
2306	t-Butyl Formate	C5H10O2	1112.6492	12.5866
1303	Propyl Formate	C4H8O2	1176.9026	9.9803
2305	sec-ButylFormate	C5H10O2	1215.0154	11.6299
2311	CYCLOHEXL FORMAT	C7H12O2	981.0302	8.5838
1304	N-Butyl Formate	C5H10O2	2240.1812	20.0082
1305	Isobutyl Formate	C5H10O2	1052.6439	9.6640
2350	Benzyl Formate	C8H8O2	810.8746	5.3708
2307	n-Hexyl Formate	C7H14O2	1025.5437	7.5730
1306	N-Pentyl Formate	C6H12O2	1050.3153	8.9057
2308	n-Heptyl Formate	C8H16O2	772.7368	7.1521
1308	N-Octyl Formate	C9H18O2	912.7099	9.8301
1309	n-Nonyl Formate	C10H20O2	1061.4049	8.7940
1310	n-Decyl Formate	C11H22O2	851.8020	6.7599

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Esters

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1351	Mth Methacrylate	C5H8O2	605.3515	4.6208
1312	Methyl Acetate	C3H6O2	338.6323	2.5115
1331	Vinyl Propionate	C5H8O2	721.1871	5.9023
1321	Vinyl Acetate	C4H6O2	751.7026	6.8507
1352	Eth MthAcrylate	C6H10O2	833.7086	8.1929
1322	MethylPropionate	C4H8O2	623.7429	4.8922
1341	Methyl Acrylate	C4H6O2	755.3937	6.9655
1313	Ethyl Acetate	C4H8O2	445.8130	3.1815
1319	IsopropylAcetate	C5H10O2	938.0184	9.4916
1332	Methyl Butyrate	C5H10O2	651.2058	4.8477
1342	Ethyl Acrylate	C5H8O2	819.2638	7.8672
1318	Allyl Acetate	C5H8O2	732.0872	7.6565
1314	N-Propyl Acetate	C5H10O2	892.8544	7.4400
1323	Ethyl Propionate	C5H10O2	857.3521	6.6386
1360	I-But I-Butyrate	C8H16O2	1025.8287	10.7365
1320	Sec-ButylAcetate	C6H12O2	1041.1649	10.2601

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1336	PropylI-Butyrate	C7H14O2	1056.1437	9.1198
1353	N-C3-Mthacrylate	C7H12O2	655.0737	4.5897
1333	Ethyl Butyrate	C6H12O2	879.6884	9.1229
1347	EthylIsovalerate	C7H14O2	924.9768	8.1330
1315	N-Butyl Acetate	C6H12O2	1054.2650	8.9070
1390	Methyl Benzoate	C8H8O2	665.4406	4.7558
1388	ISOBUTYL MTHACR	C8H14O2	761.2869	8.1078
1343	1-PropylAcrylate	C6H10O2	890.2318	6.8371
1316	Isobutyl Acetate	C6H12O2	906.6518	8.0904
1344	N-Butyl Acrylate	C7H12O2	660.5276	5.7783
1357	Pentyl Acetate	C7H14O2	816.3455	7.1338
1327	N-PropN-Butyrate	C7H14O2	948.7097	8.8827
1324	N-PropPropionate	C6H12O2	791.3815	6.8555
1291	Acetic Anhydride	C4H6O3	455.1417	2.8082
1389	N-ButMthacrylate	C8H14O2	987.6085	8.8511
1359	Benzyl Acetate	C9H10O2	593.3835	4.0034
1326	N-But Propionate	C7H14O2	867.1072	6.7651
1391	Ethyl Benzoate	C9H10O2	734.4379	7.0200
1897	CH3OC3H600CH3	C6H12O3	1099.7653	8.9690
1392	DiethylCarbonate	C5H10O3	593.8736	4.3136
1385	N-But N-Butyrate	C8H16O2	649.0310	6.2306
1317	IsopentylAcetate	C7H14O2	804.1689	7.4549
1363	N-Hexyl Acetate	C8H16O2	871.8757	7.5403
1387	Ethylene Acetate	C6H10O4	687.6402	2.6203
1393	Diethyl Oxalate	C6H10O4	648.4470	4.6091
1365	Butyl Benzoate	C11H14O2	701.0837	6.1780
1361	I-C5 I-Valerate	C10H20O2	780.5506	8.9519
1367	Heptyl Acetate	C9H18O2	852.8655	6.9967
1346	N-Butyl Valerate	C9H18O2	894.3101	7.0249
1358	2-C2-C6 Acetate	C10H20O2	1056.2247	10.2271
1394	Diethyl Malonate	C7H12O4	628.5758	5.6669
1292	Propionyl Oxide	C6H10O3	1053.8914	8.0224
1364	Benzyl Benzoate	C14H12O2	300.6577	1.9654
1381	2Mth p-Phthalate	C10H10O4	498.4303	5.5849
1368	n-Octyl Acetate	C10H20O2	400.1099	3.3224
1377	DiMthI-Phthalate	C10H10O4	359.9929	4.6299
1896	Ethylene DiAcr	C8H10O4	484.5723	4.4046
1386	2-Ethylhexyl Acr	C11H20O2	954.7253	9.5669
1395	Methyl Decanoate	C11H22O2	706.5012	4.8989
1369	n-Nonyl Acetate	C11H22O2	562.1125	4.5279
1370	n-Decyl Acetate	C12H24O2	1562.4663	12.3079
1345	N-ButylNonanoate	C13H26O2	1337.1861	21.9025
1375	DiProp Phthalate	C14H18O4	715.3539	8.3266

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1376	Diisobutyl Phtha	C16H22O4	670.1165	7.1621
1396	IsopropMyristate	C17H34O2	637.7413	5.6411
1383	Butyl Stearate	C22H44O2	883.6229	12.3840
1362	Methyl Oleate	C19H36O2	281.9972	1.8892
1355	Diisooctyl Phtha	C24H38O4	344.3722	4.5354
1382	DioctylTerephtha	C24H38O4	774.0404	11.4191
1384	DIBUTYL SEBACATE	C18H34O4	638.6492	5.5632
1371	Diisodecyl Phtha	C28H46O4	344.7430	8.7829
1354	DioctylPhthalate	C24H38O4	879.7318	13.5539
2375	DiethylPhthalate	C12H14O4	638.1658	4.6594
2388	Dipropyl Maleate	C10H16O4	757.4805	6.1628
2381	Diallyl Maleate	C10H12O4	463.6780	2.6769
2370	Glyceryl Triacet	C9H14O6	1187.9889	11.5025
2382	Dibutyl Maleate	C12H20O4	469.4565	3.5792
2376	DibutylPhthalate	C16H22O4	420.3354	5.0644
2353	CetylMthacrylate	C20H38O2	400.3836	4.8299
2379	Dihexyl Adipate	C18H34O4	481.6573	4.5935
2321	T-Butyl Acetate	C6H12O2	788.5047	7.8948
2332	Methl.I-butyrate	C5H10O2	677.6457	6.1912
2354	AllylMthacrylate	C7H10O2	1075.3686	9.0617
2364	CYCLOHEXL ACETAT	C8H14O2	699.3931	6.3751
2337	EthylIsobutyrate	C6H12O2	1049.0569	12.0329
2384	IsobutylAcrylate	C7H12O2	997.2525	9.2443
2380	1,1-Diacetoxy C2	C6H10O4	737.6503	7.3463
2392	n-PropylBenzoate	C10H12O2	918.9250	8.5091
2387	Dimethyl Maleate	C6H8O4	308.2698	1.8649
2377	DiMth Phthalate	C10H10O4	564.7943	4.3569
2386	Diethyl Maleate	C8H12O4	575.0955	6.0462
2385	Mth Dodecanoate	C13H26O2	551.1062	3.9385
3379	Dioctyl Adipate	C22H42O4	290.3749	8.5413
5886	Mth Acetoacetate	C5H8O3	395.5017	1.6939
5884	Ethoxy Acetate	C6H12O3	693.9182	4.2367
5887	EthAcetoAcetate	C6H10O3	564.8931	3.8033
5885	Carbitol Acetate	C8H16O4	873.5203	7.1465

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Ketones

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1096	Methyl Isopropen	C5H8O	752.6946	4.6970
1079	Cyclopentanone	C5H8O	484.0488	1.9486

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1051	Acetone	C3H6O	306.7821	1.6568
1052	MEK	C4H8O	571.8956	3.4785
1065	Mesityl Oxide	C6H10O	748.2644	4.9527
1066	T-But Mth Ketone	C6H12O	827.0163	5.6916
1060	2-Pentanone	C5H10O	752.8402	4.6387
1061	Mth iC3 Ketone	C5H10O	656.6491	4.4747
1053	Diethyl Ketone	C5H10O	1049.8035	6.8506
1059	3-Hexanone	C6H12O	1202.5818	7.5173
1099	Diketene	C4H4O2	63.6251	0.1618
1055	Sec-ButMthKetone	C6H12O	815.6224	5.5777
1054	MIBK	C6H12O	860.2175	5.4929
1095	EthIsopropKetone	C6H12O	1261.3799	7.4153
1063	2-Heptanone	C7H14O	878.1642	5.2267
1064	5-Mth-2-Hexanone	C7H14O	1467.1275	8.0385
1058	4-Heptanone	C7H14O	1618.6174	11.3710
1057	3-Heptanone	C7H14O	1159.1395	6.4281
1076	2,4-Pentanedione	C5H8O2	1059.7528	18.2354
1068	DiisobutylKetone	C9H18O	1296.7522	8.8234
1097	2-CycC6 CycC6one	C12H20O	596.3291	2.3227
1083	2-Octanone	C8H16O	851.7118	5.2100
1073	Dibutyl Ketone	C9H18O	1125.2610	7.1602
1062	2-Hexanone	C6H12O	472.8477	2.8476
1077	Isophorone	C9H14O	392.5188	3.4372
1090	Acetophenone	C8H8O	591.6343	2.9801
1080	Cyclohexanone	C6H10O	496.8660	2.2397
1074	2-Nonanone	C9H18O	859.7227	5.2650

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Alcohol-Ethers

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
2862	2-Butoxyethanol	C6H14O2	1127.5114	14.6700
4857	butyl carbitol	C8H18O3	709.2970	8.5189
2898	2-Chloroethanol	C2H5ClO	767.2962	8.6015
2864	Carbitol	C6H14O3	615.5729	6.2483
3854	Methyl propasol	C4H10O2	1680.2278	27.2721
2860	2-Methoxyethanol	C3H8O2	1230.6023	14.4377
2854	DiacetoneAlcohol	C6H12O2	1512.1238	25.0022
2861	2-Ethoxyethanol	C4H10O2	971.1480	12.0479
2889	HydroxyAcetone	C3H6O2	905.4103	10.1626

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

3856	1tButoxy2Propnol	C7H16O2	2834.3889	35.3704
3858	PROPGLYC2tBUTYL	C7H16O2	1647.4546	17.9970
4855	2-Propoxyethanol	C5H12O2	1223.3355	17.3162
4849	Acetovanillone	C9H10O3	841.9962	4.5667
5883	Ethyl Lactate	C5H10O3	1376.7717	31.9001
6883	2-HydroxyEth Acr	C5H8O3	350.6966	2.2907
2863	Methyl Carbitol	C5H12O3	529.4507	4.6795
3855	Dowanol DPM	C7H16O3	2318.4214	45.7544
3857	TriPropGlymEthlE	C10H22O4	1696.8491	22.5292

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Hydrocarbons

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
404	DiMth-Acetylene	C4H6	760.9132	3.3560
202	Propylene	C3H6	209.1577	3.2649
412	2-Pentyne	C5H8	3725.2173	56.1304
207	2-Methylpropene	C4H8	488.6202	4.8073
204	1-Butene	C4H8	627.4612	7.4490
205	Cis-2-Butene	C4H8	415.3007	3.3387
402	Propyne	C3H4	500.6878	5.0595
406	3-Hexyne	C6H10	1285.4575	7.2514
206	Trans-2-Butene	C4H8	480.8611	4.4663
407	2-Hexyne	C6H10	1164.2898	5.5958
231	33-2Mth-1-Butene	C6H12	841.4801	7.5014
230	23-2Mth-1-Butene	C6H12	724.6617	4.9973
229	2-Ethyl-1-Butene	C6H12	835.8781	5.6675
8	I-Pentane	C5H12	549.1915	4.9297
14	2,2-DiMth-Butane	C6H14	639.1982	5.1407
232	23-2Mth-2-Butene	C6H12	742.1875	4.1484
213	3-Mth-1-Butene	C5H10	761.7011	7.6750
212	2-Mth-1-Butene	C5H10	533.2553	4.1877
211	Trans-2-Pentene	C5H10	796.5944	6.0111
210	Cis-2-Pentene	C5H10	693.8309	5.0766
223	4-Mth-1-Pentene	C6H12	819.8145	7.1490
221	2-Mth-1-Pentene	C6H12	961.4535	6.8600
248	2-t-Butylpropene	C7H14	794.4637	5.0033
227	Cs-4-Mth-2-C5H10	C6H12	875.2022	6.2320
224	2-Mth-2-Pentene	C6H12	852.3209	7.1359
403	1-Butyne	C4H6	1144.5049	11.3495
15	2,3-DiMth-Butane	C6H14	536.0986	3.6377
214	2-Mth-2-Butene	C5H10	585.7404	5.3827
228	Ts-4-Mth-2-C5H10	C6H12	820.2162	5.4628

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

225	Cs-3-Mth-2-C5H10	C6H12	828.0789	7.2685
218	Trans-2-Hexene	C6H12	919.1182	6.1623
2226	3-METH-Tr-2Pente	C6H12	764.6365	5.9606
222	3-Mth-1-Pentene	C6H12	884.7848	7.7536
257	2-Diisobutylene	C8H16	901.8458	6.7606
256	1-Diisobutylene	C8H16	947.3821	6.4674
217	Cis-2-Hexene	C6H12	876.9214	6.0839
2414	1-Heptyne	C7H12	1446.9382	12.0049
13	3-Methylpentane	C6H14	699.7515	5.0620
219	Cis-3-Hexene	C6H12	923.0663	6.6155
12	2-Methylpentane	C6H14	787.0113	6.1335
220	Trans-3-Hexene	C6H12	943.0886	6.4633
405	1-Pentyne	C5H8	1448.2875	14.7692
209	1-Pentene	C5H10	929.4326	9.2316
11	N-Hexane	C6H14	1270.9672	9.3387
235	Cis-2-Heptene	C7H14	936.7815	6.4205
249	Cis-3-Heptene	C7H14	1749.6188	11.8833
216	1-Hexene	C6H12	991.1184	8.2274
239	3-Eth-1-Pentene	C7H14	964.8020	6.7131
226	4-Mth-1-Hexene	C7H14	962.0899	6.4711
240	3-Mth-1-Hexene	C7H14	922.5925	6.4460
419	3-Mth-1-Butyne	C5H8	1372.7240	13.9610
233	2-Eth-1-Pentene	C7H14	960.3794	6.1584
238	2-Mth-1-Hexene	C7H14	1075.9714	7.2736
416	1-Octyne	C8H14	1331.7172	9.9914
289	2,3Dimeth Hexene	C8H16	973.4207	5.8369
234	1-Heptene	C7H14	822.3983	6.0946
413	1-Hexyne	C6H10	1274.8709	11.3153
237	Trans-3-Heptene	C7H14	973.3873	6.5503
236	Trans-2-Heptene	C7H14	881.7102	5.8310
251	Trans-2-Octene	C8H16	1016.7978	6.7987
279	Trans-4-Octene	C8H16	1058.6658	7.0700
277	Trans-3-Octene	C8H16	972.9921	6.5378
2252	2Methl-1-Heptene	C8H16	1014.6453	6.9472
250	1-Octene	C8H16	669.7783	4.4761
258	2-Ethyl-1-Hexene	C8H16	1019.5159	6.8164
280	3-Octene	C8H16	1001.9083	6.9470
278	4-Octene	C8H16	1077.6316	7.5765
276	2-Octene	C8H16	546.2018	3.6310
259	1-Nonene	C9H18	865.3846	5.2805
262	1-Dodecene	C12H24	811.9012	4.7496
263	1-Tridecene	C13H26	744.0794	4.2239
264	1-Tetradecene	C14H28	439.6608	2.4215
265	1-Pentadecene	C15H30	546.8505	3.1316
266	1-Hexadecene	C16H32	608.4171	3.2891
267	1-Octadecene	C18H36	352.2235	1.9982
281	1-Heptadecene	C17H34	1049.6652	5.9257
284	1-Eicosene	C20H40	344.4896	2.0847

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

283	1-Nonadecene	C19H38	515.9973	2.8624
3	Propane	C3H8	184.5212	2.7848
4	I-Butane	C4H10	232.8096	2.5132
9	Neopentane	C5H12	623.1749	7.5874
5	N-Butane	C4H10	494.7538	5.6659
7	pentane	C5H12	717.4470	6.4384
44	Hexamethylethane	C8H18	506.8287	2.5727
25	223-TriMthButane	C7H16	534.6146	3.3614
24	3,3-DiMthPentane	C7H16	717.8739	5.0190
51	2,2,3,3-4Mth-C5	C9H20	455.5736	2.0273
21	2,2-DiMthPentane	C7H16	839.6978	6.2561
42	2,3,3-TriMth-C5	C8H18	515.0343	2.7910
22	2,3-DiMthPentane	C7H16	581.0256	3.4360
40	2,2,3-TriMth-C5	C8H18	612.6115	3.4602
23	2,4-DiMthPentane	C7H16	813.8251	5.6874
41	2,2,4-TriMth-C5	C8H18	791.5992	5.6588
39	3-Mth-3-Eth-C5	C8H18	665.5958	4.0371
20	3-Ethylpentane	C7H16	836.2272	5.3676
52	2,2,3,4-4Mth-C5	C9H20	535.1506	2.7270
54	2334TetrMethPent	C9H20	342.2661	1.4444
53	2,2,4,4-4Mth-C5	C9H20	684.2601	4.3513
43	2,3,4-TriMth-C5	C8H18	540.7432	2.7971
36	3,3-DiMth-Hexane	C8H18	897.1989	5.7201
19	3-Methylhexane	C7H16	829.8415	5.5279
18	2-Methylhexane	C7H16	816.5574	5.5733
38	2-Mth-3-Eth-C5	C8H18	812.7235	4.6829
190	2,2-2C1-3-C2-C5	C9H20	685.3833	3.8399
32	2,2-DiMth-Hexane	C8H18	730.3134	4.9912
37	3,4-DiMth-Hexane	C8H18	492.3479	2.6982
50	3,3-DiEthPentane	C9H20	681.6677	4.0598
34	2,4-DiMth-Hexane	C8H18	1571.0217	9.8996
33	2,3-DiMth-Hexane	C8H18	787.5145	4.3744
17	N-Heptane	C7H16	909.0734	6.0721
49	244TriMethHexane	C9H20	796.4338	4.9368
192	2,4-2C1-3-C2-C5	C9H20	591.5528	3.1553
47	2,2,5-TriMth-C6	C9H20	611.7513	3.9496
35	2,5-DiMth-Hexane	C8H18	784.4144	4.9068
31	3-Ethylhexane	C8H18	676.7500	4.2667
30	4-Methylheptane	C8H18	661.5574	4.1436
29	3-Methylheptane	C8H18	727.4683	4.5162
28	2-Methylheptane	C8H18	670.4443	4.2278
96	2,2-DiMthHeptane	C9H20	957.8078	6.3601
176	2,6-DiMthHeptane	C9H20	518.4513	2.9578
27	N-Octane	C8H18	972.0426	6.0057
94	3-Ethylheptane	C9H20	897.4841	5.4411
92	3-Methyloctane	C9H20	844.8926	4.8616
93	4-Methyloctane	C9H20	951.4219	5.7209
91	2-Methyloctane	C9H20	901.4349	5.1447

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

72	2,2-DiMthOctane	C10H22	873.4928	5.2982
2095	2,3Dimethloctane	C10H22	1049.6306	5.5415
2096	2,4Dimethloctane	C10H22	893.8437	5.2050
2098	2,6DimethlOctane	C10H22	846.9406	4.7525
2097	2,5Dimethloctane	C10H22	844.5473	4.8721
2099	2,7DimethlOctane	C10H22	966.8665	5.4230
46	N-Nonane	C9H20	577.5956	3.3525
88	5-Methylnonane	C10H22	901.5903	5.1786
85	3-Methylnonane	C10H22	1077.9319	6.0205
87	4-Methylnonane	C10H22	873.8801	5.2298
86	2-Methylnonane	C10H22	924.2854	4.9259
56	N-Decane	C10H22	1491.2892	8.1122
63	N-Undecane	C11H24	681.2265	3.8372
64	N-Dodecane	C12H26	452.9149	2.3626
65	N-Tridecane	C13H28	668.0196	3.5787
66	N-Tetradecane	C14H30	349.2902	1.9168
67	N-Pentadecane	C15H32	1080.3825	5.6783
68	N-Hexadecane	C16H34	751.3525	4.1032
69	N-Heptadecane	C17H36	438.2883	2.3724
70	N-Octadecane	C18H38	543.5309	3.0982
71	N-Nonadecane	C19H40	786.8715	4.5540
73	N-Eicosane	C20H42	831.4055	5.0808
74	n-HENEICOSANE	C21H44	479.8703	3.0040
75	n-DOCOSANE	C22H46	307.5565	2.0056
76	n-TRICOSANE	C23H48	631.2638	4.1258
77	n-Tetracosane	C24H50	194.3734	1.3416
78	n-PENTACOSANE	C25H52	240.9232	1.6646
79	n-HEXACOSANE	C26H54	580.1410	4.1038
81	n-Octacosane	C28H58	394.2544	3.0178
2081	n-TRICONTANE	C30H62	162.8984	1.4648
2082	n-Dotriacontane	C32H66	579.8841	5.6516

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Cyclic Hydrocarbons

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
269	Cyclopentene	C5H8	657.1893	6.0956
270	Cyclohexene	C6H10	506.5924	3.7257
287	3MthCyclopentene	C6H10	698.8736	6.4232
286	1-MthCyclPentene	C6H10	691.9996	6.0143
288	4MthCyclopenten	C6H10	689.8736	6.2193
273	Cycloheptene	C7H12	612.0283	4.2712

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

274	Cyclooctene	C8H14	615.5087	4.0403
101	Cyclopropane	C3H6	148.3219	1.9407
810	ADAMANTANE	C10H16	314.6932	2.9348
102	Cyclobutane	C4H8	330.1531	3.0710
104	Cyclopentane	C5H10	517.0115	3.9509
137	Cyclohexane	C6H12	660.6732	4.8321
105	MthCyclopentane	C6H12	606.3383	4.9439
146	Cs-1,4-2C1-CycC6	C8H16	595.9589	4.4807
142	Cs-1,2-2C1-CycC6	C8H16	536.3889	3.6819
141	1,1-2C1-CycC6	C8H16	675.5442	7.0926
145	Ts-1,3-2C1-CycC6	C8H16	588.5169	4.3841
144	Cs-1,3-2C1-CycC6	C8H16	678.7746	5.6235
147	Ts-1,4-2C1-CycC6	C8H16	666.0830	5.7613
143	Ts-1,2-2C1-CycC6	C8H16	596.9538	4.8602
138	MthCyclohexane	C7H14	667.6303	5.0779
159	Cycloheptane	C7H14	590.8111	3.4031
140	Ethylcyclohexane	C8H16	647.6224	4.4421
154	Trans-Decalin	C10H18	439.3016	2.8488
149	N-PropylCyc-C6	C9H18	678.1313	4.3713
109	Cs-1,2-2C1-CycC5	C7H14	401.2047	2.7906
110	Ts-1,2-2C1-CycC5	C7H14	552.5039	4.4723
112	Ts-1,3-2C1-CycC5	C7H14	359.9054	2.9281
107	Eth-Cyclopentane	C7H14	844.7434	5.6487
114	N-PropCycPentane	C8H16	473.5495	3.0047
108	1,1-DiMthCycC5	C7H14	759.0651	8.3120
111	Cs-1,3-2C1-CycC5	C7H14	833.0736	7.1340
152	N-ButylCycHexane	C10H20	610.4778	3.7207
160	Cyclooctane	C8H16	470.1019	2.4558
153	Cis-Decalin	C10H18	594.1322	3.1621
115	ISOPROPYLCYCLOPENTANE	C8H16	558.3613	3.4913
150	Isopropyl-CycC6	C9H18	636.1206	3.6786
116	1-C1-1-C2-CycC5	C8H16	630.6071	5.8919
122	Butylcyclpentane	C9H18	641.5776	3.7066
155	1,1-Bicyclohexyl	C12H22	504.2154	3.0571
158	N-Decylcyclo-C6	C16H32	648.0307	3.4721

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Aromatic Hydrocarbons

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
307	1,4-Pentadiene	C5H8	1020.2441	9.8579
306	1-ts3-Pentadiene	C5H8	558.1040	3.4416
414	2-Methyl-1-Butenyne	C5H6	1428.2579	18.1703

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

305	Cs1,3-Pentadiene	C5H8	545.7374	3.0584
309	Isoprene	C5H8	665.7938	4.6579
421	1-Pentene-4-yne	C5H6	1304.0664	15.3046
303	1,3-Butadiene	C4H6	560.2226	5.6608
332	1,4-CyclHexadien	C6H8	540.0121	1.8832
501	Benzene	C6H6	698.5517	5.6501
315	Cyclopentadiene	C5H6	726.7128	7.6422
319	Diisopropenyl	C6H10	655.0987	3.2620
615	Ethynylbezene	C8H6	1345.6017	11.9030
601	Styrene	C8H8	1113.1934	5.9982
331	1,3-CycHexadiene	C6H8	676.2994	3.3891
310	1,5-Hexadiene	C6H10	1105.7240	10.5798
312	MthCycPentadiene	C6H8	812.5090	5.4818
420	1-Pentene-3-yne	C5H6	1262.2996	6.5552
502	Toluene	C7H8	769.8374	5.6974
521	T-Butylbenzene	C10H14	1644.6308	10.7057
320	Dipropylene	C6H10	551.6388	2.3351
520	Sec-Butylbenzene	C10H14	1201.7567	8.7365
313	1,4-Hexadiene	C6H10	974.0783	6.9508
314	Dipropylene	C6H10	686.2478	2.6723
316	DiCycPentadiene	C10H12	434.5720	2.9345
333	1,5-CycOctadiene	C8H12	511.9489	1.7163
701	Naphthalene	C10H8	676.4252	6.0857
504	Ethylbenzene	C8H10	826.1223	5.4674
820	Indan	C9H10	694.4551	3.0208
505	O-Xylene	C8H10	659.1170	3.6717
612	P-Methylstyrene	C9H10	1639.0360	7.8519
330	DIISOCROTYL	C8H14	626.5082	3.3477
507	P-Xylene	C8H10	835.1789	5.3296
329	DIISOBUTENYL	C8H14	1011.2352	5.9955
506	M-Xylene	C8H10	815.0713	5.0455
603	Methylstyrene	C9H10	933.4943	4.5076
613	Alpha-MthStyrene	C9H10	924.8652	5.1630
510	Isopropylbenzene	C9H12	1166.5424	8.1621
724	2-Methylindene	C10H10	540.6955	2.7486
285	Vinylcyclohexene	C8H12	1315.7976	8.3353
803	Indene	C9H8	949.1855	8.1225
706	Tetralin	C10H12	389.2102	1.5750
511	O-Ethyltoluene	C9H12	727.5091	3.9214
723	1-Methylindene	C10H10	391.8800	1.7179
738	Fluorene	C13H10	550.9621	3.1825
619	Tr-1PropenylBz	C9H10	730.6405	3.2349
525	O-Diethylbenzene	C10H14	807.8287	4.3556
618	Propenyl Bz(cis)	C9H10	677.7211	3.4462
602	O-Methylstyrene	C9H10	911.7234	4.2339
702	1-MthNaphthalene	C11H10	549.9902	4.2366
509	N-Propylbenzene	C9H12	713.9072	4.8431
526	M-Diethylbenzene	C10H14	824.1436	4.7128

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

583	Cs-2-PhnButene-2	C10H12	775.5706	4.8171
543	M-DiisopropylBz	C12H18	921.8437	6.7669
584	Ts-2-PhnButene-2	C10H12	1306.6381	10.9587
580	1,2-DiC1-3C2-Bz	C10H14	676.8310	2.9631
704	1-EthNaphthalene	C12H12	499.5058	1.8679
512	M-Ethyltoluene	C9H12	805.6768	4.8154
522	1-Mth-2-iC3-Benz	C10H14	865.7361	5.9389
513	P-Ethyltoluene	C9H12	586.1821	3.4849
514	1,2,3-Mesitylene	C9H12	587.8032	2.7026
614	M-Divinylbenzene	C10H10	1140.0701	5.2540
524	1-Mth-4-iC3-Benz	C10H14	544.7035	3.5157
822	Gamma-Terpinene	C10H16	549.6293	3.4357
821	Alpha-Terpinene	C10H16	706.8921	5.3795
523	1-Mth-3-iC3-Benz	C10H14	860.9457	5.9081
703	2-MthNaphthalene	C11H10	636.4990	4.9966
557	CycHexylBenzene	C12H16	466.3067	2.0758
515	1,2,4-Mesitylene	C9H12	722.0662	3.6679
519	Isobutylbenzene	C10H14	783.3228	5.4540
424	DiPhnAcetylene	C14H10	525.5081	3.0232
544	P-DiisopropylBz	C12H18	807.3239	4.8933
518	N-Butylbenzene	C10H14	759.2471	4.7419
516	1,3,5-Mesitylene	C9H12	854.8451	4.4912
809	Acenaphthalene	C12H8	662.7669	5.2134
725	123-TriMthIndene	C12H14	733.2082	5.4029
527	1,4-DiEthBenzene	C10H14	1082.6148	5.7692
558	Diphenyl	C12H10	576.7648	4.8700
576	2-Ethyl-m-Xylene	C10H14	961.6071	4.6548
620	p-ISOPROPENYLSTY	C11H12	639.1288	2.6276
585	o-PropylToluene	C10H14	735.2198	4.4062
577	2-Ethyl-p-Xylene	C10H14	804.6647	4.1359
579	4-Ethyl-o-Xylene	C10H14	978.9670	4.7271
586	m-Propyltoluene	C10H14	794.6274	4.7535
587	p-Propyltoluene	C10H14	773.2227	4.5961
578	4-Ethyl-m-Xylene	C10H14	772.8249	3.9295
575	5-Ethyl-m-Xylene	C10H14	480.3182	2.4959
530	Prehnitene	C10H14	540.1133	1.8003
709	2,6-2Mth-Naphtha	C12H12	533.8580	3.9235
715	2,7-2Mth-Naphtha	C12H12	543.2010	3.9971
719	2-Ethylnaphthalene	C12H12	807.2980	6.7100
621	p-tert-BUTYLSTY	C12H16	739.5108	3.9400
532	1,2,4,5-TetMthBz	C10H14	677.2087	2.8083
531	1,2,3,5-TetMthBz	C10H14	687.0116	2.7079
533	p-tert-BUTYL ET	C12H18	1579.8390	9.3226
567	N-Pentylbenzene	C11H16	680.3894	4.1130
718	1-n-PROPYLNAPHTH	C13H14	727.0129	6.6285
562	1,1-DiPhnEthane	C14H14	558.0706	3.6726
616	4-ISOBUTYLSTYRE	C12H16	513.2015	1.7797
260	1-Decene	C10H20	982.6500	5.7663

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

735	Cis-Stilbene	C14H12	642.4468	5.2080
568	Hexylbenzene	C12H18	659.2317	4.0228
563	Diphenylmethane	C13H12	588.4033	3.1052
564	1,2-DiPhnEthane	C14H14	569.4384	3.3270
804	Anthracene	C14H10	258.4336	2.5079
736	Trans-Stilbene	C14H12	348.3438	1.2323
805	Phenanthrene	C14H10	330.7582	3.0284
713	1-ButNaphthalene	C14H16	345.1278	2.5403
807	Pyrene	C16H10	215.3414	2.3629
261	1-Undecene	C11H22	1269.4087	7.3949
581	23-2C1-23-2PhnC4	C18H22	352.8066	2.8696
549	N-Heptylbenzene	C13H20	741.9866	4.5256
710	1-PhnNaphthalene	C16H12	511.8276	5.9024
566	2,4-Diphenyl-4-M	C18H20	735.0011	4.4988
561	O-Terphenyl	C18H14	988.4920	16.5596
569	N-Octylbenzene	C14H22	674.2335	4.0599
565	Triphenylmethane	C19H16	462.7401	3.4537
714	N-C6-Naphthalene	C16H20	846.6723	5.7867
717	Fluoranthene	C16H10	528.0330	7.8555
716	1-Hexyl-Tetralin	C16H24	623.3870	4.7320
731	TriPhnEthylene	C20H16	274.5054	1.9690
806	Chrysene	C18H12	119.2010	0.8235
588	1,1,2TriPhenEth	C20H18	641.7711	6.3225
711	1-n-NonylNaphtha	C19H26	383.6954	3.7307
570	N-Nonylbenzene	C15H24	730.5053	4.3360
712	1-Decyl Naphtha	C20H28	344.8561	3.4426
559	P-Terphenyl	C18H14	262.9617	2.0666
560	M-Terphenyl	C18H14	358.4781	3.7896
589	TetraPhenylMetha	C25H20	121.7719	1.5588
554	Decylbenzene	C16H26	321.9496	1.9290
732	TetraPhnEthylene	C26H20	92.5479	0.9421
574	N-Dodecylbenzene	C18H30	234.8687	1.4401
571	N-Undecylbenzene	C17H28	614.9252	3.6043
572	Tridecylbenzene	C19H32	700.8633	4.2254
573	n-TETRADECYLBENZ	C20H34	310.2633	2.1377
2575	n-PENTADECYLBENZ	C21H36	259.3879	1.7282
2576	n-HEXADECYLBENZ	C22H38	255.1656	1.7395
2577	n-HEPTADECYLBENZ	C23H40	426.7813	3.2274
2578	n-OCTADECYLBENZE	C24H42	481.0075	3.8321

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Halocarbons

DipID	Name	Formula	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1544	Allyl Chloride	C3H5Cl	713.8774	7.4435
1595	2-Chloropropene	C3H5Cl	890.7331	14.0421

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1531	3-Chloropropyne	C3H3Cl	1036.9621	12.8020
1535	T-Butyl Chloride	C4H9Cl	790.2403	5.8931
1583	Chloroprene	C4H5Cl	1076.5013	12.9949
1530	Isopropyl Cl	C3H7Cl	728.2461	4.9351
1572	O-DiCl-Benzene	C6H4Cl2	664.1317	4.5571
1585	Propyl Chloride	C3H7Cl	718.8790	6.9170
1684	Isopropyl Iodide	C3H7I	821.1155	7.2523
1598	13-2Cl-ts-2-C4H8	C4H6Cl2	912.9868	9.9795
1651	2-Bromopropane	C3H7Br	741.6132	5.2625
1691	Iodobenzene	C6H5I	934.9746	7.2321
1860	Fluorobenzene	C6H5F	606.5746	4.8181
1571	Chlorobenzene	C6H5Cl	764.8672	6.0702
1680	Bromobenzene	C6H5Br	1120.2724	8.4557
1526	1,2-DiCl-Propane	C3H6Cl2	1201.0980	10.7961
1683	Propyl Iodide	C3H7I	845.5471	7.2409
1576	Benzotrichloride	C7H5Cl3	753.9541	6.7877
1536	2,3-DICHLOROBUT	C4H8Cl2	924.2845	4.3381
2638	2-Bromobutane	C4H9Br	786.7161	4.1292
1586	1-Chlorobutane	C4H9Cl	874.2856	7.5778
1573	M-DiCl-Benzene	C6H4Cl2	828.9688	6.9499
2634	Benzotrifluoride	C7H5F3	2438.6827	16.6465
1574	P-DiCl-Benzene	C6H4Cl2	785.2074	5.9131
1650	1-Bromopropane	C3H7Br	749.2945	4.9664
1587	2-Chlorobutane	C4H9Cl	893.2782	6.1315
2653	8F-2-Butene	C4F8	4123.4710	245.8766
1678	M-Dibromobenzene	C6H4Br2	1069.2706	8.2931
1537	1,2-DiCl-Butane	C4H8Cl2	1358.8129	12.6084
1597	34-DiCl-1-Butene	C4H6Cl2	1310.1638	8.5248
1577	O-Chlorotoluene	C7H7Cl	780.5137	5.1880
1532	123-3Cl-Propane	C3H5Cl3	988.9402	8.8606
1578	P-Chlorotoluene	C7H7Cl	584.6014	3.2671
1562	Benzyl Chloride	C7H7Cl	833.8780	5.4332
2661	P-Bromotoluene	C7H7Br	1002.0199	6.7158
1508	1,4-DiCl-Butane	C4H8Cl2	566.2547	3.9398
1655	1-Bromobutane	C4H9Br	914.6990	5.7454
1599	BenzylDichloride	C7H6Cl2	593.0664	4.8012
2652	Perfluoropropane	C3F8	739.8340	6.3038
1505	2-Butylene DiCl	C4H6Cl2	338.8333	1.5974
1593	14-2Cl-cs-2-C4H8	C4H6Cl2	635.7387	4.1102
1588	1-Chloropentane	C5H11Cl	845.0569	7.6545
2654	OctaF-CycButane	C4F8	3.1164	0.0171
1592	1,2,4-TriCl-Bz	C6H3Cl3	741.1344	6.6432
1579	2,4-2Cl-Toluene	C7H6Cl2	692.7015	4.2251
2593	1,3,5-TriCl-BZ	C6H3Cl3	793.3171	7.5706
1697	1-Br-Naphthalene	C10H7Br	537.4605	2.2299
1622	Perfluorobutane	C4F10	845.3889	4.8334
1857	P-Cl-Benzo-TriF	C7H4ClF3	2143.5389	16.0000
1509	1,5-DiCl-Pentane	C5H10Cl2	491.6506	3.0463

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

1589	1-Cl-Naphthalene	C10H7Cl	472.9070	3.8306
1864	Perfluorobenzene	C6F6	779.3898	6.1928
1858	2,4-2Cl-Benzo-3F	C7H3Cl2F3	1872.0516	13.1523
1667	1-Bromoheptane	C7H15Br	1053.4316	5.6131
1575	HexaCl-Benzene	C6Cl6	402.5635	1.0265
2640	Freon 123B1	C2HBrClF3	4392.9186	53.3336
1504	Vinyl Chloride	C2H3Cl	771.9464	6.9559
1672	1,1-DiBr-Ethane	C2H4Br2	1009.0301	5.0098
1580	Acetylene DiCl	C2H2Cl2	1056.1965	5.6477
1692	Diiodomethane	CH2I2	625.4125	2.7247
1698	Bromoform	CHBr3	1176.5949	8.6138
2687	Freon 13B1	CBrF3	8164.3918	261.5476
2690	Br-3F-Ethylene	C2BrF3	2386.4272	101.4938
1649	Tetrabromoethane	C2H2Br4	557.8804	2.5679
2686	Freon 12B1	CBrClF2	5155.3923	199.7275
1503	Ethyl Chloride	C2H5Cl	522.1798	5.9798
2641	Br-TriCl-Methane	CBrCl3	1413.0191	16.4246
1641	Methyl Bromide	CH3Br	347.5934	2.7545
2688	Freon 12B2	CBr2F2	3671.6432	103.3912
2545	2,3-DiCl-Propene	C3H4Cl2	814.4916	4.0852
1673	1,2-DiBr-Ethane	C2H4Br2	736.2393	4.6662
2637	Dibromomethane	CH2Br2	834.4083	4.3681
1542	TetraCl-Ethylene	C2Cl4	3007.3245	102.7801
1541	TriCl-Ethylene	C2HCl3	2319.3773	70.9505
1527	111-TriCl-Ethane	C2H3Cl3	727.5664	5.6995
1612	Cl-2F-Ethylene	C2HClF2	485.5904	5.1047
1617	Ethyl Fluoride	C2H5F	0.8632	0.0167
2639	Br-Cl-Methane	CH2BrCl	1141.5758	10.2286
1581	Ts-1,2-DiCl-C2H4	C2H2Cl2	2036.1934	14.5302
1682	Ethyl Iodide	C2H5I	824.7483	7.2509
1522	1,1-DiCl-Ethane	C2H4Cl2	560.4143	4.2379
2695	1-Cl-1,1-DiF-C2	C2H3ClF2	46.8408	0.1976
1525	Hexachloroethane	C2Cl6	717.8858	3.9047
1528	1112-4Cl-Ethane	C2H2Cl4	966.4763	8.7971
1590	Penta-Cl-Ethane	C2HCl5	795.1199	7.5794
1529	1122-4Cl-Ethane	C2H2Cl4	802.0417	6.5314
2693	Perfluoroethane	C2F6	710.2540	10.2353
1611	Freon 114B2	C2Br2F4	4828.4425	110.8496
2692	Cl-PentaF-Ethane	C2ClF5	895.8506	8.8899
2655	122-3Cl-112-3FC2	C2Cl3F3	791.0080	7.6729
1609	12-2Cl-1122-4FC2	C2Cl2F4	674.9641	5.0167
2526	1,1-DiCl-Propane	C3H6Cl2	671.7112	4.7350
1645	Ethyl Bromide	C2H5Br	605.2609	4.2456
2658	1112-4Cl-22-2FC2	C2Cl4F2	1305.6115	9.5821
1619	111-3F-Ethane	C2H3F3	6.5231	0.0265
1524	1,1,2-3Cl-Ethane	C2H3Cl3	970.7948	9.5798
1640	1,1-DiF-Ethane	C2H4F2	0.0000	0.0000
2691	Genetron 1113	C2ClF3	1388.7854	74.7851

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

2694	Vinyl Bromide	C2H3Br	1247.1769	16.5444
1694	Refrigerant 123	C2HCl2F3	2378.2984	29.1342
1523	1,2-DiCl-Ethane	C2H4Cl2	733.6967	7.7465
2656	1122-4Cl-12-2FC2	C2Cl4F2	710.4014	7.6238
2527	1,3-DiCl-Propane	C3H6Cl2	771.8384	6.6992

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

Acids

DipID	**Name**	**Formula**	$P_{Gani}^{760mmHg}$	P_{Gani}^{10mmHg}
1277	Acrylic Acid	C3H4O2	738.0194	3.1443
1274	Ts-Crotonic Acid	C4H6O2	263.5439	0.2646
1279	Oleic Acid	C18H34O2	380.2510	2.2750
1278	Methacrylic Acid	C4H6O2	827.6449	1.7811
2271	Cinnamic Acid	C9H8O2	297.4596	0.2800
1266	n-UNDECANOIC ACI	C11H22O2	499.7422	1.9084
1282	O-Toluic Acid	C8H8O2	652.6748	2.1353
2283	IBUPROFEN	C13H18O2	819.1345	3.5899
1261	Isovaleric Acid	C5H10O2	937.7221	2.7153
1264	1,4-CychexDicarboxAcid	C8H12O4	52.4590	0.0519
1283	P-Toluic Acid	C8H8O2	405.2221	0.9923
1257	3-MthButyricAcid	C5H10O2	783.9888	2.7332
1288	Isophthalic Acid	C8H6O4	5.8402	0.0014
2871	4CarboxAcidBzldhyde	C8H6O3	10.8251	0.0047
1256	N-Butyric Acid	C4H8O2	814.5032	2.2424
1276	Stearic Acid	C18H36O2	659.8515	4.3014
1285	Adipic Acid	C6H10O4	211.0040	0.3615
1273	Cs-Crotonic Acid	C4H6O2	600.5361	1.4568
4851	Diglycolic Acid	C4H6O5	188.6846	0.1267
1286	Maleic Acid	C4H4O4	197.6661	0.2177
2277	Citraconic Acid	C5H6O4	62.2202	0.0455
2278	Itaconic Acid	C5H6O4	165.7443	0.1856
2281	Glutaric Acid	C5H8O4	211.1712	0.2333
1271	TetradecylicAcid	C14H28O2	406.6774	1.8226
1259	N-Nonanoic Acid	C9H18O2	1319.1241	4.3885
1280	Linoleic Acid	C18H32O2	455.4956	2.9215
1260	Isobutyric Acid	C4H8O2	495.7119	1.4823
2268	Fumaric Acid	C4H4O4	246.1393	0.1945
1287	Phthalic Acid	C8H6O4	890.5399	2.7529
1289	TerephthalicAcid	C8H6O4	1.1691	0.0000
2280	Succinic Acid	C4H6O4	142.3665	0.1086
1270	Tridecanoic Acid	C13H26O2	315.7333	1.3264
1254	N-Decanoic Acid	C10H20O2	410.8657	1.2706

Table E.3 Vapor Pressures Calculated by the Gani Method (Continued)

2270	Suberic Acid	C8H14O4	182.8368	0.4651
2255	Linolenic Acid	C18H30O2	594.5584	3.3637
1262	N-Hexanoic Acid	C6H12O2	1056.4646	2.4649
4852	Levulinic Acid	C5H8O3	232.3867	0.3811
2275	Sebacic Acid	C10H18O4	200.8429	0.6328
1255	Oxalic Acid	C2H2O4	68.7041	0.0294
2259	PentadecylicAcid	C15H30O2	500.6355	2.6602
2266	NonadecanoicAcid	C19H38O2	908.1856	6.3739
2269	Pimelic Acid	C7H12O4	197.8347	0.3041
1252	Acetic Acid	C2H4O2	744.1016	4.2509
3268	Malonic Acid	C3H4O4	120.4823	0.0747
2279	2-EthButyricAcid	C6H12O2	1005.1442	3.9766
1265	N-Octanoic Acid	C8H16O2	670.3071	1.7767
2258	NeopentanoicAcid	C5H10O2	1387.9187	2.7919
2257	Azelaic Acid	C9H16O4	204.5892	0.5206
1281	Benzoic Acid	C7H6O2	571.9568	1.2183
1269	Dodecanoic Acid	C12H24O2	1241.2333	4.4149
2261	Heptanoic Acid	C7H14O2	512.9566	1.3399
1258	N-Valeric Acid	C5H10O2	1142.7823	2.8531
2265	HeptadecylicAcid	C17H34O2	394.2199	2.3960
2267	N-Eicosanic Acid	C20H40O2	626.8244	4.7653
1253	Propionic Acid	C3H6O2	816.4347	3.1407
5877	Ascorbic Acid	C6H8O6	478.1965	0.1330
1272	HexadecanoicAcid	C16H32O2	528.3554	3.0169

APPENDIX F.

A DETAILED LIST OF OMITTED COMPOUNDS

RELATED TO CHAPTER IV

Table F. 1 Boiling Temperatures and Vapor Pressures Calculated from the Proposed correlations for the omitted compounds

Dip ID	Name	Formula	$T_{b,Calc}^{760\,mmHg}$	$T_{b,Calc}^{10\,mmHg}$	$P_{calc}^{760\,mmHg}$	$P_{Calc}^{10\,mmHg}$
	Alcohols[a]					
1250	Sorbitol	C6H14O6	672.83	534.52	438.108	0.615
1249	Inositol	C6H12O6	667.79	534.46	569.234	0.865
	Silanes[b]					
3985	Dimethyl Silane	C2H8Si	251.48	178.45	746.518	8.823
3984	Methyl Silane	CH6Si	216.22	151.57	759.999	10.009
3986	Trimethyl Silane	C3H10Si	277.65	195.95	753.905	8.510
1984	TetraMth Silane	C4H12Si	298.68	212.16	760.917	8.398
2994	TETRAETHYL Si	C8H20Si	409.01	298.73	464.903	5.334
1965	HexMthDisiloxane	C6H18OSi2	378.37	271.80	820.842	9.562
1966	6C1Cyc3Siloxane	C6H18O3Si3	403.13	296.48	632.149	7.508
1988	8C1Cyc4Siloxane	C8H24O4Si4	463.92	341.48	759.995	9.991
3991	DecaMethcyclpenS	C10H30O5Si5	323.92	277.99	1.494	0.050
3992	DodecaMethCyHexS	C12H36O6Si6	561.10	414.92	977.351	18.074

[a] These compounds have been excluded from database because they have anormous deviations in vapor pressure by The Joback method

[b] Joback and Gani models both do not have Si groups

Table F.1 Boiling Temperatures and Vapor Pressures Calculated from the Proposed correlations for the omitted compounds (Continued)

	Imines[c]					
1754	N-Methylpyrrole	C5H7N	343.40	255.99	176.102	1.311
3740	Acridine	C13H9N	568.43	429.79	562.672	6.584
	Tert-Ns[c]					
1703	Trimethylamine	C3H9N	266.49	194.96	760.006	10.047
2856	DiMth Acetamide	C4H9NO	366.73	273.31	69.261	0.329
	Nitrates[d]					
1779	P-Nitrotoluene	C7H7NO2	492.53	366.39	726.556	7.391
1886	Nitrobenzene	C6H5NO2	469.11	348.06	520.272	6.060
1778	O-Nitrotoluene	C7H7NO2	492.53	366.39	723.120	9.857
1780	M-Nitrotoluene	C7H7NO2	492.53	366.39	630.941	8.454
1891	O-Nitroanisole	C7H7NO3	517.63	386.38	334.009	2.116
2740	M-Dinitrobenzene	C6H4N2O4	554.84	417.95	498.393	5.697
2742	P-Dinitrobenzene	C6H4N2O4	554.84	417.95	823.512	10.005
2741	O-Dinitrobenzene	C6H4N2O4	554.84	417.95	301.629	3.244
2749	3,5-DiNitToluene	C7H6N2O4	573.35	432.57	517.391	6.850
2743	DNT	C7H6N2O4	573.35	432.57	645.318	10.133
2745	3,4-DiNitToluene	C7H6N2O4	573.35	432.57	350.317	5.190
2744	2,6-DiNitToluene	C7H6N2O4	573.35	432.57	1096.570	21.814
2748	2,5-DiNitToluene	C7H6N2O4	573.35	432.57	535.875	8.866
2746	1,3,5-TrinitroBz	C6H3N3O6	623.76	474.71	541.113	6.214
3748	(NO2)C6H4)2NC6H5	C18H13N3O4	737.93	564.18	1237.788	8.683
2747	Trinitrotoluene	C7H5N3O6	639.03	486.90	1264.331	24.135
	Hydrocarbon[a]					
2086	n-Hexatriacontane	C36H74	775.78	595.40	1172.881	11.848
	Halocarbons[e]					
1561	6Cl-1,3Butadiene	C4Cl6	484.00	349.85	759.518	6.559
1582	6ClCycPentadiene	C5Cl6	496.43	363.16	499.694	4.992
1591	Vinylidene DiCl	C2H2Cl2	307.52	222.45	796.003	10.000
1614	Difluoromethane	CH2F2	134.62	44.01	0.265	0.000
	Acids[a]					
2282	PyromelliticAcid	C10H6O8	765.51	609.70	1822.574	15.986

[c] Gani approach do not have –N< group

[d] Koska et al. method do not have ACNO2 for prediction the heat of vaporization

[e] Koska et al. method do not have CCl2 for prediction the heat of vaporization

APPENDIX G.

DETAILED VAPOR PRESSURES CALCULATED

BY THE ASHER METHOD

Table G. 1 Detailed estimated vapor pressures for 68 compounds at 10 mmHg by the presented method and Asher, 2006.(all temperatures are in the scope of Asher et al. regression, i.e. between 290 and 320).

	No. of Compounds	DipID	Name	Tb at 10 mmHg /K	$P_{This}^{10\,mmHg}$	$P_{Asher}^{10\,mmHg}$
Alcohos	12	1111	2-Mth-2-Butanol	290.71	13.26	6.26
		1123	3-Mth-1-Butanol	314.15	3.51	13.09
		1115	2-Hexanol	318.24	10.91	6.14
		1130	4-Mth-2-Pentanol	308.10	11.54	6.49
		1106	Isobutanol	297.46	3.40	14.69
		1105	N-Butanol	303.84	1.96	9.55
		1109	1-Pentanol	317.63	5.33	7.81
		1113	T-Butylcarbinol	298.93	4.89	10.53
		1124	3-Mth-2-Butanol	299.42	3.77	11.59
		1110	2-Pentanol	304.95	5.47	7.40
		1120	3-Pentanol	300.99	15.00	5.69
		1112	2-Mth-1-Butanol	312.45	3.97	11.82
Ave %PAAD						
Aldehyde	4	1009	1-Hexanal	296.77	8.06	17.30
		1016	2-Methylhexanal	308.78	8.61	8.35
		1017	3-Methylhexanal	307.06	9.03	9.62
		1008	1-Heptanal	314.31	7.73	8.50
Ave %PAAD						
ketone	9	1065	Mesityl Oxide	296.49	9.24	67.01

Table G.1 Detailed estimated vapor pressures for 68 compounds at 10 mmHg by the presented method and Asher, 2006 (Continued)

		1059	3-Hexanone	292.55	9.76	19.30
		1063	2-Heptanone	313.82	9.32	19.08
		1064	5-Mth-2-Hexanone	309.00	15.79	37.80
		1058	4-Heptanone	307.42	15.21	66.53
		1057	3-Heptanone	312.30	8.73	6.83
		1076	2,4-Pentanedione	291.74	34.93	8.84
		1062	2-Hexanone	295.58	5.15	6.26
		2889	HydroxyAcetone	314.86	6.55	3.36
Ave %PAAD						
Hydrocarbones	21	259	1-Nonene	308.59	6.91	3.49
		51	2,2,3,3-4Mth-C5	299.06	2.48	23.07
		52	2,2,3,4-4Mth-C5	293.85	4.17	19.45
		54	2334TetrMethPent	300.36	2.25	26.70
		190	2,2-2C1-3-C2-C5	296.04	5.33	9.36
		50	3,3-DiEthPentane	303.80	5.19	6.51
		49	244TriMethHexane	292.88	6.81	7.83
		192	2,4-2C1-3-C2-C5	298.16	5.41	11.47
		96	2,2-DiMthHeptane	295.83	8.11	4.00
		176	2,6-DiMthHeptane	299.20	4.64	5.45
		27	N-Octane	292.27	7.84	2.53
		94	3-Ethylheptane	304.90	7.86	3.48
		92	3-Methyloctane	306.16	7.07	3.79
		93	4-Methyloctane	304.71	8.29	3.44
		91	2-Methyloctane	305.91	7.49	3.72
		72	2,2-DiMthOctane	315.48	7.05	3.94
		2096	2,4Dimethloctane	315.79	8.30	4.47
		2098	2,6DimethlOctane	318.56	7.58	5.36
		2097	2,5Dimethloctane	317.12	7.79	4.89
		2099	2,7DimethlOctane	318.17	8.68	5.22
		46	N-Nonane	312.11	4.55	2.60
Ave %PAAD						
Cyclic	8	274	Cyclooctene	303.04	8.25	12.6
Hydrocarbons		142	Cs-1,2-2C1-CycC6	291.44	6.69	25.86
		140	Ethylcyclohexane	293.67	8.90	12.59
		149	N-PropylCyc-C6	313.31	8.59	10.80
		114	N-PropCycPentane	294.42	6.19	4.61
		160	Cyclooctane	308.21	5.52	107.60
		150	Isopropyl-CycC6	311.01	8.02	20.09
		122	Butylcyclpentane	314.72	7.49	4.46
Ave %PAAD						

Table G.1 Detailed estimated vapor pressures for 68 compounds at 10 mmHg by the presented method and Asher, 2006 (Continued)

Aromatics	12	601	Styrene	306.52	9.50	7.89
		333	1,5-CycOctadiene	310.35	5.63	3.03
		504	Ethylbenzene	298.88	10.01	4.16
		505	O-Xylene	305.24	8.39	2.91
		330	DIISOCROTYL	301.43	4.85	7.72
		507	P-Xylene	300.40	11.90	2.27
		506	M-Xylene	301.19	11.30	2.37
		510	Isopropylbenzene	311.55	11.14	3.10
		285	Vinylcyclohexene	290.32	19.17	1.82
		509	N-Propylbenzene	316.33	8.78	3.52
		512	M-Ethyltoluene	318.16	10.64	3.51
		513	P-Ethyltoluene	318.67	7.85	3.61