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Predicting flash points of pure compounds and mixtures with help of COSMO-RS

Jens Reinisch[#,1] *and Andreas Klamt*[1,2]

[1] COSMOlogic GmbH&CoKG, Imbacher Weg 46, Leverkusen, Germany

[2] Inst. of Physical and Theoretical Chemistry, University of Regensburg, Germany

[#] corresponding author: reinisch@cosmologic.de

Abstract: The flash point (FP) is an important parameter for safety assessment of chemical compounds. Many empirical approaches have been developed to predict the FP based on the molecular structure, sometimes involving a large number of descriptors and resulting in class specific equations. We demonstrate in this work that a satisfying and rather general prediction of the saturation pressure at the FP can be achieved using the molecular surface area only. This relation in combination with any experimental or computational method for calculating the temperature dependent vapor pressures thus allows for the prediction of the FP. In a second step we calculate the FP of mixtures by using COSMO-RS activity coefficients. By using the proposed method, the flash points can be calculated without need for data typically generated from experiments such as the normal boiling point or the enthalpy of combustion, while experimental pure compound FPs and vapor pressure data still can be used to increase the prediction quality.

1) INTRODUCTION

The flash point (FP) of a liquid is the temperature at which the vapor over the liquid will completely combust after ignition. It is an important parameter for the safety assessment of chemical compounds or their mixtures. Unfortunately, two different experimental setups for the measurement of flash points are in use, one with an open ignition cup, the other using a closed cup. Usually FPs from open cup measurements are 50 K – 100 K higher. The closed-cup setup appears to have the better reproducibility and is more widely accepted. Hence in this paper we only consider closed-cup FPs. Still the scatter between flash points measured independently and reported in different literature sources or material safety data sheets can differ substantially. The experimental data thus need to be considered with care.

In this situation predictive methods for the FP can be used for two purposes: they allow to cross-check experimental data vs. predicted data and to directly predict FPs for compounds and mixtures where no experimental data are available. Especially the FPs for mixtures of two or more compounds are rarely available from measurements. It is also common that flash point related experimental data, e.g. boiling points or enthalpies of vaporization, are not available for new molecules and mixtures, so that models depending on these data cannot be applied. The scope of this paper is to provide a simple flash point model for pure compounds and their mixtures without the mandatory usage of any experimental input.

2) PREDICTING THE PURE COMPOUND FLASH POINT

In the last 15 years many prediction methods for the FP have been published, partly based on relations involving typically measured data such as enthalpies of vaporization, enthalpies of combustion and vapor pressures. Among these data the normal boiling point (BP) appears to be

of special value as descriptor. A second group of methods is most often based on quantitative structure property relationships (QSPR) where large numbers of all kinds of molecular descriptors and many different statistical regression methods ranging from classical multiple-linear regression, via genetic algorithms to artificial neural networks have been applied. Many of these methods are restricted to a single compound class for which they have been developed, and some are themselves collections of class specific QSPR equations for narrow compound classes. A review on several approaches has been given by Liu and Liu[1] and more references can be found in table 2 of a review on mixture flash points by Phoon et. al.[2]. The typical accuracy of descriptor based methods is in the range of 10 K – 20 K for medium sized data sets with more than 500 compounds, see table 3 of Liu and Liu[1]. If an experimental uncertainty of greater 5 K is assumed, an accuracy of 10 K can already be considered a good model. An exact comparison of the various models is difficult as they are fitted and tested on highly different data sets and the errors are sometimes given in absolute average deviation (AAD), standard deviation, relative error or just as a correlation coefficient.

In this paper we present a model which avoids using extensive QSPR and which is independent of experimental data. It is just based on a single molecular size descriptor, i.e. the molecular surface area, which can be considered at least as a physically plausible descriptor because several relevant aspects, such as the heat of combustion and the number of combustion products naturally increase with the size of the compounds. This descriptor combined with a prediction model to interconvert vapor pressure and temperature is the foundation of the presented concept. The conversion is required as the presented models will natively predict the saturation vapor pressure at the flash point and the flash point is only calculated from this pressure. This is possible because each FP of a compound *i* corresponds to a saturation pressure ($P_{i,fp}^{sat}$), which theoretically

is identical to the lower flammability limit (LFL) at the FP. This is a natural relation as lower concentrations of compound *i* will not ignite. To establish the prediction model for pure compound FPs a two step procedure is applied. As a first step, we assume that a certain compound specific saturation pressure is required to flash and that the FP is just the temperature to reach it. We calculate this pressure ($P_{i,fp}^{sat}$) with the COSMO-RS[3–6] implementation COSMO*therm*[6–8] (version C30_1401) for a set of molecules for which experimental FPs are available. In a second step this experiment based saturation pressures are correlated with the molecular surface area of the molecules, which is calculated with the conductor like screening model (COSMO)[9] implementation of TURBOMOLE 6.6[10]. The resulting correlation can now be used to predict the saturation pressure for other organic compounds, which can subsequently be transformed into the flash points by use of COSMO*therm*. As the prediction of the vapor pressure and thus the interconversion of pressure and temperature is not a native results of the COSMO-RS theory, a few explanatory words have to be said. COSMO-RS is a theory for dense liquids and provides the chemical potential in liquids. Together with an estimate of the change of chemical potential when entering the gas phase, the vapor pressure can be directly calculated. The applied COSMO*therm* software uses an approximate equation to calculate the required differen in the chemical potentials, which has been published[6,11] before. The used approach is fully predictive and can be used without external data. It is, however, limited to ideal gases and bound to the used COSMO-RS implementation. The above described approach to predict the flash points has basically three sources of error:

1) The transformation of experimental FPs into saturation pressures to establish the correlation
2) The rather simple correlation of the saturation pressure to the molecular surface
3) The back-transformation of predicted saturation pressures to FPs

To reduce the error of step 1 and to establish an optimal correlation, the available experimental normal boiling points (BP) are used for the calibration of the COSMO*therm* vapor pressure, where the predictions of the vapor pressure are scaled in such a way that the vapor pressure at the normal boiling point is exactly reproduced:

$$P_{pred}^{scaled}(T) = P_{pred}(T) \cdot \frac{1atm}{P_{pred}(T_{BP})} \quad (1)$$

This leads to a general improvement of the predicted vapor pressures as the COSMO-RS error usually deviates systematically over a wide temperature range. By applying this compound specific calibration COSMO*therm* is not predicting the absolute value of the vapor pressure, but only the difference between the vapor pressure at the normal boiling point and the flash point. In this way BPs or other experimental vapor pressure data can also be used in step 3 to get an improved back transformation of saturation pressure to FP.

To establish the model, a high quality data set of experimental flash points is required. For this purpose we use the data set collected by J. Rowley[12] and cured it for likely experimental errors. We added BPs from the PhysProp database 2002 and several other sources, but also took care not to use wrong or at least questionable BPs. After this procedure 931 normal boiling points were finally used. 13 compounds were excluded from the original set of Rowley: four compounds because they were not present in our molecule database, one compound could not be exactly identified, five compounds are solid at the FP, which cannot be easily handled by COSMO*therm*, one compound showed a large variation in experimental data, one compound very likely decomposes around FP and one compound has an unreasonable FP as compared to a series of similar compounds. A list of the excluded compounds is given in the supporting information (table S1). The final set contains 1056 molecules and their flash points. The full table of used pure compound data is given in the supporting information (table S3).

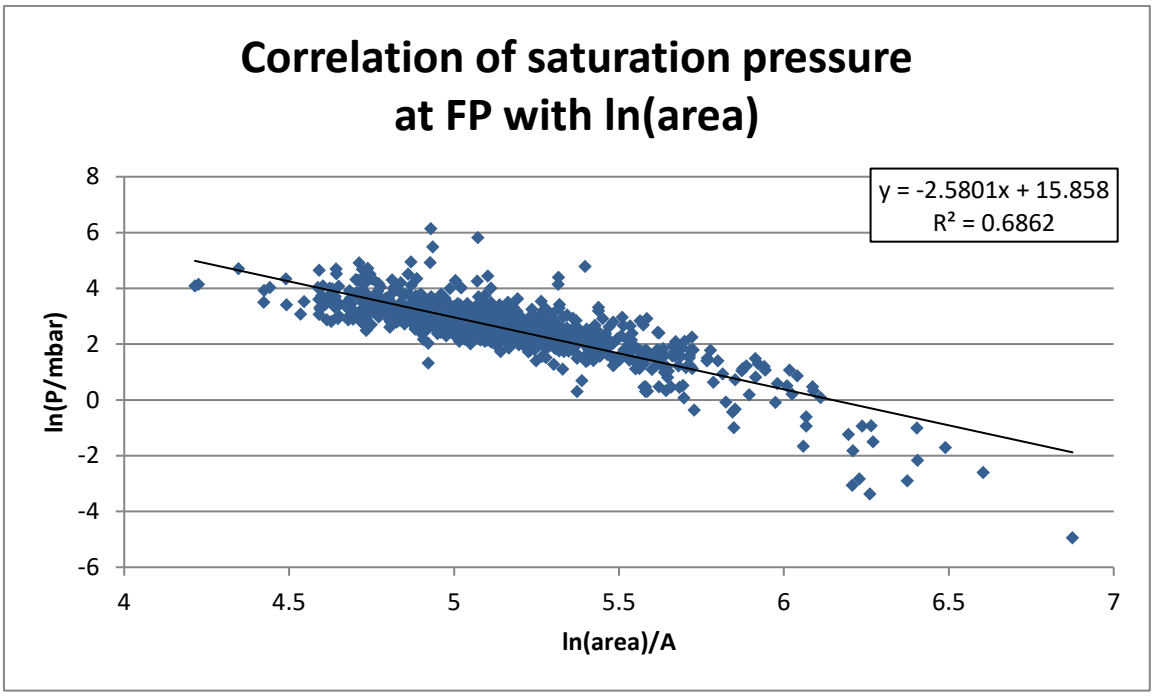

Figure 1. Correlation of predicted logarithmic saturation pressures at experimental FP with ln(area) for 1056 molecules. The vapor pressure prediction is done with a correction based on experimental normal boiling points.

Figure 1 shows the correlation between the saturation vapor pressure at the FP and the molecule surface area. To first order the data show a linear trend resulting in the equation:

$$\ln(P_{i,fp}^{sat}) = 15.86 - 2.58\ln(area_i) \qquad (2)$$

A quadratic correction could improve the correlation, but this would be strongly influenced by the few, very large compounds for which the experimental data and the predicted vapor pressures may be more questionable. Therefore we decided to stay with this linear model for the logarithmic flash point pressure as a function of logarithmic surface area. The resulting correlation of the experimental FP to the predicted FP is shown in figures 2 and 3. The two different approaches presented in figure 2 and 3 demonstrate the expected accuracy if no BP is available (fig 2) and if a BP can be used for calibrating the COSMO-RS prediction (fig 3).

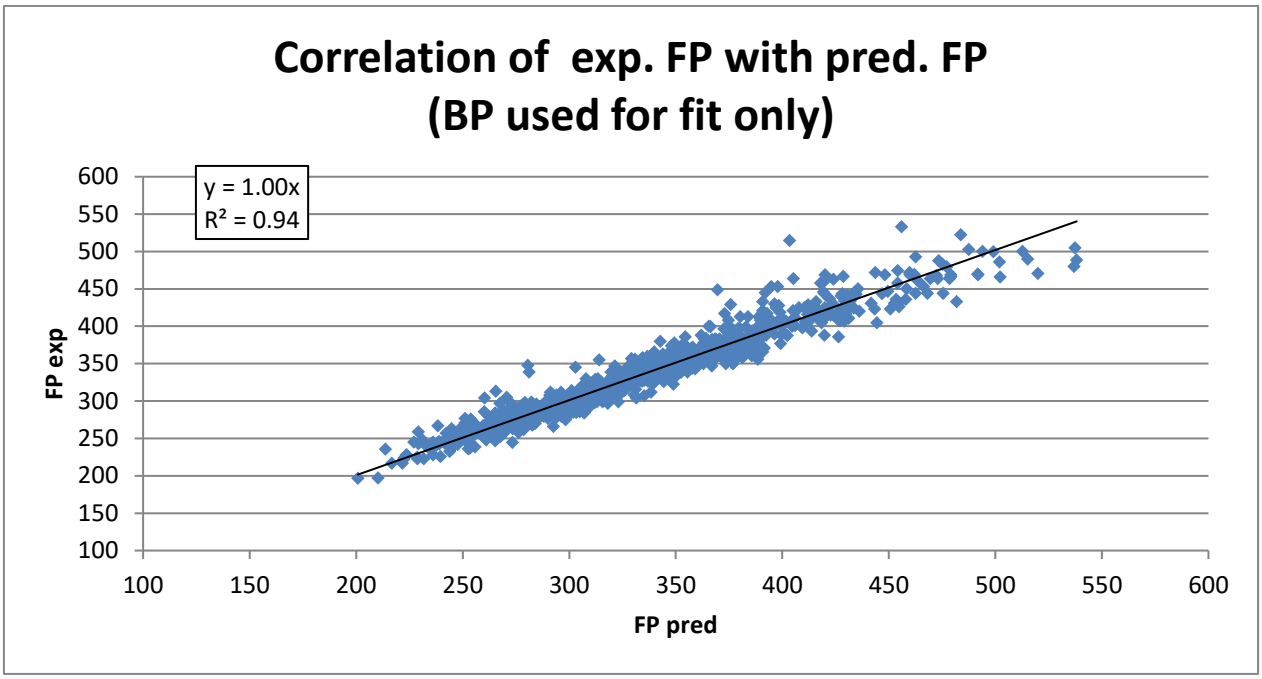

Figure 2. The data have been predicted without calibration with experimental normal boiling points in step 3. The BPs are thus only used in step 1 to establish the experiment based vapor pressures at the flash points used for fitting eq. 2. The RMSE and AAD are 14.32 K and 10.02 K.

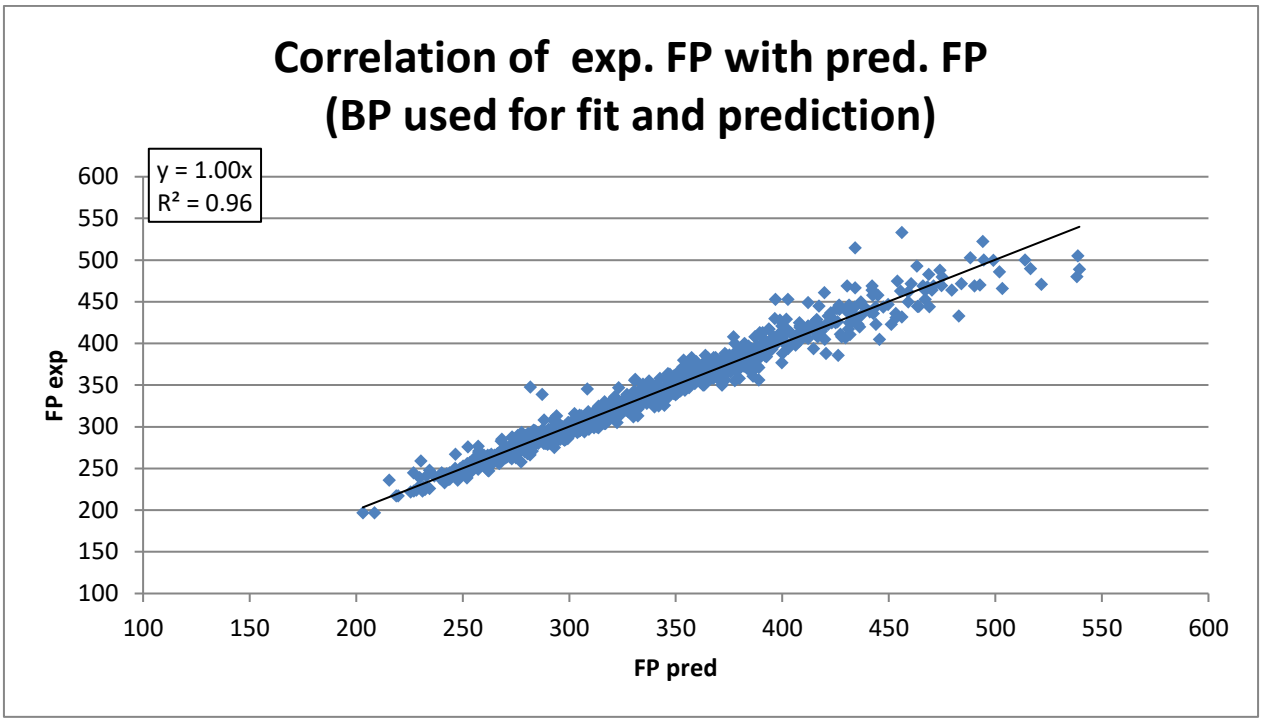

Figure 3. The data have been predicted using the experimental normal boiling points in step 1 and step 3. The BPs thus are used for fitting eq. 2 and transforming predicted saturation pressures into FPs. The RMSE and AAD are 11.20 K and 7.48 K.

The root mean square error (RMSE) for the prediction (fig. 2) is 14.32 K and the absolute average deviation (AAD) is 10.02 K. If the experimental boiling points are also used for transforming the predicted saturation pressure into FPs, the RMSE is 11.20 K and the AAD is 7.48 K. It has to be noted, that these values are calculated for predicting the fitting set and not for a validation set. As only a single descriptor is used and only two parameters are adjusted to the 1056 data points, the model can hardly be over-fitted and should hold for the entire range of organic chemistry represented by the experimental data set. The better correlation in figures 2 and 3 as compared to the underlying correlation in figure 1 is caused by the non-linear transformation of saturation pressures to flash points, which decrease the relative error and thus increases the correlation coefficient. We also estimated the experimental error of FP measurements by using the DIPPR data as presented by Gharagheizi[13] in comparison to the data of Rowley. We

calculated the deviations between the Rowley FP and the DIPPR FP to their mean value for all compounds where the two FPs are different (N=511) as it is assumed that numerically identical points stem from the same source. This leads to an estimated experimental RMSE of 5.3 K and an AAD of 3.5 K.

The presented model performs with roughly the same quality as other methods[1] as far as a comparison can be conducted. Please refer to the review by Liu and Liu[1] for accuracy details on other methods, which use different data sets and accuracy indicators and are thus not directly comparable with the presented work. Though providing no significant improvement in accuracy, the presented method has several other advantages: once the model is established, its usage does not require any experimental input for predicting the FPs (though it can benefit from it), it uses only one descriptor and two parameters and is fitted and tested with a comparably large data set. Despite providing a generally good accuracy, the simple correlation to molecular surface area and the (predictive) transformation of saturation pressure to FPs with COSMO*therm* introduces some errors. Two major error sources can be identified by taking a look at the worst predictions. There are 10 compounds having a prediction error of more than 50 K (if no experimental BP is used for FP prediction), see table S2. These may be labeled as outliers.

The outliers can be roughly categorized into two categories: molecules with one or many chlorine atoms (Cl-type) and molecules with several spatially close OH-groups (polyol-type). The physical reason for the Cl-type outliers is assumed to be the rather inert nature of Cl, which does not significantly contribute to the combustion enthalpy as compared to H and C. If one just neglects the area of the Cl-atoms, the FP prediction improves significantly, see table 1. If one evaluates only those molecules of the complete set having at least a single chlorine atom, the RMSE and AAD increase to 20.85 K and 12.72 K with a mean deviation of -9.99 K, supporting the special role of chlorine. We also checked if COSMO*therm* generally overestimates the Cl-

compounds vapor pressure, which is not the case as the vapor pressures mean deviation is just 9% for the chlorine compounds.

Table 1. Error reduction by neglecting of chlorine area.

	Area / A^2		Flash point error / K	
Cl-type outliers	With Cl	Without Cl	With Cl	Without Cl
Terephthaloyl Chloride	203.7	133.9	-58	-33
Hexachlorobenzene	220.9	34.5	-112	-19
Trichloroacetaldehyde	138.3	38.0	-68	-7
Dichloroacetyl Chloride	139.2	37.4	-58	-19
Isophthaloyl Chloride	203.5	133.0	-55	-30

The flash point predictions are done without experimental vapor pressure data on the original fit (eq. 2). The error is calculated as predicted FP minus exp. FP.

For the polyol-type outliers the main reason is that the vapor pressure prediction of COSMO*therm* systematically provides too high vapor pressures, which will result in too low FPs. In addition one might assume that oxygen (in analogy to chlorine) will not provide a large contribution to the heat of combustion and molecules with a significant amount of oxygen will thus have larger errors. This assumption, however, is not consistent with the error of Triethylenglycol bis(2-ethylhexanoate), as the flash point is overestimated and thus the vapor pressure is underestimated. The chlorine outliers demonstrate that further improvement of the model can be expected by introducing element specific scaling of the surface areas. Such improvements will be considered in a forthcoming paper.

3) PREDICTING MIXTURE FLASH POINTS

A recent review[2] by Phoon et al. on flash point prediction models for mixtures presents an overview on available methods and their strength and weaknesses. According to this review the

equations by Liaw[14] are currently the most commonly used approach to predict mixture flash points. The Liaw model uses the assumption of temperature independent LFL and requires mixture activity coefficients and pure compound P(T) data. It has been extended and tested for partly miscible systems[15], ternary systems[16] and water organic systems[17,18].

The equations used by Liaw are

$$LFL_i = \frac{P_{i,fp}^{sat}}{P_{external}} \tag{3}$$

$$\sum_{i \neq k} \frac{y_i P_{mix,fpmix}^{sat}}{P_{external} LFL_i} = \sum_{i \neq k} \frac{x_i \gamma_i P_{mix,fpmix}^{sat}}{P_{i,fp}^{sat}} = 1 \tag{4}$$

These equations use the fact that at the flash point the LFL should be identical to the saturation vapor pressure. If one or more compounds are not flammable (index k), their contributions within the sum of eq. 4 are ignored. This makes eq. 4 applicable for mixtures with inert substances. If liquid mixtures show a phase separation, the activity of each compound in each phase is the same within the region of phase separation. If one enters the activity for any phase into the equation for the whole region of phase separation, eq. 4 stays valid and provides a constant flash point. An assumption made is that the LFL is not temperature dependent, which introduces a slight inaccuracy, but ensures that only the temperature dependent activity coefficients, the temperature dependent pure compound vapor pressures and the pure compound flash points are required to calculate the mixture flash points. We use this model in combination with COSMO-RS to predict mixture flash points, where COSMO-RS is used to calculate the mixture activity coefficients and in a second model also the pure compound vapor pressure.

In addition to the above temperature independent model we analyze the effect of considering temperature dependent flash points on the results. Looking at the question how much fuel must be burned to promote the flash inside the gaseous phase and neglecting kinetic effects, one can assume that the combustion of one equivalent of fuel/air mixture needs to heat up another

equivalent to ignite it and again produce the same amount of heat. If this condition is not fulfilled, the flame would cool down while propagating and the flash cannot continue through the whole fuel/air mixture. This can be expressed by the following general equation which divides the heat of combustion for a certain amount of fuel by the total heat capacity required to heat up another equivalent volume of mixture to calculate the flame temperature required to flash.

$$T_{i,fp} + \frac{n_i H_i^C}{n_{fuel/air} C_{fuel/air}} = T_i^{flame} \tag{5}$$

where H_i^C is the heat of combustion available to heat up the surrounding fuel/air mixture and $C_{fuel/air}$ is the heat capacity of the fuel/air mixture. At constant pressure this can be rewritten by using the partial pressure P_i and contracting everything else into a compound specific constant a_i.

$$T_{i,fp} + a_i \frac{n_i}{n_{fuel/air}} = T_{i,fp} + a_i P_{i,fp}^{sat} = T_i^{flame} \tag{6}$$

Writing this equation for a general temperature T and combining it with eq. 6 yields

$$P_i^{sat}(T) = \frac{P_{i,fp}^{sat}(T_i^{flame} - T)}{(T_i^{flame} - T_{i,fp})} = \frac{P_{i,fp}^{sat}(T_{i,fp} + a_i P_{i,fp}^{sat} - T)}{(T_i^{flame} - T_{i,fp})} = \frac{P_{i,fp}^{sat}(T_{i,fp} - T)}{(T_i^{flame} - T_{i,fp})} + P_{i,fp}^{sat} \tag{7}$$

Comparing this with the Zabetakis[19] equation for the flammability limits of hydrocarbons

$$LFL_i(T) = LFL_i^{25°} - \frac{LFL_i^{25°}(T - 25°)}{(1300° - 25°)} \tag{8}$$

we can estimate the flame temperature to be about 1573 K and approximately compound independent. If available, an experimental substance specific adiabatic flame temperature could be used replacing the 1573 K. By applying equation 6 to a mixture

$$T_{fpmix} + a_{mix} P_{mix,fpmix}^{sat} = T^{flame} \tag{9}$$

and decomposing the total saturation pressure into the contributions of the individual compounds

$$T_{fpmix} + \sum_i a_i y_i P^{sat}_{mix,fpmix} = T^{flame} \quad (10)$$

we derive a temperature dependent version of eq. 4

$$\frac{P^{sat}_{mix,fpmix}}{(T^{flame} - T_{fpmix})} \sum_{i \neq k} \frac{x_i \gamma_i (T^{flame} - T_{i,fp})}{P^{sat}_{i,fp}} = 1 \quad (11)$$

As T^{flame} is set equal to 1573 K and the flash point for each compound is used as input, the temperature independent eq. 4 and the temperature dependent eq. 11 can be solved if the temperature dependent mixture activity coefficient and pure compound vapor pressure of each compound are known. These data are often taken from correlations to experimental data, e.g. Antoine equation for the vapor pressure and Wilson equation[20] or the non-random two-liquid (NRTL) model[21] for the activity coefficients. Because correlation based equations limit the applicability of the model to already measured compounds (vapor pressure data) or investigated binary systems (activity coefficient data), Liaw[22] has also used UNIFAC[23,24] to obtain the required activity coefficients for unknown mixtures and could thus broaden the applicability of eq. 4 to non ideal and not yet measured mixtures, though pure compound vapor pressures are still required in the approach by Liaw.

To further broaden the applicability, it is beneficial to not only use the mixture activity coefficients from predictive models, e.g. UNIFAC as used by Liaw and COSMO-RS in this work, but also to have a predictive model for calculating the vapor pressure of the pure compounds in dependence of temperature, which is also tested in this work.

For predicting mixture flash points we use four different models: The first model (label 1401) uses the COSMO-RS software COSMO*therm* with parameterization BP_TZVPD_FINE_C30_1401, which is the same level used for the pure compound flash points. It makes use of eq. 4 and takes experimental pure compound vapor pressure data and

experimental pure compound flash points into account. It uses COSMO-RS to predict the mixture activity coefficients only. The second model (label 1501) is basically the same as the first one, but uses the newer BP_TZVPD_FINE_C30_1501 parameterization. The third variant (label 1501(T)) uses model two, but with the temperature dependent eq. 11 and the last model (label 1501(T)P) uses the temperature dependent eq. 11 and a predicted pure compound vapor pressure dependency instead of experimental data. The fourth model does not need pure compound vapor pressure data and the only experimental input is thus the pure compound flash points. Equation 4 and 11 have been solved by converting the experimental flash points into saturation vapor pressures as for the pure compounds and then conducting COSMO-RS calculations at 40 temperature points in 0.5 K steps above and below the experimental mixture flash point. Each COSMO-RS calculation provides a total vapor pressure over the mixture as well as activity coefficients for each compound in mixture. At each test temperature eq. 4 or eq. 11 have been evaluated and the single temperature where the result is closest to 1 is taken as result for each equation. By using steps of 0.5 K, the mixture flash point can be determined with an accuracy of 0.25 K on average, which should be well below the general accuracy of the models and measurements.

Tables 2 and 3 present a summary of the prediction error for a series of mixture systems, with experimental data taken from several papers by Liaw[15,17,22], where the water / n-propanol and water / isopropanol data have been extracted graphically. The deviations are given as AAD for better comparison with the literature data. Table 4 presents some UNIFAC based data from[22] for comparison. Figure 4 and 5 illustrate how the flash points of a typical non ideal, but still miscible system, and a partially miscible system vary with composition. The experimental and predicted data for all cases can be found in the supporting information (table S4).

Table 2. FP prediction errors for several miscible systems

Fully miscible systems		N	AAD 1401	1501	1501(T)	1501(T) P
Octane	Ethanol	21	2.55	2.19	2.14	2.19
Octane	Heptane	9	0.17	0.17	0.17	0.17
Octane	1-butanol	13	0.86	0.77	0.73	0.69
Octane	2-butanol	16	0.56	0.34	0.34	0.34
Octane	isopropanol	19	1.92	0.74	0.68	0.74
Methylacetate	Methylacrylate	9	0.44	0.39	0.44	0.39
Methanol	Methylacrylate	11	0.36	0.68	0.73	0.55
Isoamylalcohol	Isoamlyacetate	9	1.00	1.11	1.11	0.67
Water	n-propanol	16	3.78	1.97	2.09	2.06
Water	iso-propanol	15	6.87	6.70	6.37	5.13
Total (miscible systems)		138	2.12	1.67	1.63	1.46

The absolute average deviation (AAD) is calculated over all available data points N with $0<x_1<1$. Model 1401 uses the COSMO*therm* parameterization BP_TZVPD_FINE_C30_1401. It uses eq. 4 and takes experimental pure compound vapor pressure data and experimental pure compound flash points into account. Model 1501 uses the BP_TZVPD_FINE_C30_1501 parameterization. Model 1501(T) uses model 1501, but with the temperature dependent eq. 11 and model 1501(T)P also applies a predicted pure compound vapor pressure dependency instead of experimental data.

Table 3. FP prediction errors for several partially miscible systems.

Partially miscible systems		N	AAD 1401	1501	1501(T)	1501(T)P
Methanol	Octane	12	5.50	4.37	4.29	4.37
Methanol	Decane	6	11.75	6.42	6.42	6.42
Acetone	Decane	10	7.30	1.00	1.10	1.30
Methanol	2,2,4-trimethylpentane	4	3.62	3.37	3.37	2.87
Ethanol	Tetradecane	8	8.25	6.12	6.12	6.44
Water	1-butanol	14	2.04	3.39	3.14	2.50
Water	2-butanol	10	2.40	3.15	2.85	2.60
Water	isobutanol	8	4.19	2.50	2.81	2.31
Water	1-pentanol	6	1.00	1.75	1.58	1.50
Total (partially miscible systems)		78	4.90	3.50	3.44	3.28

The region of phase separation is excluded from the absolute average deviation calculation, as the flash point is constant and no additional information is gained. The models 1401 to 1501(T)P are the same as in table 2.

Table 4: Literature[22] Data for comparison.

Fully miscible systems		N	AAD for UNIFAC original	Do	Lyngby	Bastos
Octane	Ethanol	21	0.58	0.78	0.66	1.33
Octane	Heptane	9	0.15	0.16	0.16	0.16
Octane	1-butanol	13	0.1	0.36	0.2	0.46
Octane	2-butanol	16	0.34	0.26	0.35	0.49
Octane	isopropanol	19	0.91	0.39	0.93	1.32
Methylacetate	Methylacrylate	9	0.27	0.64		
Methanol	Methylacrylate	11	0.16	0.81	0.58	2.06
Isoamylalcohol	Isoamlyacetate	9	0.28	0.29		
Water	n-propanol	16	2.3	2.63	2.06	4.66
Water	iso-propanol	15	3.91	1.6	2.27	6.22
Total (miscible systems)		138	1.01	0.85	0.81	1.95

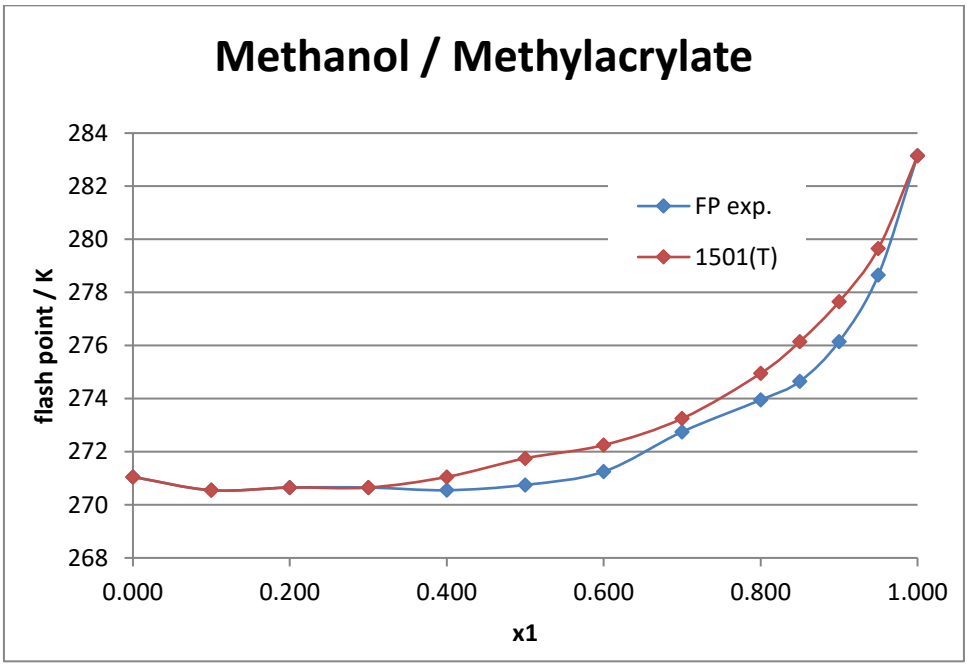

Figure 4. The system methanol / methylacrylate shows a broad region of an almost constant flash point. The lines are a guide to the eye.

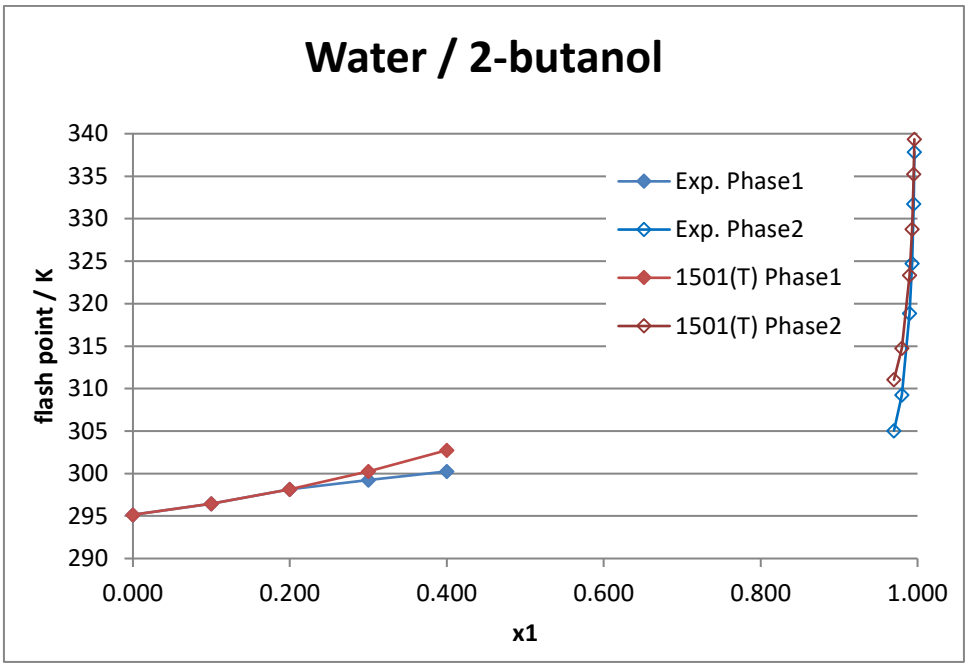

Figure 5. The system water / 2-butanol shows a miscibility gap, in which the flash point is not plotted. The flash point should be constant inside this region. The shown experimental concentrations do not include the exact LLE concentrations. The lines are a guide to the eye.

From the observed AADs it can be concluded that the activity coefficients predicted by COSMO-RS are slightly less accurate than three of the four tested UNIFAC variants for the miscible systems. This result is not surprising, because the mixtures for which such data are available, consist of simple and mono-functional compounds, which fall into the center of the applicability domain of UNIFAC and for which it is known to be more accurate than COSMO-RS methods. The mixture flash points predicted by model 1501 are about 0.8K worse than those from UNIFAC(Do). It is also noteworthy that the 1501 parameterization seems to perform better than the 1401, especially for the miscible systems water / n-propanol and octane / isopropanol and the partially miscible systems methanol / decane and acetone / decane. The temperature dependence of model three (1501(T)) provides a slight increase in prediction quality, which is, however, insignificant as compared to the general error. As using eq. 11 is not more complicated

than using eq. 4 and it allows for entering the compound specific adiabatic flame temperate (instead of the general value 1573K), eq. 11 might still be preferable over eq. 4. The results of the fourth model (1501(T)P), which does not use any vapor pressure equation for the pure compounds, but uses purely predicted vapor pressures, are somewhat surprising as the accuracy is even slightly better than for the third model. This can only be attributed to an error compensation for some compounds, where the vapor pressure prediction error cancels the error of the activity coefficient prediction. It can at least be concluded that using predicted vapor pressures instead of experimental vapor pressure does not seem to significantly reduce the prediction quality of mixture flash points when using COSMO*therm*. By using the mixture model 1501(T)P, the need for experimental pure compound vapor pressure data can be completely eliminated with only little or no loss in prediction accuracy.

4) CONCLUSIONS

With the presented two parameter model based solely on the molecular surface area in combination with the COSMO-RS method, the pure compound flash points of organic molecules can be predicted with an accuracy of about 10 K AAD, if no exp. data is available and 7.5 K if experimental normal boiling points are used. Despite its simplicity and the comparably large data set, the model shows a similar error as more complex and structurally more restricted, descriptor based models. In addition, further improvements seem possible, though at the cost of an increased complexity. A major strength of the model is its independence of any typically measured data combined with the ability to profit from available boiling points or vapor pressure data. By combining the presented models for pure compound FP estimation and mixture FP prediction a single method to predict pure compound flash points and mixture flash points can be constructed, which can be applied fully predictive, i.e. without pure compound flash points, activity

coefficients and vapor pressures. The only requirement is to have a COSMO-RS implementation able to predict vapor pressures. This makes the model broadly applicable, even for virtual screening purposes. In addition, the same model can make use of experimental boiling points, pure compound flash points and vapor pressures without any changes and in a straight forward manner.

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SUPPORTING INFORMATION

Table S1: Excluded compounds from Rowley set

Table S2: Outliers in pure compound estimation

Table S3: Pure compound data

Table S4: Mixture data

REFERENCES

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Supporting Information

Predicting flash points of pure compounds and mixtures with help of COSMO-RS

Jens Reinisch[#,1] *and Andreas Klamt*[1,2]

[1] COSMOlogic GmbH&CoKG, Imbacher Weg 46, Leverkusen, Germany

[2] Inst. of Physical and Theoretical Chemistry, University of Regensburg, Germany

[#] corresponding author: reinisch@cosmologic.de

Table S1. Excluded compounds from Rowley set.

	CAS	Name used by Rowley	Comment
1		Di(2-Ethylhexyl)Terephthalate	Not in COSMObase
2		1,4-Dichloro-cis-2-Butene	Not in COSMObase
3	4420-74-0	3-(trimethoxysilyl)-1-Propanethiol	Not in COSMObase
4		Octamethylcyclotetrasiloxane	Not in COSMObase
5		Nonylphenol	Could not be uniquely identified
6	74-90-8	Hydrogen Cyanide	FP is for the solid
7	281-23-2	Adamantane	FP is for the solid
8	100-21-0	Terephthalic Acid	FP is for the solid
9	88-99-3	Phthalic Acid	FP is for the solid
10	280-33-1	bicyclo[2,2,2]octane	FP is probably for the solid
11	64-18-6	Formic Acid	Large variation in exp. FP
12	3319-31-1	Trioctyl Trimellitate	Decomposition around FP
13	123-63-7	Paraldehyde	FP too low as compared to various other 6-rings (dioxane, cyclohexane, 2,6-dimethyl-1,4-Dioxane, etc.)

Table S2. Outliers. Molecules with a prediction error of greater 50 K if no experimental normal boiling point is used for the prediction.

Cl-type	**Polyol-type**	**Others**
Terephthaloyl Chloride	Glycerol	Triethylene Glycol bis(2-Ethylhexanoate)
Hexachlorobenzene	Trimethylolpropane	
Trichloroacetaldehyde	Diethanolamine	
Dichloroacetyl Chloride	Triethylene Glycol	
Isophthaloyl Chloride	Pentaerythritol	

Table S3. Pure compound data. Area in Angstrom, pressure in mbar, FP and BP in K, BP sources are:

CAS	Name	FP/K	FP/K DIPPR	BP / K		ln(area)	ln(P) at FP	Pred. ln(P)	Pred. FP		Deviation to exp. FP	
									no BP	BP	no BP	BP
000100-00-5	p-Chloronitrobenzene	397.15	400.15	515.15	a	5.13	3.19	2.63	379.18	384.15	-17.97	-13.00
000100-18-5	p-Diisopropylbenzene	349.82	354.15	483.45	a	5.44	2.00	1.82	343.12	346.42	-6.70	-3.40

000100-37-8	Diethylethanolamine	330.15	321.15	436.15	a	5.15	3.10	2.56	307.90	319.60	-22.25	-10.55
000100-40-3	Vinylcyclohexene	288.15	289.00	401.15	a	5.11	2.32	2.68	292.26	294.65	4.11	6.50
000100-41-4	Ethylbenzene	296.15	288.15	409.25	a	5.08	2.31	2.75	304.73	304.23	8.58	8.08
000100-42-5	Styrene	305.00	305.00	418.15	a	5.04	2.49	2.84	309.53	311.70	4.53	6.70
000100-44-7	Benzyl Chloride	333.15	333.15	452.15	a	5.08	2.45	2.74	340.61	338.86	7.46	5.71
000100-46-9	Benzylamine	338.15	333.15	458.15	a	5.05	2.47	2.83	340.76	345.32	2.61	7.17
000100-47-0	Benzonitrile	348.15	344.15	464.25	a	4.99	2.76	2.99	359.76	352.94	11.61	4.79
000100-51-6	Benzyl Alcohol	366.15	366.15	478.45	a	5.02	2.45	2.90	376.04	374.63	9.89	8.48
000100-52-7	Benzaldehyde	337.00	335.15	452.15	a	4.98	2.76	3.01	339.51	342.04	2.51	5.04
000100-53-8	Benzyl Mercaptan	343.15	343.15	467.65	a	5.11	2.29	2.67	350.96	350.55	7.81	7.40
000100-54-9	Nicotinonitrile	357.15	357.15	480.05	a	4.96	2.43	3.06	378.41	370.29	21.26	13.14
000100-60-7	N-Methylcyclohexylamine	308.15	302.15	420.15	a	5.12	2.47	2.64	308.31	311.34	0.16	3.19
000100-61-8	N-Methylaniline	351.00		469.35	a	5.05	2.82	2.84	346.94	351.47	-4.06	0.47
000100-64-1	Cyclohexanone Oxime	362.15	362.00	479.15	a	5.04	2.26	2.84	367.36	373.02	5.21	10.87
000100-66-3	Anisole	318.65	325.15	426.85	a	5.02	2.76	2.90	323.97	321.24	5.32	2.59
000100-68-5	Methyl Phenyl Sulfide	345.15	342.00	466.15	a	5.10	2.43	2.70	353.26	350.59	8.11	5.44
000100-74-3	N-Ethyl-Morpholine	304.15		411.65	a	5.07	3.20	2.77	260.21	295.17	-43.94	-8.98
000100-80-1	m-Methylstyrene	324.15	324.15	437.15	a	5.16	2.60	2.54	324.51	323.05	0.36	-1.10
010025-78-2	Trichlorosilane	259.15		304.95	a	4.87	4.95	3.30	229.15	230.33	-30.00	-28.82
001003-03-8	Cyclopentylamine	284.65	290.15	381.15	a	4.90	2.57	3.21	293.19	294.96	8.54	10.31
010061-01-5	cis-1,3-Dichloropropene	294.15		377.45	a	4.89	3.63	3.25	283.19	286.90	-10.96	-7.25
010061-02-6	trans-1,3-Dichloropropene	300.15		385.15	a	4.91	3.59	3.20	289.14	292.61	-11.01	-7.54
000101-54-2	p-Aminodiphenylamine	466.50	466.48	627.15	a	5.44	1.76	1.83	479.07	468.14	12.57	1.64
000101-81-5	Diphenylmethane	400.00	403.15	538.15	a	5.39	2.21	1.94	404.61	394.24	4.61	-5.76
000101-83-7	Dicyclohexylamine	372.65	377.00	528.95	a	5.48	1.23	1.71	382.81	382.14	10.16	9.49
000101-84-8	Diphenyl Ether	388.15	369.00	531.15	a	5.36	1.95	2.02	392.38	389.64	4.23	1.49
000101-97-3	Ethyl Phenyl Acetate	372.15		500.15	a	5.38	2.11	1.98	382.95	369.59	10.80	-2.56
000102-25-0	1,3,5-Triethylbenzene	354.15	354.15	489.05	a	5.47	2.03	1.75	344.12	348.80	-10.03	-5.35
000102-69-2	Tripropylamine	314.00	302.04	429.15	a	5.43	2.36	1.85	301.11	304.95	-12.89	-9.05
000102-70-5	Triallylamine	312.15		428.65	a	5.36	2.24	2.04	308.09	308.62	-4.06	-3.53
000102-71-6	Triethanolamine	463.15	453.00	608.55	a	5.21	2.73	2.42	423.90	455.46	-39.25	-7.69
000102-82-9	Tri-n-Butylamine	353.15	359.26	489.65	a	5.66	1.58	1.25	344.34	347.13	-8.81	-6.02
000103-09-3	2-Ethylhexyl Acetate	344.15	344.15	472.15	a	5.52	1.81	1.63	347.93	340.81	3.78	-3.34
000103-11-7	2-Ethylhexyl Acrylate	355.15	355.15	486.65	a	5.56	1.77	1.52	360.31	350.49	5.16	-4.66
000103-23-1	Di(2-Ethylhexyl)Adipate	469.15	466.00	690.15	a	6.20	-1.23	-0.13	491.86	490.15	22.71	21.00
000103-29-7	1,2-Diphenylethane	398.15	402.04	557.15	a	5.49	1.30	1.70	409.47	406.29	11.32	8.14
000103-50-4	Dibenzyl Ether	408.15	408.15	571.15	a	5.55	1.12	1.54	426.32	416.63	18.17	8.48
000103-65-1	n-Propylbenzene	312.15	303.15	432.35	a	5.20	2.11	2.45	319.76	318.30	7.61	6.15
000103-69-5	N-Ethylaniline	358.15		476.15	a	5.17	2.73	2.52	355.80	354.00	-2.35	-4.15
000103-71-9	Phenyl Isocyanate	324.15	324.15	436.15	a	5.06	2.78	2.81	321.02	324.64	-3.13	0.49
000103-73-1	Phenetole	328.00	325.00	442.95	a	5.15	2.48	2.57	335.17	329.66	7.17	1.66
000103-76-4	N-(2-Hydroxyethyl)Piperazine	397.15	397.15	519.15	a	5.15	2.93	2.58	380.09	389.59	-17.06	-7.56

000103-84-4	Acetanilide	434.15	446.15	577.15	a	5.18	2.35	2.48	429.17	437.15	-4.98	3.00
000104-46-1	Anethole	362.15	362.15	508.15	a	5.31	1.84	2.17	361.71	368.87	-0.44	6.72
000104-57-4	Benzyl Formate	355.00	355.00	476.15	a	5.18	2.58	2.49	352.28	353.23	-2.72	-1.77
000104-76-7	2-Ethyl-1-Hexanol	346.00	346.00	457.75	a	5.31	2.08	2.16	344.05	347.23	-1.95	1.23
000104-87-0	p-Tolualdehyde	353.00	353.00	477.65	a	5.10	2.57	2.69	353.31	355.53	0.31	2.53
000105-05-5	p-Diethylbenzene	330.00	329.15	456.85	a	5.29	2.17	2.20	326.33	330.60	-3.67	0.60
000105-30-6	2-Methyl-1-Pentanol	323.15	319.00	422.15	a	5.10	2.25	2.70	327.52	330.25	4.37	7.10
000105-34-0	Methyl Cyanoacetate	380.65	383.15	473.65	a	4.93	3.66	3.13	377.81	369.20	-2.84	-11.45
000105-37-3	Ethyl Propionate	285.00	285.00	372.25	a	5.04	3.13	2.84	293.81	280.13	8.81	-4.87
000105-38-4	Vinyl Propionate	281.00	274.00	364.35	a	5.01	3.25	2.93	282.02	275.73	1.02	-5.27
000105-39-5	Ethylchloroacetate	327.15	311.00	417.45	a	5.05	3.28	2.84	332.49	318.95	5.34	-8.20
000105-45-3	Methyl Acetoacetate	343.00	343.00	444.85	a	5.06	2.98	2.80	348.29	339.45	5.29	-3.55
000105-46-4	sec-Butyl Acetate	289.00		385.15	a	5.14	2.80	2.59	291.40	285.41	2.40	-3.59
000105-53-3	Diethyl Malonate	358.15	366.15	473.15	a	5.36	2.29	2.04	372.75	353.62	14.60	-4.53
000105-54-4	Ethyl n-Butyrate	297.15	297.15	394.65	a	5.17	2.74	2.53	301.11	293.63	3.96	-3.52
000105-56-6	Ethyl Cyanoacetate	383.15	383.15	483.15	a	5.08	3.48	2.76	377.49	367.87	-5.66	-15.28
000105-57-7	Acetal	286.15		375.35	a	5.20	2.99	2.44	284.52	276.94	-1.63	-9.21
000105-58-8	Diethyl Carbonate	298.15		399.15	a	5.12	2.58	2.64	296.98	299.14	-1.17	0.99
000105-59-9	Methyl Diethanolamine	399.82	399.82	520.15	a	5.09	3.08	2.71	366.23	391.71	-33.59	-8.11
000105-60-2	epsilon-Caprolactam	412.65	425.15	543.15	a	5.02	2.77	2.90	412.88	415.81	0.23	3.16
000105-66-8	Propyl Butyrate	310.15	305.00	416.15	a	5.27	2.45	2.25	317.87	306.70	7.72	-3.45
000105-67-9	2,4-Xylenol	368.15	368.15	484.05	a	5.13	2.91	2.62	348.60	362.27	-19.55	-5.88
000105-76-0	Dibutyl Maleate	413.00	413.00	554.15	a	5.71	1.59	1.12	425.45	403.88	12.45	-9.12
000106-31-0	Butyric Anhydride	355.00	355.00	473.15	a	5.39	2.27	1.96	367.36	349.13	12.36	-5.87
000106-35-4	3-Heptanone	310.15	310.15	420.15	a	5.20	2.50	2.43	310.88	309.00	0.73	-1.15
000106-36-5	Propyl Propionate	294.15	292.15	395.65	a	5.17	2.54	2.53	302.81	294.04	8.66	-0.11
000106-38-7	p-Bromotoluene	343.15	358.15	457.45	a	5.11	2.73	2.67	343.12	341.74	-0.03	-1.41
000106-42-3	p-Xylene	299.00	298.15	411.45	a	5.08	2.43	2.74	303.67	304.82	4.67	5.82
000106-43-4	p-Chlorotoluene	322.15	325.00	435.55	a	5.08	2.67	2.75	321.71	323.60	-0.44	1.45
000106-44-5	p-Cresol	359.15	368.00	475.05	a	5.02	2.52	2.91	362.02	366.62	2.87	7.47
000106-46-7	p-Dichlorobenzene	339.00	339.00	447.15	a	5.08	3.00	2.75	331.80	333.80	-7.20	-5.20
000106-47-8	p-Chloroaniline	386.00	386.00	505.15	a	5.05	2.92	2.84	385.97	384.09	-0.03	-1.91
000106-49-0	p-Toluidine	360.00	360.00	473.55	a	5.05	2.94	2.84	353.74	357.91	-6.26	-2.09
000106-50-3	p-Phenylenediamine	428.70	428.70	540.15	a	5.01	3.46	2.93	412.11	416.11	-16.59	-12.59
000106-63-8	Isobutyl Acrylate	304.26	304.26	405.15	a	5.23	2.57	2.37	311.82	300.75	7.56	-3.51
000106-65-0	Dimethyl Succinate	358.15	358.15	469.55	a	5.23	2.72	2.37	361.61	351.47	3.46	-6.68
000106-88-7	1,2-Epoxybutane	258.15	251.15	336.45	a	4.79	3.65	3.49	248.00	255.37	-10.15	-2.78
000106-89-8	alpha-Epichlorohydrin	304.00	304.00	389.26	a	4.80	3.60	3.48	298.05	301.69	-5.95	-2.31
000106-92-3	Allyl Glycidyl Ether	321.15	318.15	427.15	a	5.13	2.79	2.61	316.11	317.81	-5.04	-3.34
000106-99-0	1,3-Butadiene	197.15		268.75	a	4.69	2.90	3.75	210.28	208.68	13.13	11.53
001067-08-9	3-Methyl-3-Ethylpentane	276.00	276.00	391.35	a	5.18	2.26	2.50	266.37	280.13	-9.63	4.13
001067-20-5	3,3-Diethylpentane	294.00	294.00	419.45	a	5.26	2.11	2.30	280.33	297.52	-13.67	3.52

001068-87-7	2,4-Dimethyl-3-Ethylpentane	291.15	288.00	409.85	a	5.28	2.27	2.23	276.43	290.44	-14.72	-0.71
000107-02-8	Acrolein	247.15	247.15	325.75	a	4.59	3.07	4.01	265.17	262.25	18.02	15.10
000107-03-9	Propyl Mercaptan	253.15	253.15	340.95	a	4.83	2.84	3.40	262.99	262.30	9.84	9.15
000107-05-1	3-Chloropropene	244.15	241.15	318.25	a	4.74	3.37	3.62	252.53	248.19	8.38	4.04
000107-06-2	1,2-Dichloroethane	286.00	286.00	356.65	a	4.77	4.17	3.55	260.13	273.89	-25.87	-12.11
000107-07-3	2-Chloroethanol	328.15	313.71	401.75	a	4.68	3.92	3.77	319.12	325.38	-9.03	-2.77
000107-13-1	Acrylonitrile	268.15	273.15	350.45	a	4.59	3.33	4.00	282.63	280.33	14.48	12.18
000107-15-3	Ethylenediamine	311.00	306.15	390.15	a	4.67	3.48	3.80	308.99	316.59	-2.01	5.59
000107-18-6	Allyl Alcohol	294.00		370.15	a	4.65	3.02	3.86	305.67	307.12	11.67	13.12
000107-19-7	Propargyl Alcohol	305.15	309.26	386.75	a	4.61	2.88	3.95	320.33	322.47	15.18	17.32
000107-21-1	Ethylene Glycol	384.15	383.15	470.45	a	4.59	3.60	4.01	379.68	392.61	-4.47	8.46
000107-25-5	Methyl Vinyl Ether	217.15	217.15	278.65	a	4.64	3.71	3.89	221.69	219.78	4.54	2.63
000107-29-9	Acetaldoxime	313.15	313.15	388.15	a	4.61	3.42	3.97	319.43	322.54	6.28	9.39
000107-30-2	Chloromethyl Methyl Ether	265.15	255.00	332.65	a	4.71	3.86	3.72	264.81	262.67	-0.34	-2.48
000107-39-1	2,4,4-Trimethyl-1-Pentene	269.10	267.15	374.55	a	5.17	2.46	2.51	262.74	269.92	-6.36	0.82
000107-40-4	2,4,4-Trimethyl-2-Pentene	272.15	272.15	378.05	a	5.19	2.43	2.47	266.88	272.91	-5.27	0.76
000107-41-5	Hexylene Glycol	366.00	366.00	471.15	a	5.11	2.07	2.66	383.74	375.84	17.74	9.84
000107-46-0	Hexamethyldisiloxane	271.15		372.15	a	5.43	2.68	1.86	251.15	257.54	-20.00	-13.61
000107-47-1	Di-tert-Butyl Sulfide	304.15	300.00	422.25	a	5.29	1.92	2.21	313.81	309.21	9.66	5.06
000107-51-7	Octamethyltrisiloxane	308.15	302.15	426.15	a	5.70	2.11	1.15	290.88	292.19	-17.27	-15.96
000107-87-9	2-Pentanone	280.00	280.00	375.35	a	4.96	2.83	3.06	286.65	283.99	6.65	3.99
000107-88-0	1,3-Butanediol	382.00	382.00	480.65	a	4.90	2.85	3.22	388.26	388.92	6.26	6.92
000107-92-6	n-Butyric Acid	345.15	345.00	436.85	a	4.89	3.22	3.25	341.47	345.74	-3.68	0.59
000107-93-7	trans-Crotonic Acid	363.15	368.00	457.85	a	4.85	3.27	3.33	358.94	364.41	-4.21	1.26
000107-98-2	Propylene Glycol Monomethyl Ether	305.00	305.00	392.15	a	4.94	3.14	3.12	302.49	304.73	-2.51	-0.27
001070-87-7	2,2,4,4-Tetramethylpentane	278.15	276.00	395.35	a	5.26	1.97	2.29	276.04	283.57	-2.11	5.42
001071-26-7	2,2-Dimethylheptane	292.15	297.00	405.85	a	5.34	2.17	2.09	286.50	290.69	-5.65	-1.46
001072-05-5	2,6-Dimethylheptane	290.65	299.00	408.35	a	5.35	1.97	2.06	287.61	292.05	-3.04	1.40
001072-16-8	2,7-Dimethyloctane	310.93	306.00	433.05	a	5.44	1.91	1.82	312.25	309.44	1.32	-1.49
001077-16-3	Hexylbenzene	356.15	353.15	499.25	a	5.48	1.51	1.71	348.23	359.96	-7.92	3.81
001078-71-3	n-Heptylbenzene	370.65	368.15	513.15	a	5.56	1.49	1.50	373.84	370.85	3.19	0.20
000108-01-0	Dimethylethanolamine	312.15		407.15	a	4.93	3.48	3.14	291.18	305.34	-20.97	-6.81
000108-03-2	1-Nitropropane	308.15	306.15	404.25	a	4.86	3.31	3.33	302.39	308.56	-5.76	0.41
000108-05-4	Vinyl Acetate	265.37	265.00	345.65	a	4.87	3.17	3.29	273.05	267.25	7.68	1.88
000108-10-1	Methyl Isobutyl Ketone	286.15	286.15	389.65	a	5.06	2.56	2.79	291.70	290.12	5.55	3.97
000108-11-2	4-Methyl-2-Pentanol	314.00	314.00	404.75	a	5.09	2.29	2.72	325.96	320.34	11.96	6.34
000108-18-9	Diisopropylamine	266.15	266.15	357.05	a	5.12	2.74	2.66	269.16	264.86	3.01	-1.29
000108-20-3	Diisopropyl Ether	245.00		341.65	a	5.11	2.10	2.67	273.37	253.46	28.37	8.46
000108-21-4	Isopropyl Acetate	274.82	275.00	361.75	a	5.03	2.97	2.88	281.95	273.28	7.13	-1.53
000108-22-5	1-Methylvinyl Acetate	283.00	283.00	370.15	a	5.00	3.11	2.96	286.50	280.57	3.50	-2.43
000108-24-7	Acetic Anhydride	322.59	322.59	412.65	a	4.94	3.32	3.11	348.88	318.67	26.28	-3.92
000108-30-5	Succinic Anhydride	425.00	424.00	534.15	a	4.81	3.80	3.45	407.76	415.59	-17.24	-9.41

000108-31-6	Maleic Anhydride	375.15	375.15	475.15	a	4.77	3.75	3.55	363.99	370.45	-11.16	-4.70
000108-32-7	Propylene Carbonate	408.15		515.15	a	4.86	3.79	3.31	394.90	395.86	-13.25	-12.29
000108-36-1	m-Dibromobenzene	366.15	366.15	491.15	a	5.14	2.39	2.59	372.91	370.25	6.76	4.10
000108-38-3	m-Xylene	298.15	298.15	412.25	a	5.08	2.36	2.75	303.38	305.19	5.23	7.04
000108-39-4	m-Cresol	359.15	368.00	475.35	a	5.02	2.54	2.91	361.96	366.29	2.81	7.14
000108-43-0	m-Chlorophenol	370.15	364.00	487.15	a	5.02	2.72	2.91	371.37	374.06	1.22	3.91
000108-44-1	m-Toluidine	359.00	359.15	476.45	a	5.05	2.79	2.84	356.09	359.94	-2.91	0.94
000108-45-2	m-Phenylenediamine	411.15	411.15	558.15	a	5.01	2.23	2.93	418.10	427.35	6.95	16.20
000108-46-3	1,3-Benzenediol	444.00	400.00	553.15	a	4.95	3.51	3.08	428.24	433.99	-15.76	-10.01
000108-48-5	2,6-Dimethylpyridine	306.00	306.00	417.25	a	5.06	2.36	2.80	322.41	314.11	16.41	8.11
000108-55-4	Glutaric Anhydride	446.15	386.00	560.15	a	4.93	3.69	3.14	434.02	431.38	-12.13	-14.77
000108-59-8	Dimethylmalonate	358.15	363.15	454.55	a	5.13	3.28	2.62	343.11	345.30	-15.04	-12.85
000108-64-5	Ethyl Isovalerate	299.15	298.15	408.15	a	5.25	2.30	2.31	304.55	299.37	5.40	0.22
000108-65-6	Propylene Glycol Monomethyl Ether Acetate	316.00	316.00	418.15	a	5.22	2.54	2.39	331.14	313.41	15.14	-2.59
000108-67-8	Mesitylene	317.55	317.55	437.85	a	5.19	2.43	2.46	311.27	318.10	-6.28	0.55
000108-70-3	1,3,5-Trichlorobenzene	380.15	400.00	481.15	a	5.19	3.63	2.46	342.71	353.76	-37.44	-26.39
000108-75-8	2,4,6-Trimethylpyridine	327.15	330.15	443.75	a	5.18	2.38	2.50	336.92	329.45	9.77	2.30
000108-82-7	2,6-Dimethyl-4-Heptanol	339.15	339.00	447.65	a	5.38	2.08	1.98	341.39	337.61	2.24	-1.54
000108-83-8	Diisobutyl Ketone	322.15	322.15	442.55	a	5.36	2.23	2.02	311.34	318.34	-10.81	-3.81
000108-86-1	Bromobenzene	324.26	324.26	429.15	a	4.99	2.88	2.98	331.46	326.21	7.20	1.95
000108-87-2	Methylcyclohexane	269.15	267.15	374.05	a	5.03	2.48	2.87	272.43	275.89	3.28	6.74
000108-88-3	Toluene	279.15	277.15	383.75	a	4.95	2.47	3.07	292.49	289.88	13.34	10.73
000108-89-4	4-Methylpyridine	312.15	329.15	418.45	a	4.92	2.81	3.16	322.27	318.94	10.12	6.79
000108-90-7	Monochlorobenzene	301.15	305.00	404.85	a	4.95	2.80	3.08	308.26	306.41	7.11	5.26
000108-91-8	Cyclohexylamine	299.65	304.15	407.15	a	5.00	2.38	2.95	306.90	309.41	7.25	9.76
000108-93-0	Cyclohexanol	334.15	341.00	433.95	a	4.98	2.30	3.02	350.35	345.93	16.20	11.78
000108-94-1	Cyclohexanone	316.15	317.00	428.55	a	4.95	2.72	3.10	325.41	323.72	9.26	7.57
000108-95-2	Phenol	352.15	353.00	454.95	a	4.88	2.91	3.26	358.66	358.92	6.51	6.77
000108-98-5	Phenyl Mercaptan	328.15		442.25	a	4.99	2.57	2.99	337.73	336.48	9.58	8.33
000108-99-6	3-Methylpyridine	309.15	309.15	417.25	a	4.92	2.73	3.16	318.95	317.36	9.80	8.21
000109-06-8	2-Methylpyridine	299.15	299.15	402.45	a	4.93	2.63	3.15	315.71	308.57	16.56	9.42
000109-21-7	Butyl Butyrate	323.15	326.48	439.15	a	5.37	2.21	2.00	324.11	319.45	0.96	-3.70
000109-49-9	5-Hexen-2-one	296.15	296.15	402.65	a	5.06	2.48	2.80	304.53	301.80	8.38	5.65
000109-52-4	Pentanoic Acid	359.15	358.15	459.25	a	5.03	3.06	2.88	345.97	355.72	-13.18	-3.43
000109-55-7	3-(N,N-Dimethylamino) Propylamine	308.15		406.15	a	5.11	3.04	2.68	294.04	301.82	-14.11	-6.33
000109-60-4	n-Propyl Acetate	283.71	288.00	374.65	a	5.05	2.93	2.83	300.52	281.99	16.81	-1.71
000109-65-9	1-Bromobutane	283.00	291.15	374.75	a	4.97	3.09	3.02	282.42	281.74	-0.58	-1.26
000109-66-0	n-Pentane	224.15	233.15	309.15	a	4.94	2.86	3.12	222.63	228.30	-1.52	4.15
000109-67-1	1-Pentene	222.00		303.05	a	4.90	2.98	3.21	222.21	225.61	0.21	3.61
000109-69-3	Butyl Chloride	263.75	263.75	351.75	a	4.94	3.06	3.12	264.78	264.77	1.03	1.02
000109-73-9	n-Butylamine	266.15	261.00	350.15	a	4.90	2.89	3.22	265.19	271.19	-0.96	5.04
000109-74-0	Butyronitrile	291.15	289.15	390.75	a	4.82	3.02	3.42	296.94	298.93	5.79	7.78

000109-75-1	Vinylacetonitrile	296.15	296.15	392.15	a	4.76	3.10	3.57	304.19	305.11	8.04	8.96
000109-76-2	1,3-Propanediamine	322.15	321.15	412.95	a	4.86	3.34	3.32	306.68	321.85	-15.47	-0.30
000109-77-3	Malononitrile	385.15	385.15	491.65	a	4.69	3.47	3.76	386.03	392.01	0.88	6.86
000109-78-4	Hydracrylonitrile	402.15	383.15	494.15	a	4.73	3.82	3.64	393.27	398.04	-8.88	-4.11
000109-79-5	Butyl Mercaptan	274.15	274.82	371.65	a	4.98	2.71	3.02	278.06	279.52	3.91	5.37
000109-83-1	Methylethanolamine	345.15	345.15	431.15	a	4.81	3.46	3.44	334.20	344.85	-10.95	-0.30
000109-86-4	2-Methoxyethanol	312.00	312.00	397.25	a	4.79	3.24	3.49	309.73	316.44	-2.27	4.44
000109-87-5	Methylal	241.15	255.00	315.15	a	4.79	3.48	3.49	237.57	241.33	-3.58	0.18
000109-89-7	Diethylamine	245.15	234.15	328.65	a	4.91	2.70	3.20	252.26	252.40	7.11	7.25
000109-93-3	Divinyl Ether	226.15	226.15	301.45	a	4.80	2.88	3.46	239.55	234.38	13.40	8.23
000109-94-4	Ethyl Formate	254.15		327.55	a	4.75	3.42	3.61	261.42	257.17	7.27	3.02
000109-97-7	Pyrrole	312.00	312.00	402.85	a	4.67	3.35	3.80	321.49	320.95	9.49	8.95
000109-99-9	Tetrahydrofuran	259.15	259.00	338.15	a	4.73	3.64	3.65	256.11	259.33	-3.04	0.18
000110-00-9	Furan	237.00	237.00	304.65	a	4.64	3.50	3.89	253.38	243.10	16.38	6.10
000110-01-0	Tetrahydrothiophene	291.00	285.15	394.15	a	4.83	2.91	3.38	294.99	300.23	3.99	9.23
000110-02-1	Thiophene	266.45	266.45	357.15	a	4.75	2.71	3.60	292.59	281.53	26.14	15.08
000110-05-4	Di-t-Butyl Peroxide	277.15	291.00	384.15	a	5.33	1.90	2.11	293.49	280.44	16.34	3.29
000110-12-3	5-Methyl-2-Hexanone	308.15	309.15	417.15	a	5.18	2.47	2.49	312.75	308.36	4.60	0.21
000110-18-9	Tetramethylethylenediamine	290.15		394.15	a	5.20	2.60	2.43	283.71	287.23	-6.44	-2.92
000110-19-0	Isobutyl Acetate	291.00	291.00	389.65	a	5.15	2.68	2.57	306.85	289.26	15.85	-1.74
000110-42-9	Methyl Decanoate	367.15	367.15	497.15	a	5.62	1.80	1.37	369.35	359.37	2.20	-7.78
000110-43-0	2-Heptanone	312.15	312.15	424.15	a	5.21	2.41	2.42	314.76	312.24	2.61	0.09
000110-54-3	n-Hexane	250.15	251.50	341.85	a	5.07	2.85	2.78	242.43	248.84	-7.72	-1.31
000110-56-5	1,4-Dichlorobutane	325.15	313.15	434.15	a	5.05	2.97	2.82	310.94	322.20	-14.21	-2.95
000110-57-6	1,4-Dichloro-trans-2-Butene	326.15	326.15	428.55	a	5.05	3.01	2.83	321.62	322.62	-4.53	-3.53
000110-58-7	n-Pentylamine	280.15	272.15	377.45	a	5.04	2.52	2.86	278.65	285.46	-1.50	5.31
000110-59-8	Valeronitrile	307.15	305.00	414.45	a	4.97	2.87	3.04	307.53	310.34	0.38	3.19
000110-61-2	Succinonitrile	405.00	405.00	539.15	a	4.85	2.73	3.35	418.39	419.92	13.39	14.92
000110-62-3	Pentanal	279.15	285.15	376.15	a	4.96	2.93	3.05	275.92	281.29	-3.23	2.14
000110-63-4	1,4-Butanediol	407.15	407.15	508.15	a	4.88	3.15	3.26	401.68	409.51	-5.47	2.36
000110-65-6	2-Butyne-1,4-Diol	425.00	425.00	511.15	a	4.89	3.72	3.24	410.51	415.10	-14.49	-9.90
000110-66-7	Pentyl Mercaptan	291.15	291.00	399.75	a	5.11	2.41	2.69	293.33	296.03	2.18	4.88
000110-67-8	3-Methoxypropionitrile	338.15	338.15	436.15	a	4.91	3.42	3.19	334.19	333.41	-3.96	-4.74
000110-71-4	1,2-Dimethoxyethane	271.48	271.48	358.15	a	4.97	3.17	3.04	263.78	269.39	-7.70	-2.09
000110-71-4	1,2-Dimethoxyethane	271.48	271.48	358.15	a	4.97	3.17	3.04	263.78	269.39	-7.70	-2.09
000110-71-4	1,2-Dimethoxyethane	271.48	271.48	358.15	a	4.97	3.17	3.04	263.78	269.39	-7.70	-2.09
000110-74-7	n-Propyl Formate	270.15	270.00	354.05	a	4.91	3.28	3.20	283.95	268.74	13.80	-1.41
000110-77-0	Ethylthioethanol	350.15	350.15	457.15	a	5.00	3.07	2.95	333.07	347.73	-17.08	-2.42
000110-80-5	2-Ethoxyethanol	316.00	316.00	408.15	a	4.95	3.09	3.08	310.80	315.82	-5.20	-0.18
000110-81-6	Diethyl Disulfide	313.15	313.15	427.25	a	5.11	2.47	2.67	313.80	317.08	0.65	3.93
000110-82-7	Cyclohexane	255.93	253.15	353.85	a	4.91	2.73	3.19	258.26	263.83	2.33	7.90
000110-83-8	Cyclohexene	256.15	243.15	356.05	a	4.88	2.62	3.26	263.25	267.25	7.10	11.10

000110-85-0	Piperazine	338.15		419.15	a	4.85	3.78	3.34	327.50	329.80	-10.65	-8.35
000110-86-1	Pyridine	293.15	293.15	388.35	a	4.77	2.97	3.55	309.84	303.80	16.69	10.65
000110-88-3	Trioxane	318.15	318.15	387.65	a	4.73	4.14	3.66	316.97	308.99	-1.18	-9.16
000110-89-4	Piperidine	280.15	276.15	379.35	a	4.88	2.55	3.26	288.12	292.02	7.97	11.87
000110-91-8	Morpholine	308.15	308.15	401.15	a	4.83	3.08	3.41	315.18	314.11	7.03	5.96
000110-96-3	Diisobutylamine	297.35	294.15	412.75	a	5.33	2.01	2.10	298.23	298.83	0.88	1.48
000110-97-4	Diisopropanolamine	408.15	397.00	523.15	a	5.24	2.48	2.35	404.97	405.67	-3.18	-2.48
000111-13-7	2-Octanone	329.15	324.15	445.65	a	5.31	2.34	2.15	329.35	325.67	0.20	-3.48
000111-14-8	n-Heptanoic Acid	388.15	382.00	495.35	a	5.26	3.05	2.28	361.88	373.09	-26.27	-15.06
000111-15-9	2-Ethoxyethyl Acetate	327.15	328.00	429.55	a	5.24	2.64	2.33	334.25	321.73	7.10	-5.42
000111-26-2	Hexylamine	300.15	281.15	405.95	a	5.16	2.48	2.55	292.49	301.18	-7.66	1.03
000111-27-3	1-Hexanol	333.15	333.00	430.75	a	5.13	2.42	2.61	333.40	336.22	0.25	3.07
000111-29-5	1,5-Pentanediol	409.15	402.15	512.15	a	5.07	2.86	2.76	399.66	407.36	-9.49	-1.79
000111-31-9	Hexyl Mercaptan	305.65	293.15	424.15	a	5.22	2.08	2.39	308.68	311.21	3.03	5.56
000111-34-2	Butyl Vinyl Ether	272.00	272.00	367.15	a	5.10	2.78	2.69	271.66	270.47	-0.34	-1.53
000111-36-4	Butyl Isocyanate	295.65	290.15	388.15	a	5.04	3.46	2.85	273.15	283.86	-22.50	-11.79
000111-40-0	Diethylenetriamine	367.15	372.00	480.15	a	5.09	2.97	2.73	349.86	362.13	-17.29	-5.02
000111-41-1	N-Aminoethyl Ethanolamine	417.15	375.00	512.15	a	4.99	4.00	2.99	372.92	393.58	-44.23	-23.57
000111-42-2	Diethanolamine	445.15	425.00	541.95	a	5.02	4.06	2.91	392.02	417.24	-53.13	-27.91
000111-44-4	Di(2-Chloroethyl)Ether	348.15	328.15	451.65	a	5.15	2.98	2.58	347.07	340.33	-1.08	-7.82
000111-46-6	Diethylene Glycol	413.15	397.00	518.95	a	5.02	3.42	2.91	383.86	402.08	-29.29	-11.07
000111-47-7	Di-n-Propyl Sulfide	305.15	301.00	416.05	a	5.20	2.42	2.44	304.68	305.48	-0.47	0.33
000111-48-8	Thiodiglycol	433.15	433.15	555.15	a	5.05	3.30	2.82	390.78	421.50	-42.37	-11.65
000111-49-9	Hexamethyleneimine	301.15	310.00	411.15	a	4.99	2.44	2.98	302.70	310.73	1.55	9.58
000111-55-7	Ethylene Glycol Diacetate	361.15	361.15	463.15	a	5.26	2.93	2.29	366.09	349.16	4.94	-11.99
000111-65-9	n-Octane	287.15	286.00	398.75	a	5.30	2.29	2.20	290.19	285.48	3.04	-1.67
000111-66-0	1-Octene	284.65	281.00	394.35	a	5.27	2.36	2.26	277.35	282.93	-7.30	-1.72
000111-68-2	n-Heptylamine	317.15	308.15	429.15	a	5.27	2.43	2.26	306.69	314.26	-10.46	-2.89
000111-70-6	1-Heptanol	346.15	345.00	449.55	a	5.25	2.38	2.32	342.42	345.23	-3.73	-0.92
000111-71-7	Heptanal	308.15	308.15	425.95	a	5.21	2.27	2.41	304.47	310.77	-3.68	2.62
000111-76-2	2-Butoxyethanol	334.15	333.15	441.55	a	5.20	2.66	2.44	324.65	330.12	-9.50	-4.03
000111-77-3	2-(2-Methoxyethoxy)Ethanol	360.15	357.04	466.15	a	5.16	3.19	2.55	336.65	347.35	-23.50	-12.80
000111-78-4	1,5-Cyclooctadiene	308.15	308.15	423.95	a	5.06	2.48	2.80	310.84	314.29	2.69	6.14
000111-84-2	n-Nonane	304.15	304.00	423.95	a	5.39	2.05	1.95	294.61	302.37	-9.54	-1.78
000111-86-4	Octylamine	333.00	333.00	452.75	a	5.37	2.29	2.01	320.05	328.01	-12.95	-4.99
000111-87-5	1-Octanol	359.70	357.00	468.25	a	5.35	2.28	2.06	352.12	356.03	-7.58	-3.67
000111-88-6	Octyl Mercaptan	341.15	341.15	472.25	a	5.42	1.87	1.88	337.36	341.41	-3.79	0.26
000111-90-0	2-(2-Ethoxyethoxy)Ethanol	363.15	356.45	469.15	a	5.27	3.07	2.25	343.92	347.30	-19.23	-15.85
000111-91-1	Di-(2-Chloroethoxy)Methane	383.15	383.15	491.15	a	5.30	3.08	2.19	370.52	364.97	-12.63	-18.18
000111-92-2	Di-n-Butylamine	315.00	312.15	432.75	a	5.37	2.18	1.99	306.00	311.69	-9.00	-3.31
000111-96-6	Diethylene Glycol Dimethyl Ether	330.15	335.93	435.15	a	5.28	2.78	2.23	323.34	320.05	-6.81	-10.10
000111-96-6	Diethylene Glycol Dimethyl Ether	330.15	335.93	435.15	a	5.28	2.78	2.23	323.34	320.05	-6.81	-10.10

000111-96-6	Diethylene Glycol Dimethyl Ether	330.15	335.93	435.15	a	5.28	2.78	2.23	323.34	320.05	-6.81	-10.10
001112-39-6	Dimethyldimethoxysilane	263.15	258.15	355.15	a	5.14	3.03	2.61	244.86	255.90	-18.29	-7.25
001116-76-3	Tri-n-Octylamine	444.50	457.00	639.15	a	6.27	-1.50	-0.32	475.42	464.14	30.92	19.64
000112-05-0	Nonanoic Acid	413.15	401.00	527.65	a	5.45	2.92	1.79	380.28	390.75	-32.87	-22.40
000112-07-2	Ethylene Glycol Monobutyl Ether Acetate	344.15	344.15	465.15	a	5.43	1.91	1.84	356.64	342.83	12.49	-1.32
000112-14-1	Octyl Acetate	356.15	359.15	483.15	a	5.55	1.84	1.55	364.27	350.92	8.12	-5.23
000112-15-2	Diethylene Glycol Ethyl Ether Acetate	368.15		491.65	a	5.48	2.03	1.71	378.39	362.28	10.24	-5.87
000112-17-4	Decyl Acetate	386.50	377.00	517.15	a	5.69	1.87	1.17	385.90	373.56	-0.60	-12.94
000112-20-9	n-Nonylamine	343.15	335.15	475.35	a	5.46	1.86	1.78	333.46	341.61	-9.69	-1.54
000112-24-3	Triethylenetetramine	408.15	408.15	539.65	a	5.39	2.04	1.94	413.09	406.23	4.94	-1.92
000112-25-4	2-Hexoxyethanol	363.15	355.00	481.15	a	5.40	2.54	1.92	346.10	351.56	-17.05	-11.59
000112-27-6	Triethylene Glycol	429.15	429.15	558.15	a	5.32	3.30	2.14	375.71	401.92	-53.44	-27.23
000112-30-1	1-Decanol	377.15	355.37	504.25	a	5.52	1.69	1.61	375.90	375.81	-1.25	-1.34
000112-31-2	Decanal	356.15	358.15	481.65	a	5.50	2.20	1.68	347.15	346.35	-9.00	-9.80
000112-32-3	Octyl Formate	349.50	337.00	471.95	a	5.46	2.24	1.77	340.81	340.59	-8.69	-8.91
000112-34-5	2-(2-Butoxyethoxy)Ethanol	378.15	351.00	504.15	a	5.46	2.38	1.77	364.83	366.40	-13.32	-11.75
000112-35-6	2-(2-(2-Methoxyethoxy)Ethoxy)Ethanol	391.48	387.55	522.15	a	5.43	2.44	1.86	374.71	379.72	-16.77	-11.76
000112-36-7	Diethylene Glycol Diethyl Ether	344.15		461.15	a	5.48	2.00	1.73	357.68	339.56	13.53	-4.59
000112-41-4	1-Dodecene	346.15	340.00	486.95	a	5.62	1.44	1.37	340.18	344.84	-5.97	-1.31
000112-42-5	1-Undecanol	386.15	388.00	516.15	a	5.60	1.56	1.41	386.12	383.66	-0.03	-2.49
000112-49-2	Triethylene Glycol Dimethyl Ether	383.15	383.15	489.15	a	5.51	2.97	1.64	368.74	357.50	-14.41	-25.65
000112-50-5	2-(2-(2-Ethoxyethoxy)Ethoxy)Ethanol	408.15	408.15	528.95	a	5.51	2.67	1.63	390.40	387.36	-17.75	-20.79
000112-53-8	1-Dodecanol	400.00	398.00	532.15	a	5.67	1.58	1.23	399.65	394.00	-0.35	-6.00
006047-69-4	5-o-Tolyl-2-Pentene	361.00		500.15	b	5.44	1.86	1.82	355.44	360.11	-5.56	-0.89
000077-99-6	Trimethylolpropane	449.15	445.15	570.15	c	5.11	4.01	2.67	369.64	412.19	-79.51	-36.96
000112-88-9	1-Octadecene	421.15	421.15	588.15	d	5.98	0.59	0.43	416.30	418.10	-4.85	-3.05
000112-92-5	1-Octadecanol	458.15	450.00	608.15	e	6.02	1.07	0.33	454.11	444.86	-4.04	-13.29
002084-19-7	2-Pentanethiol	282.46	282.46	374.15	f	5.08	2.92	2.76	284.13	279.72	1.67	-2.74
002150-02-9	Dimercaptoethyl Ether	371.15	371.15	490.15	f	5.19	2.73	2.45	361.42	365.51	-9.73	-5.64
002530-87-2	(3-Chloropropyl)Trimethoxy-Silane	351.48		468.15	f	5.47	2.62	1.74	333.27	334.64	-18.21	-16.84
000585-07-9	tert-Butyl Methacrylate	300.15	300.15	405.15	f	5.28	2.42	2.22	301.36	296.81	1.21	-3.34
000608-23-1	3-Chloro-o-Xylene	346.00		467.15	f	5.16	2.70	2.55	333.82	342.77	-12.18	-3.23
000763-69-9	Ethyl-3-Ethoxypropionate	331.15	331.15	439.15	f	5.34	2.37	2.09	347.08	326.33	15.93	-4.82
000919-30-2	gamma-Aminopropyltriethoxysilane	369.26		490.15	f	5.68	1.86	1.21	378.95	358.20	9.69	-11.06
000931-88-4	Cyclooctene	298.15	298.15	419.15	f	5.08	2.22	2.75	301.64	308.25	3.49	10.10
000100-20-9	Terephthaloyl Chloride	453.15		539.20	g	5.32	4.40	2.14	394.87	396.72	-58.28	-56.43
000100-50-5	1,2,3,6-Tetrahydrobenzaldehyde	320.15		437.20	g	5.04	2.71	2.85	313.90	323.05	-6.25	2.90
000105-08-8	1,4-Cyclohexanedimethanol	434.15	434.15	556.20	g	5.25	2.34	2.32	431.99	433.66	-2.16	-0.49
000106-48-9	p-Chlorophenol	389.00	389.00	493.15	g	5.02	3.40	2.91	374.83	378.27	-14.17	-10.73
000112-55-0	Dodecyl Mercaptan	393.00	360.15	547.70	g	5.72	1.13	1.09	389.58	392.27	-3.42	-0.73

000127-17-3	Pyruvic Acid	355.15	355.15	438.20	g	4.75	4.35	3.61	314.02	337.48	-41.13	-17.67
013151-06-9	7-Methyl-1-Octene	289.65	291.00	412.14	g	5.35	1.75	2.06	290.43	294.87	0.78	5.22
001694-31-1	t-Butyl Acetoacetate	339.15		457.00	g	5.34	2.13	2.09	355.51	338.47	16.36	-0.68
003048-64-4	Vinylnorbornene	295.15	300.15	414.20	g	5.13	2.08	2.62	304.64	304.91	9.49	9.76
004390-04-9	2,2,4,4,6,8,8-Heptamethylnonane	368.15	368.15	513.20	g	5.71	1.51	1.12	353.11	360.70	-15.04	-7.45
000592-44-9	1,2-Hexadiene	254.15	253.00	348.00	g	5.02	2.90	2.92	245.55	254.41	-8.60	0.26
006163-64-0	Methyl t-Butyl Sulfide	270.15	270.15	373.00	g	5.03	2.34	2.88	281.44	279.16	11.29	9.01
006434-78-2	trans-2-Nonene	305.15		417.70	g	5.37	2.32	2.00	295.93	299.50	-9.22	-5.65
006863-58-7	Di-sec-Butyl Ether	285.65	288.00	394.00	g	5.30	2.26	2.19	289.44	284.52	3.79	-1.13
000702-79-4	1,3-Dimethyladamantane	325.15	325.15	471.00	g	5.30	1.28	2.18	338.10	341.99	12.95	16.84
000926-54-5	trans-2-Methyl-1,3-Pentadiene	255.15	253.15	348.70	g	4.99	2.98	2.99	244.82	255.37	-10.33	0.22
000929-06-6	2-Aminoethoxyethanol	397.00		494.20	g	4.97	3.66	3.03	372.57	383.21	-24.43	-13.79
000096-17-3	2-Methylbutyraldehyde	269.15	271.00	365.00	g	4.93	2.89	3.13	268.59	273.29	-0.56	4.14
000096-35-5	Methyl Glycolate	339.15	339.15	423.20	g	4.82	4.00	3.43	324.30	327.07	-14.85	-12.08
000099-04-7	m-Toluic Acid	419.15		536.20	g	5.15	3.06	2.56	398.89	408.34	-20.26	-10.81
000112-57-2	Tetraethylenepentamine	436.00	436.00	614.65	a	5.62	0.47	1.35	457.90	453.21	21.90	17.21
000112-58-3	Di-n-Hexyl Ether	354.65	350.15	496.15	a	5.68	1.22	1.20	353.03	354.30	-1.62	-0.35
000112-59-4	2-(2-Hexoxyethoxy)Ethanol	408.15	408.15	533.15	a	5.62	2.43	1.36	391.47	387.21	-16.68	-20.94
000112-60-7	Tetraethylene Glycol	469.00	469.00	601.15	a	5.44	3.32	1.83	420.12	430.39	-48.88	-38.61
000112-72-1	1-Tetradecanol	421.15	416.00	562.15	a	5.80	1.40	0.89	415.39	412.11	-5.76	-9.04
000112-73-2	Diethylene Glycol Di-n-Butyl Ether	391.15	391.15	529.15	a	5.77	1.41	0.98	401.01	383.37	9.86	-7.78
000112-80-1	Oleic Acid	462.00	462.00	633.15	a	6.01	0.51	0.35	463.34	459.17	1.34	-2.83
001120-21-4	n-Undecane	339.05	338.15	469.05	a	5.56	1.82	1.51	337.29	333.51	-1.76	-5.54
001123-00-8	Cyclopentylacetic Acid	382.15	382.15	501.15	a	5.15	2.69	2.58	370.76	379.97	-11.39	-2.18
001127-76-0	1-Ethylnaphthalene	384.15	384.15	531.75	a	5.31	2.08	2.15	373.76	385.63	-10.39	1.48
000115-11-7	Isobutene	197.04		266.25	a	4.73	3.24	3.66	200.85	203.15	3.81	6.11
000115-21-9	Ethyltrichlorosilane	288.15		373.65	a	5.11	3.49	2.67	268.79	273.22	-19.36	-14.93
000116-09-6	Acetol	329.00	329.00	418.65	a	4.72	3.84	3.69	312.22	325.80	-16.78	-3.20
000118-74-1	Hexachlorobenzene	515.00	515.00	598.15	a	5.40	4.79	1.93	403.35	434.12	-111.65	-80.88
000118-91-2	o-Chlorobenzoic Acid	446.00	435.00	560.15	a	5.14	3.42	2.60	419.30	426.66	-26.70	-19.34
001186-53-4	2,2,3,4-Tetramethylpentane	284.00	284.00	406.15	a	5.25	2.03	2.31	275.20	288.90	-8.80	4.90
000119-36-8	Methyl Salicylate	369.00		496.05	a	5.20	2.52	2.45	367.83	367.50	-1.17	-1.50
000119-64-2	1,2,3,4-Tetrahydronaphthalene	344.00	344.00	480.75	a	5.18	2.09	2.49	344.37	352.16	0.37	8.16
000119-65-3	Isoquinoline	380.15	380.15	516.35	a	5.11	2.44	2.69	379.24	385.65	-0.91	5.50
001191-99-7	2,3-Dihydrofuran	249.15	249.15	327.65	a	4.69	3.26	3.76	261.05	257.30	11.90	8.15
000120-12-7	Anthracene	458.15	394.00	613.05	a	5.37	2.60	1.99	417.93	442.46	-40.22	-15.69
000120-51-4	Benzyl Benzoate	431.00	418.15	596.65	a	5.56	1.31	1.53	441.75	435.57	10.75	4.57
000120-61-6	Dimethyl Terephthalate	414.15	414.15	561.15	a	5.43	1.99	1.85	416.27	411.17	2.12	-2.98
000120-80-9	1,2-Benzenediol	400.00	400.00	518.15	a	4.94	3.01	3.11	396.53	402.27	-3.47	2.27
000120-82-1	1,2,4-Trichlorobenzene	378.15	378.71	486.65	a	5.18	3.34	2.49	349.34	359.22	-28.81	-18.93
000120-92-3	Cyclopentanone	299.00	299.00	403.65	a	4.84	2.87	3.38	308.42	309.06	9.42	10.06
000120-94-5	N-Methylpyrrolidine	259.00	259.00	354.15	a	4.91	2.87	3.19	260.18	264.55	1.18	5.55

000121-14-2	2,4-Dinitrotoluene	442.00	480.15	573.15	a	5.26	2.96	2.29	430.45	425.69	-11.55	-16.31
000121-17-5	4-Chloro-3-Nitrobenzotrifluoride	374.15	374.15	495.15	a	5.32	2.61	2.13	373.22	364.45	-0.93	-9.70
000121-43-7	Trimethyl Borate	260.15		340.65	a	5.03	3.20	2.89	262.79	255.21	2.64	-4.94
000121-44-8	Triethylamine	262.15	258.15	362.15	a	5.12	2.57	2.64	255.48	263.32	-6.67	1.17
000121-69-7	N,N-Dimethylaniline	348.15	335.15	466.60	a	5.14	2.72	2.59	343.64	345.53	-4.51	-2.62
000121-73-3	m-Chloronitrobenzene	388.00	400.15	508.65	a	5.13	3.00	2.63	376.72	379.59	-11.28	-8.41
000122-39-4	Diphenylamine	426.00	426.00	575.15	a	5.37	2.00	2.00	431.68	425.97	5.68	-0.03
000122-51-0	Triethyl Orthoformate	308.15		416.15	a	5.37	2.06	2.00	330.59	307.19	22.44	-0.96
000122-52-1	Triethyl Ester Phosphorous Acid	317.15		431.05	a	5.39	2.17	1.94	325.05	313.24	7.90	-3.91
000122-60-1	1,2-Epoxy-3-Phenoxypropane	387.00	383.15	516.15	a	5.27	2.46	2.26	388.20	382.80	1.20	-4.20
000122-79-2	Phenyl Acetate	349.15		469.15	a	5.18	2.45	2.50	347.34	349.97	-1.81	0.82
000122-97-4	3-Phenyl-1-Propanol	382.15	373.15	508.15	a	5.25	1.98	2.31	388.64	388.04	6.49	5.89
000123-05-7	2-Ethylhexanal	317.59	317.15	436.15	a	5.29	2.38	2.22	309.50	314.54	-8.09	-3.05
000123-07-9	p-Ethylphenol	373.15	373.15	491.05	a	5.14	2.61	2.60	367.94	372.99	-5.21	-0.16
000123-19-3	4-Heptanone	307.15	321.15	417.15	a	5.20	2.52	2.43	305.07	305.59	-2.08	-1.56
000123-25-1	Diethyl Succinate	369.15	363.00	490.85	a	5.43	2.20	1.84	381.93	362.55	12.78	-6.60
000123-31-9	p-Hydroquinone	438.00	438.00	560.15	a	4.95	2.94	3.08	430.49	441.10	-7.51	3.10
000123-38-6	Propanal	247.15	243.15	321.15	a	4.63	3.58	3.90	248.75	252.67	1.60	5.52
000123-39-7	N-Methylformamide	384.15	376.00	472.65	a	4.59	4.03	4.02	364.14	383.86	-20.01	-0.29
000123-42-2	Diacetone Alcohol	334.00	331.00	441.05	a	5.09	2.69	2.72	344.69	334.48	10.69	0.48
000123-51-3	3-Methyl-1-Butanol	316.00	316.00	404.25	a	4.98	2.59	3.02	322.31	322.58	6.31	6.58
000123-54-6	Acetylacetone	307.15	307.15	411.15	a	4.97	2.44	3.03	335.23	317.51	28.08	10.36
000123-62-6	Propionic Anhydride	336.00	336.00	443.15	a	5.19	2.75	2.48	339.64	330.85	3.64	-5.15
000123-72-8	Butanal	262.15	262.15	347.95	a	4.81	3.24	3.44	260.33	265.62	-1.82	3.47
000123-73-9	trans-Crotonaldehyde	286.15	281.15	375.35	a	4.78	3.20	3.52	294.48	292.09	8.33	5.94
000123-75-1	Pyrrolidine	276.00		359.65	a	4.76	3.25	3.57	274.40	281.38	-1.60	5.38
000123-76-2	Levulinic Acid	410.00	410.00	518.65	a	5.01	2.91	2.93	426.94	410.30	16.94	0.30
000123-86-4	n-Butyl Acetate	298.15	295.00	399.25	a	5.17	2.60	2.52	312.14	296.86	13.99	-1.29
000123-91-1	1,4-Dioxane	284.15	285.00	374.65	a	4.80	3.12	3.48	293.10	290.71	8.95	6.56
000123-92-2	Isopentyl Acetate	306.15	298.15	415.65	a	5.25	2.28	2.32	315.35	306.80	9.20	0.65
000123-96-6	2-Octanol	344.15	344.26	451.65	a	5.34	2.02	2.09	348.31	345.25	4.16	1.10
000124-02-7	Diallylamine	289.00	284.15	384.15	a	5.11	2.90	2.67	284.86	285.11	-4.14	-3.89
000124-04-9	Adipic Acid	469.26	436.00	610.65	a	5.23	2.51	2.37	459.88	466.07	-9.38	-3.19
000124-07-2	Octanoic Acid	400.15	393.00	512.15	a	5.36	2.93	2.03	375.21	382.25	-24.94	-17.90
000124-09-4	Hexamethylenediamine	354.15	366.00	478.15	a	5.24	2.31	2.33	338.37	354.63	-15.78	0.48
000124-11-8	1-Nonene	299.15	295.00	420.05	a	5.36	2.03	2.03	292.05	299.14	-7.10	-0.01
000124-13-0	Octanal	327.15	324.15	444.15	a	5.31	2.43	2.14	319.42	321.87	-7.73	-5.28
000124-17-4	Diethylene Glycol Monobutyl Ether Acetate	389.15	375.15	518.15	a	5.63	1.85	1.32	399.48	379.56	10.33	-9.59
000124-18-5	n-Decane	322.85	319.00	447.25	a	5.48	2.02	1.72	311.01	317.44	-11.84	-5.41
000124-40-3	Dimethylamine	223.15		279.95	a	4.55	3.52	4.13	228.69	231.12	5.54	7.97
000124-70-9	Methyl Vinyl Dichlorosilane	276.15		365.65	a	5.10	3.08	2.71	273.15	269.87	-3.00	-6.28
000126-30-7	Neopentyl Glycol	380.15	371.15	481.15	a	4.98	2.82	3.00	377.37	383.59	-2.78	3.44

000126-33-0	Sulfolane	438.15	446.15	560.45	a	4.95	3.37	3.08	429.24	430.61	-8.91	-7.54
000126-98-7	Methacrylonitrile	274.25	286.00	363.45	a	4.77	3.22	3.55	281.54	280.27	7.29	6.02
000126-99-8	Chloroprene	253.15		332.55	a	4.84	3.49	3.38	245.95	251.26	-7.20	-1.89
000127-00-4	1-Chloro-2-Propanol	324.82		400.15	a	4.84	3.80	3.37	315.21	316.81	-9.61	-8.01
000127-19-5	N,N-Dimethylacetamide	336.15	336.15	438.15	a	4.90	3.44	3.22	323.50	331.43	-12.65	-4.72
000127-91-3	beta-Pinene	310.65	304.00	439.15	a	5.22	2.09	2.39	307.20	316.38	-3.45	5.73
000128-37-0	2,6-Di-tert-Butyl-p-Cresol	390.15	390.15	538.15	a	5.61	1.46	1.37	396.40	388.36	6.25	-1.79
000129-00-0	Pyrene	472.00	472.00	677.15	a	5.42	1.42	1.87	443.68	483.98	-28.32	11.98
000131-11-3	Dimethyl Phthalate	419.00	419.00	556.85	a	5.41	2.23	1.89	426.35	411.79	7.35	-7.21
000132-64-9	Dibenzofuran	403.15	403.15	560.15	a	5.29	1.99	2.21	394.52	408.11	-8.63	4.96
013269-52-8	trans-3-Hexene	248.15	261.15	340.25	a	5.05	2.84	2.84	241.79	248.19	-6.36	0.04
013360-61-7	1-Pentadecene	385.15	385.00	541.35	a	5.81	0.94	0.86	380.77	383.64	-4.38	-1.51
013389-42-9	trans-2-Octene	287.15	294.26	398.15	a	5.27	2.34	2.25	279.05	285.59	-8.10	-1.56
000135-01-3	o-Diethylbenzene	330.37	330.37	457.15	a	5.26	2.22	2.28	326.37	331.67	-4.00	1.30
000135-98-8	sec-Butylbenzene	325.00	325.00	446.65	a	5.27	2.17	2.26	327.94	326.71	2.94	1.71
000136-60-7	n-Butyl Benzoate	379.15	379.15	523.45	a	5.46	1.63	1.76	388.54	381.62	9.39	2.47
000137-32-6	2-Methyl-1-Butanol	316.15	316.15	401.15	a	4.97	2.79	3.04	318.73	319.95	2.58	3.80
000138-86-3	d-Limonene	321.00	318.15	449.15	a	5.29	2.03	2.21	319.03	324.38	-1.97	3.38
000140-11-4	Benzyl Acetate	363.15	363.15	486.15	a	5.29	2.31	2.21	370.31	361.11	7.16	-2.04
000140-29-4	Phenylacetonitrile	374.15	374.15	506.65	a	5.11	2.44	2.67	380.23	379.23	6.08	5.08
000140-31-8	N-Aminoethyl Piperazine	372.15	366.15	493.15	a	5.18	2.60	2.50	367.89	370.00	-4.26	-2.15
000140-88-5	Ethyl Acrylate	280.93	282.15	372.55	a	5.01	2.87	2.93	296.04	281.79	15.11	0.86
000141-05-9	Diethyl Maleate	366.15	366.15	496.15	a	5.41	1.83	1.91	384.88	367.59	18.73	1.44
000141-32-2	Butyl Acrylate	310.15	312.00	418.15	a	5.25	2.34	2.32	318.00	309.73	7.85	-0.42
000141-43-5	Monoethanolamine	366.55	358.15	444.15	a	4.62	4.01	3.93	354.40	364.83	-12.15	-1.72
000141-59-3	tert-Octyl Mercaptan	304.00	304.00	433.15	a	5.28	1.52	2.24	315.71	316.42	11.71	12.42
000141-62-8	Decamethyltetrasiloxane	336.15	335.00	467.15	a	5.91	1.49	0.60	330.52	321.38	-5.63	-14.77
000141-63-9	Dodecamethylpentasiloxane	352.15	352.15	505.15	a	6.09	0.47	0.15	356.28	346.99	4.13	-5.16
000141-78-6	Ethyl Acetate	269.00	269.00	350.25	a	4.91	3.16	3.19	277.66	269.45	8.66	0.45
000141-79-7	Mesityl Oxide	301.00	301.00	403.15	a	5.04	2.92	2.86	299.55	300.00	-1.45	-1.00
000141-93-5	m-Diethylbenzene	329.00	329.00	454.25	a	5.29	2.17	2.21	327.46	329.70	-1.54	0.70
000141-97-9	Ethyl Acetoacetate	343.15	330.37	453.95	a	5.19	2.53	2.48	355.83	342.21	12.68	-0.94
000142-28-9	1,3-Dichloropropane	305.15	294.15	394.05	a	4.91	3.47	3.19	299.79	299.76	-5.36	-5.39
000142-29-0	Cyclopentene	244.00	244.00	317.35	a	4.76	3.65	3.57	241.57	242.61	-2.43	-1.39
000142-62-1	n-Hexanoic Acid	375.15	375.00	478.35	a	5.15	3.13	2.57	352.95	364.05	-22.20	-11.10
000142-82-5	n-Heptane	269.00	269.00	371.65	a	5.19	2.55	2.47	260.59	267.65	-8.41	-1.35
000142-84-7	Di-n-Propylamine	280.65	290.15	382.45	a	5.17	2.56	2.53	279.35	280.10	-1.30	-0.55
000143-08-8	1-Nonanol	369.15	368.00	486.45	a	5.44	2.00	1.83	364.79	366.34	-4.36	-2.81
000143-10-2	Decyl Mercaptan	371.15	371.15	513.75	a	5.58	1.59	1.46	364.35	368.61	-6.80	-2.54
000143-13-5	Nonyl Acetate	372.15	372.15	483.15	a	5.62	2.40	1.35	373.93	353.41	1.78	-18.74
000143-15-7	Dodecyl Bromide	417.15	383.15	549.15	a	5.72	2.25	1.10	392.96	393.76	-24.19	-23.39
000143-22-6	2-(2-(2-Butoxyethoxy)Ethoxy)Ethanol	416.00	416.00	551.15	a	5.66	1.94	1.24	411.83	402.59	-4.17	-13.41

000143-24-8	Tetraethylene Glycol Dimethyl Ether	414.15	414.15	548.45	a	5.72	1.79	1.11	420.79	401.30	6.64	-12.85
000143-24-8	Tetraethylene Glycol Dimethyl Ether	414.15	414.15	548.45	a	5.72	1.79	1.11	420.79	401.30	6.64	-12.85
000144-19-4	2,2,4-Trimethyl-1,3-Pentanediol	382.65	383.15	508.15	a	5.26	2.00	2.30	381.51	388.20	-1.14	5.55
001455-21-6	n-Nonyl Mercaptan	351.15	351.15	493.15	a	5.50	1.46	1.66	350.83	354.89	-0.32	3.74
001459-93-4	Dimethyl Isophthalate	411.15	411.15	555.15	a	5.43	1.99	1.85	416.73	408.11	5.58	-3.04
014686-13-6	trans-2-Heptene	272.00	272.00	371.15	a	5.17	2.75	2.53	262.01	268.26	-9.99	-3.74
014686-14-7	trans-3-Heptene	267.15	267.15	368.85	a	5.17	2.59	2.53	259.47	266.09	-7.68	-1.06
014850-23-8	trans-4-Octene	285.65	281.00	395.45	a	5.27	2.40	2.25	276.37	283.05	-9.28	-2.60
000149-57-5	2-Ethyl Hexanoic acid	383.15	387.15	501.15	a	5.32	2.52	2.12	363.44	375.54	-19.71	-7.61
000149-74-6	Phenylmethyldichlorosilane	353.15		479.65	a	5.34	2.30	2.09	351.54	348.99	-1.61	-4.16
014919-01-8	trans-3-Octene	287.15	282.00	396.45	a	5.28	2.43	2.25	277.14	283.91	-10.01	-3.24
000150-76-5	p-Methoxyphenol	398.00	398.00	516.15	a	5.08	2.82	2.74	392.94	396.47	-5.06	-1.53
000151-56-4	Ethyleneimine	262.04	262.04	329.15	a	4.44	4.03	4.40	250.09	268.71	-11.95	6.67
001551-27-5	2-n-Propylthiophene	317.59	317.59	431.15	a	5.16	2.42	2.55	322.84	320.08	5.25	2.49
000156-43-4	p-Phenetidine	389.00	389.00	527.15	a	5.23	2.18	2.37	392.39	393.03	3.39	4.03
000156-59-2	cis-1,2-Dichloroethylene	277.00	277.00	333.25	a	4.72	4.69	3.67	251.07	257.31	-25.93	-19.69
000156-60-5	trans-1,2-Dichloroethylene	267.15	275.00	321.85	a	4.74	4.72	3.63	238.33	246.57	-28.82	-20.58
000156-87-6	3-Amino-1-Propanol	374.15	352.59	460.65	a	4.78	4.05	3.53	347.95	362.38	-26.20	-11.77
001569-01-3	Propylene Glycol n-Propyl Ether	321.15	321.15	423.15	a	5.19	2.91	2.46	315.33	312.83	-5.82	-8.32
001569-02-4	1-Ethoxy-2-Propanol	313.15	315.15	404.15	a	5.08	3.18	2.76	306.85	305.73	-6.30	-7.42
001569-69-3	Cyclohexyl Mercaptan	312.15	316.15	432.05	a	5.07	2.24	2.78	321.11	322.34	8.96	10.19
015869-80-4	3-Ethylheptane	296.15	295.00	416.15	a	5.33	2.15	2.10	284.54	295.35	-11.61	-0.80
015869-85-9	5-Methylnonane	312.00	311.00	438.25	a	5.45	1.88	1.80	296.21	310.48	-15.79	-1.52
015870-10-7	2-Methyl-1-Heptene	283.15	283.15	392.45	a	5.25	2.38	2.30	275.59	281.75	-7.56	-1.40
001589-47-5	2-Methoxy Propanol-1	314.15	309.00	403.15	a	4.92	3.34	3.16	304.46	310.86	-9.69	-3.29
016219-75-3	5-Ethylidene-2-Norbornene	298.15	311.15	419.15	a	5.14	2.06	2.60	306.08	307.87	7.93	9.72
001634-04-4	Methyl tert-Butyl Ether	244.15	240.15	328.35	a	4.96	3.01	3.07	246.24	245.17	2.09	1.02
001639-09-4	n-Heptyl Mercaptan	323.65	319.15	450.15	a	5.32	1.94	2.12	323.16	326.99	-0.49	3.34
001640-89-7	Ethylcyclopentane	273.15	269.00	376.65	a	5.06	2.68	2.80	268.16	275.23	-4.99	2.08
001647-16-1	1,9-Decadiene	314.15	316.00	440.15	a	5.44	1.79	1.83	309.59	314.84	-4.56	0.69
016746-86-4	2,3-Dimethyl-1-Hexene	281.00	281.00	383.65	a	5.22	2.68	2.39	269.64	276.09	-11.36	-4.91
016747-30-1	2,4,4-Trimethylhexane	283.15	283.00	403.85	a	5.29	1.94	2.22	278.35	287.94	-4.80	4.79
016747-38-9	2,3,3,4-Tetramethylpentane	294.15	304.00	414.65	a	5.24	2.29	2.34	279.31	295.22	-14.84	1.07
001678-91-7	Ethylcyclohexane	291.15	295.15	405.05	a	5.14	2.37	2.58	288.85	294.96	-2.30	3.81
001678-92-8	n-Propylcyclohexane	308.15	304.00	429.85	a	5.26	2.17	2.30	304.96	310.60	-3.19	2.45
001678-93-9	n-Butylcyclohexane	325.65	321.00	454.05	a	5.35	2.02	2.04	319.44	326.03	-6.21	0.38
001678-98-4	iso-Butylcyclohexane	315.65		444.45	a	5.33	1.89	2.11	314.58	319.59	-1.07	3.94
001708-29-8	2,5-Dihydrofuran	257.15	257.15	339.65	a	4.69	3.19	3.75	269.27	266.72	12.12	9.57
001719-53-5	Dichlorodiethylsilane	297.15		402.15	a	5.21	2.79	2.42	288.56	290.28	-8.59	-6.87
017301-94-9	4-Methylnonane	317.15	311.00	438.85	a	5.45	2.06	1.80	306.55	312.52	-10.60	-4.63
001759-53-1	Cyclopropane Carboxylic Acid	360.15		456.15	a	4.81	3.35	3.46	358.30	362.30	-1.85	2.15

001795-09-1	2-Methylthiacyclopentane	300.65	295.00	407.15	a	4.97	2.74	3.04	305.25	306.27	4.60	5.62
001795-26-2	1-trans-3,5-Trimethylcyclohexane	292.15		413.65	a	5.24	1.85	2.33	299.91	300.52	7.76	8.37
002016-57-1	Decylamine	358.15	358.15	493.65	a	5.54	1.81	1.57	347.00	353.73	-11.15	-4.42
020237-34-7	trans-1,3-Hexadiene	254.15	254.15	346.35	a	5.01	2.91	2.93	247.57	254.37	-6.58	0.22
002038-03-1	4-(2-Aminoethyl) Morpholine	359.15		478.15	a	5.16	2.69	2.54	355.02	356.10	-4.13	-3.05
002039-93-2	2-Phenylbutene-1	325.15	325.00	455.15	a	5.24	2.03	2.33	325.71	331.02	0.56	5.87
002050-92-2	Diamylamine	345.65	325.15	475.65	a	5.54	1.85	1.55	337.36	340.22	-8.29	-5.43
002189-60-8	n-Octylbenzene	380.15	380.15	537.65	a	5.64	1.00	1.31	385.27	386.16	5.12	6.01
002207-04-7	trans-1,4-Dimethylcyclohexane	284.26		392.55	a	5.14	2.41	2.59	286.13	287.33	1.87	3.07
002210-28-8	n-Propyl Methacrylate	306.15	304.00	414.15	a	5.23	2.47	2.35	309.10	304.15	2.95	-2.00
002211-67-8	2,3-Dichlorobutane	291.15		391.15	a	5.01	2.87	2.92	294.25	292.13	3.10	0.98
002216-33-3	3-Methyloctane	298.65	297.00	417.35	a	5.36	2.09	2.03	290.18	297.65	-8.47	-1.00
002216-34-4	4-Methyloctane	296.15	295.00	415.55	a	5.36	2.00	2.03	289.82	296.62	-6.33	0.47
002315-68-6	Propyl Benzoate	371.15	371.15	484.15	a	5.38	2.56	1.99	380.36	360.29	9.21	-10.86
002437-56-1	1-Tridecene	365.15	352.15	505.95	a	5.69	1.56	1.18	353.96	358.14	-11.19	-7.01
002487-90-3	Trimethoxysilane	269.15		354.15	a	5.12	3.30	2.65	255.87	258.15	-13.28	-11.00
025265-71-8	Dipropylene Glycol	391.00	391.00	503.65	a	5.24	2.87	2.35	376.58	380.69	-14.42	-10.31
002550-06-3	Trichloro(3-Chloropropyl)Silane	357.15		454.65	a	5.32	3.43	2.13	329.20	330.97	-27.95	-26.18
002807-30-9	Ethylene Glycol Monopropyl Ether	322.15	322.15	422.95	a	5.09	2.80	2.74	314.96	321.02	-7.19	-1.13
000287-27-4	Trimethylene Sulfide	271.15	271.15	368.15	a	4.71	3.11	3.71	270.81	282.67	-0.34	11.52
000288-13-1	Pyrazole	355.65	355.00	460.15	a	4.63	2.81	3.92	375.47	377.75	19.82	22.10
000288-14-2	Isoxazole	285.00		368.15	a	4.59	3.27	4.00	307.19	298.26	22.19	13.26
000288-42-6	Oxazole	292.00	292.00	342.65	a	4.59	4.65	4.01	293.08	280.71	1.08	-11.29
000289-80-5	Pyridazine	358.15	358.15	481.15	a	4.74	2.67	3.64	381.28	379.81	23.13	21.66
000289-95-2	Pyrimidine	304.15	304.15	396.95	a	4.73	2.93	3.65	331.40	317.07	27.25	12.92
000291-64-5	Cycloheptane	280.15	267.15	391.55	a	5.01	2.45	2.92	281.30	288.94	1.15	8.79
000292-64-8	Cyclooctane	303.15	303.15	422.15	a	5.10	2.40	2.70	300.00	309.03	-3.15	5.88
000302-01-2	Hydrazine	313.15	311.00	386.65	a	4.21	4.09	4.98	304.44	332.21	-8.71	19.06
003031-74-1	Ethyl Hydroperoxide	305.65		368.15	a	4.63	3.99	3.91	303.22	304.30	-2.43	-1.35
003173-53-3	Cyclohexyl Isocyanate	326.00	321.15	445.15	a	5.13	2.74	2.62	314.84	323.60	-11.16	-2.40
003178-22-1	tert-Butylcyclohexane	315.15		444.65	a	5.29	1.93	2.22	313.48	320.52	-1.67	5.37
003221-61-2	2-Methyloctane	299.15	296.00	416.35	a	5.37	2.12	2.00	291.42	297.07	-7.73	-2.08
000334-48-5	Decanoic Acid	421.15	412.00	541.85	a	5.53	2.66	1.58	390.82	399.78	-30.33	-21.37
003404-61-3	3-Methyl-1-Hexene	267.15	267.15	357.05	a	5.14	3.09	2.61	254.01	258.90	-13.14	-8.25
003452-09-3	1-Nonyne	306.15	306.15	423.95	a	5.35	2.11	2.05	303.51	305.04	-2.64	-1.11
003454-07-7	p-Ethylstyrene	338.15	334.00	465.45	a	5.26	2.25	2.28	334.57	338.65	-3.58	0.50
034590-94-8	Dipropylene Glycol Monomethyl Ether	347.15	347.15	461.45	a	5.34	2.59	2.08	340.99	337.53	-6.16	-9.62
000352-93-2	Diethyl Sulfide	263.15	263.15	365.25	a	4.95	2.39	3.09	273.52	274.95	10.37	11.80
003522-94-9	2,2,5-Trimethylhexane	282.15	286.00	397.15	a	5.32	2.00	2.14	280.69	284.63	-1.46	2.48
036653-82-4	1-Hexadecanol	443.00	427.15	607.15	a	5.91	0.82	0.60	434.68	438.89	-8.32	-4.11
003710-84-7	N,N-Diethylhydroxylamine	318.15	318.15	406.15	a	4.96	2.72	3.05	321.11	323.48	2.96	5.33
003938-95-2	Ethyl Trimethyl Acetate	288.15		391.55	a	5.23	2.35	2.37	298.50	288.54	10.35	0.39

003944-36-3	1-Isopropoxy-2-Propanol	313.15	309.00	410.65	a	5.17	2.81	2.51	313.54	308.08	0.39	-5.07
004110-50-3	Ethyl Propyl Sulfide	285.65		391.75	a	5.08	2.50	2.74	286.98	289.97	1.33	4.32
004265-25-2	2-Methylbenzofuran	340.15	340.15	470.65	a	5.15	2.14	2.58	349.54	348.90	9.39	8.75
004351-54-6	Cyclohexyl Formate	324.15	324.15	436.15	a	5.13	2.72	2.62	323.16	322.22	-0.99	-1.93
004394-85-8	4-Formylmorpholine	386.15	386.15	512.15	a	4.99	2.93	2.98	380.69	387.25	-5.46	1.10
004553-62-2	Methylglutaronitrile	388.00	371.15	536.15	a	5.11	2.15	2.68	402.36	400.05	14.36	12.05
004588-18-5	2-Methyl-1-Octene	296.65	296.00	417.95	a	5.35	1.96	2.05	300.29	298.23	3.64	1.58
000462-94-2	1,5-Pentanediamine	335.15	335.15	452.15	a	5.13	2.23	2.62	329.81	342.03	-5.34	6.88
000462-95-3	Ethylal	268.15	266.00	361.15	a	5.09	2.83	2.72	268.79	266.41	0.64	-1.74
000488-23-3	1,2,3,4-Tetramethylbenzene	347.15	341.15	478.15	a	5.25	2.46	2.32	328.84	344.19	-18.31	-2.96
000493-01-6	cis-Decahydronaphthalene	334.15		468.95	a	5.22	2.16	2.40	325.79	338.95	-8.36	4.80
000493-02-7	trans-Decahydronaphthalene	327.15		460.45	a	5.24	2.00	2.35	325.79	333.87	-1.36	6.72
000496-11-7	Indane	321.65	321.65	451.05	a	5.10	2.16	2.70	325.28	332.40	3.63	10.75
000497-26-7	2-Methyl-1,3-Dioxolane	270.93		354.65	a	4.84	3.18	3.38	282.37	273.15	11.44	2.22
000498-66-8	2-Norbornene	258.15	258.15	369.15	a	4.92	2.03	3.16	276.25	277.33	18.10	19.18
000502-44-3	epsilon-Caprolactone	382.15		488.15	a	5.00	3.35	2.96	389.42	373.48	7.27	-8.67
000502-56-7	5-Nonanone	338.15	333.15	461.55	a	5.40	2.23	1.92	331.90	332.31	-6.25	-5.84
000503-64-0	cis-Crotonic Acid	353.15	352.00	442.15	a	4.83	3.42	3.39	345.39	352.53	-7.76	-0.62
000503-74-2	Isovaleric Acid	351.15	350.00	449.65	a	5.00	2.98	2.96	334.28	350.82	-16.87	-0.33
000505-22-6	1,3-Dioxane	288.15	274.15	379.25	a	4.80	3.15	3.48	297.95	294.32	9.80	6.17
000505-48-6	Suberic Acid	483.15	489.00	618.65	a	5.42	2.53	1.87	475.21	468.70	-7.94	-14.45
000512-56-1	Trimethyl Phosphate	358.15	363.00	470.35	a	5.11	3.11	2.67	349.27	348.60	-8.88	-9.55
000513-35-9	2-Methyl-2-Butene	228.15	228.15	311.65	a	4.88	3.06	3.27	223.80	231.54	-4.35	3.39
000513-44-0	Isobutyl Mercaptan	264.15	264.15	361.65	a	4.94	2.60	3.10	271.49	272.58	7.34	8.43
000513-49-5	sec-Butylamine	254.15		335.65	a	4.87	2.81	3.30	259.51	261.25	5.36	7.10
000513-81-5	2,3-Dimethyl-1,3-Butadiene	251.15	251.15	341.95	a	4.95	2.97	3.08	244.13	253.07	-7.02	1.92
005131-66-8	Propylene Glycol n-Butyl Ether	332.15		444.65	a	5.30	2.56	2.18	323.65	325.19	-8.50	-6.96
005194-50-3	Cis,trans-2,4-Hexadiene	266.15	266.15	356.65	a	5.00	3.20	2.95	252.24	261.80	-13.91	-4.35
005194-51-4	trans,trans-2,4-Hexadiene	266.15	266.15	355.35	a	5.01	3.27	2.92	249.87	259.90	-16.28	-6.25
000526-73-8	1,2,3-Trimethylbenzene	324.15	317.15	449.25	a	5.16	2.36	2.55	318.15	327.95	-6.00	3.80
000526-75-0	2,3-Xylenol	368.15	365.00	490.05	a	5.11	2.70	2.68	358.10	367.64	-10.05	-0.51
000528-29-0	o-Dinitrobenzene	423.15	423.15	591.15	a	5.16	2.03	2.53	427.78	435.56	4.63	12.41
000529-20-4	o-Tolualdehyde	340.15	340.15	473.15	a	5.08	2.25	2.75	342.46	350.53	2.31	10.38
000534-15-6	1,1-Dimethoxyethane	256.15	256.15	337.65	a	4.94	3.34	3.11	250.42	252.19	-5.73	-3.96
000536-74-3	Ethynylbenzene	304.15	304.15	416.15	a	5.03	2.53	2.87	309.95	310.57	5.80	6.42
000538-68-1	n-Pentylbenzene	339.15	338.15	478.55	a	5.40	1.52	1.93	347.24	346.86	8.09	7.71
000538-93-2	Isobutylbenzene	325.15	325.15	445.85	a	5.27	2.28	2.26	324.07	324.77	-1.08	-0.38
000539-88-8	Ethyl Levulinate	363.15		478.95	a	5.28	2.70	2.24	364.94	353.99	1.79	-9.16
000540-54-5	n-Propyl Chloride	242.15	255.37	319.65	a	4.78	3.28	3.52	247.73	246.07	5.58	3.92
000540-63-6	1,2-Ethanedithiol	318.15	317.15	419.15	a	4.87	3.03	3.29	320.25	323.29	2.10	5.14
000540-67-0	Methyl Ethyl Ether	236.00	236.00	280.55	a	4.71	4.91	3.70	213.68	215.47	-22.32	-20.53
000540-88-5	tert-Butyl Acetate	276.95	287.25	370.15	a	5.11	2.62	2.67	290.04	277.70	13.09	0.75

000540-97-6	Dodecamethylcyclohexasiloxane	366.15	366.15	518.15	a	6.09	0.33	0.15	390.78	363.19	24.63	-2.96
000541-02-6	Decamethylcyclopentasiloxane	350.15	350.15	483.15	a	5.94	1.07	0.52	373.45	341.39	23.30	-8.76
000541-05-9	Hexamethylcyclotrisiloxane	308.15	308.15	407.15	a	5.57	2.68	1.48	302.19	288.27	-5.96	-19.88
000541-41-3	Ethyl Chloroformate	289.15	275.15	368.15	a	4.91	3.62	3.18	287.52	281.25	-1.63	-7.90
000541-73-1	m-Dichlorobenzene	336.15	345.00	446.15	a	5.08	2.90	2.75	331.41	333.03	-4.74	-3.12
000542-10-9	Ethylidene Diacetate	343.15	337.00	442.15	a	5.23	3.03	2.35	354.05	330.51	10.90	-12.64
000542-18-7	Chlorocyclohexane	305.15		415.15	a	5.04	2.58	2.86	311.90	310.30	6.75	5.15
000542-55-2	Isobutyl Formate	283.15	277.00	371.35	a	5.02	3.15	2.90	280.84	278.86	-2.31	-4.29
000542-69-8	Butyl Iodide	304.15	299.00	403.75	a	5.03	2.99	2.88	299.94	302.15	-4.21	-2.00
000543-49-7	2-Heptanol	332.15	332.15	432.15	a	5.23	2.12	2.36	339.77	335.67	7.62	3.52
000543-59-9	1-Chloropentane	284.15	286.00	380.95	a	5.07	2.88	2.77	281.20	282.21	-2.95	-1.94
000544-02-5	Diisopentylsulfide	357.04	352.00	484.15	a	5.53	1.92	1.59	356.90	350.91	-0.14	-6.13
000544-40-1	Di-n-Butyl Sulfide	333.15	331.00	458.15	a	5.40	2.05	1.93	328.64	330.78	-4.51	-2.37
000544-76-3	n-Hexadecane	407.05	408.15	559.95	a	5.89	1.23	0.67	391.69	396.52	-15.36	-10.53
000547-63-7	Methyl Isobutyrate	276.15	276.15	365.65	a	5.02	3.00	2.90	278.31	274.56	2.16	-1.59
000547-64-8	Methyl Lactate	324.15		418.15	a	4.95	3.38	3.07	320.74	318.37	-3.41	-5.78
005500-21-0	Cyclopropyl Cyanide	305.15	305.15	408.25	a	4.74	3.07	3.63	316.47	316.63	11.32	11.48
000552-30-7	Trimellitic Anhydride	522.50	512.00	663.15	a	5.28	3.28	2.24	483.79	494.07	-38.71	-28.43
000554-12-1	Methyl Propionate	271.00	271.00	352.95	a	4.90	3.26	3.22	274.39	270.35	3.39	-0.65
000554-14-3	2-Methylthiophene	288.15	280.15	385.75	a	4.91	2.83	3.20	299.73	294.81	11.58	6.66
000555-10-2	beta-Phellandrene	322.15	322.15	444.65	a	5.28	2.23	2.24	319.69	322.34	-2.46	0.19
000556-67-2	Octamethylcyclotetrasiloxane	330.15	330.15	448.95	a	5.78	1.78	0.95	331.15	316.67	1.00	-13.48
000557-98-2	2-Chloropropene	239.15	239.15	295.75	a	4.73	4.24	3.66	233.55	229.78	-5.60	-9.37
000558-30-5	1,2-Epoxy-2-Methylpropane	241.15	258.15	325.15	a	4.78	3.08	3.52	245.66	248.46	4.51	7.31
000558-37-2	3,3-Dimethyl-1-Butene	241.15	245.15	314.35	a	4.98	3.53	3.01	232.60	232.95	-8.55	-8.20
000056-81-5	Glycerol	464.15	433.15	563.15	a	4.84	4.21	3.37	405.25	442.14	-58.90	-22.01
000560-21-4	2,3,3-Trimethylpentane	275.65	273.00	387.95	a	5.17	2.36	2.51	265.98	278.38	-9.67	2.73
000563-45-1	3-Methyl-1-Butene	217.15	217.15	293.25	a	4.88	3.14	3.26	216.78	218.88	-0.37	1.73
000563-79-1	2,3-Dimethyl-2-Butene	257.15	257.15	346.45	a	4.99	3.20	2.99	242.19	253.37	-14.96	-3.78
000563-80-4	Methyl Isopropyl Ketone	272.15	279.15	367.45	a	4.93	2.80	3.13	279.14	277.77	6.99	5.62
000564-02-3	2,2,3-Trimethylpentane	272.65	270.00	383.15	a	5.19	2.35	2.48	264.12	274.88	-8.53	2.23
000565-61-7	3-Methyl-2-Pentanone	285.15	285.15	391.15	a	5.06	2.46	2.81	294.04	291.26	8.89	6.11
000565-69-5	Ethyl Isopropyl Ketone	286.15	286.15	386.65	a	5.07	2.73	2.79	288.04	287.07	1.89	0.92
000565-75-3	2,3,4-Trimethylpentane	277.15	273.00	386.65	a	5.19	2.49	2.46	264.45	276.56	-12.70	-0.59
000565-80-0	Diisopropyl Ketone	288.15	288.15	398.55	a	5.16	2.38	2.55	295.95	291.05	7.80	2.90
000057-11-4	Octadecanoic Acid	469.00	476.15	656.15	a	6.03	0.21	0.31	479.15	471.05	10.15	2.05
000057-55-6	1,2-Propylene Glycol	372.00	372.00	460.75	a	4.76	3.30	3.57	369.82	377.05	-2.18	5.05
000057-57-8	beta-Propiolactone	343.15		435.15	a	4.63	3.82	3.92	339.24	345.39	-3.91	2.24
000576-26-1	2,6-Xylenol	358.15	346.15	474.15	a	5.12	2.96	2.66	346.06	351.82	-12.09	-6.33
000578-54-1	o-Ethylaniline	358.15	364.15	482.80	a	5.14	2.40	2.60	362.53	362.19	4.38	4.04
000579-66-8	2,6-Diethylaniline	382.15	396.15	508.65	a	5.32	2.54	2.13	373.84	373.60	-8.31	-8.55
000583-48-2	3,4-Dimethylhexane	280.65	277.00	390.85	a	5.22	2.46	2.39	268.23	279.41	-12.42	-1.24

000583-57-3	cis-1,2-Dimethylcyclohexane	288.15		397.15	a	5.11	2.52	2.66	286.17	290.71	-1.98	2.56
000583-59-5	trans-2-Methylcyclohexanol	331.15		437.65	a	5.08	2.15	2.75	345.31	341.07	14.16	9.92
000584-02-1	3-Pentanol	303.15	300.00	389.35	a	4.98	2.68	3.01	309.50	308.16	6.35	5.01
000584-03-2	1,2-Butanediol	366.55	363.15	467.15	a	4.91	2.84	3.19	364.04	372.98	-2.51	6.43
000584-84-9	2,4-Toluene Diisocyanate	400.15	400.15	524.15	a	5.34	3.05	2.07	365.63	377.76	-34.52	-22.39
000584-94-1	2,3-Dimethylhexane	280.15	278.48	388.75	a	5.23	2.45	2.36	269.36	278.52	-10.79	-1.63
000586-62-9	Terpinolene	329.15	311.00	459.15	a	5.29	2.10	2.20	323.37	331.09	-5.78	1.94
000587-03-1	m-Tolualcohol	378.15	378.15	488.65	a	5.14	2.71	2.60	375.34	375.95	-2.81	-2.20
005878-19-3	Methoxyacetone	297.15	293.00	389.15	a	4.91	3.17	3.20	302.24	297.54	5.09	0.39
000589-43-5	2,4-Dimethylhexane	276.15	283.15	382.65	a	5.23	2.44	2.35	267.86	274.64	-8.29	-1.51
000589-53-7	4-Methylheptane	279.15	279.15	390.85	a	5.26	2.21	2.28	273.85	280.40	-5.30	1.25
000589-81-1	3-Methylheptane	279.15	279.00	391.15	a	5.26	2.19	2.28	274.00	280.80	-5.15	1.65
000590-01-2	n-Butyl Propionate	313.15	305.37	419.95	a	5.27	2.50	2.25	315.71	308.79	2.56	-4.36
000590-66-9	1,1-Dimethylcyclohexane	280.15	276.00	392.75	a	5.11	2.22	2.67	285.07	288.05	4.92	7.90
000590-86-3	3-Methylbutyraldehyde	270.15	268.00	365.65	a	4.94	2.91	3.11	268.59	273.75	-1.56	3.60
000591-21-9	cis-1,3-Dimethylcyclohexane	283.15		395.65	a	5.14	2.24	2.59	286.68	289.17	3.53	6.02
000591-68-4	Butyl Valerate	340.00	336.00	458.95	a	5.46	2.10	1.77	343.29	334.13	3.29	-5.87
000591-76-4	2-Methylhexane	263.15	250.00	363.15	a	5.16	2.57	2.54	256.83	262.52	-6.32	-0.63
000591-78-6	2-Hexanone	296.15	296.15	400.75	a	5.09	2.59	2.72	300.96	298.43	4.81	2.28
000591-87-7	Allyl Acetate	286.15	295.37	376.65	a	5.02	2.90	2.91	302.90	286.43	16.75	0.28
005911-04-6	3-Methylnonane	319.15	311.00	441.05	a	5.45	2.11	1.80	306.31	313.41	-12.84	-5.74
000592-13-2	2,5-Dimethylhexane	275.15	271.00	382.25	a	5.25	2.35	2.32	269.30	274.62	-5.85	-0.53
000592-27-8	2-Methylheptane	279.15	277.15	390.75	a	5.27	2.17	2.25	274.43	280.52	-4.72	1.37
000592-41-6	1-Hexene	247.15		336.55	a	5.04	2.91	2.85	241.22	246.24	-5.93	-0.91
000592-42-7	1,5-Hexadiene	246.15	227.15	332.55	a	5.01	2.98	2.93	242.07	245.35	-4.08	-0.80
000592-45-0	1,4-Hexadiene	248.15	248.15	338.15	a	5.00	2.87	2.96	245.43	249.68	-2.72	1.53
000592-57-4	1,3-Cyclohexadiene	265.15	257.00	353.65	a	4.85	3.17	3.34	267.79	268.28	2.64	3.13
000592-76-7	1-Heptene	265.15	265.15	366.75	a	5.16	2.51	2.54	260.67	265.68	-4.48	0.53
000592-84-7	n-Butyl Formate	286.15	291.00	379.25	a	5.05	2.97	2.84	286.58	283.97	0.43	-2.18
000592-88-1	Diallyl Sulfide	298.65	319.15	411.75	a	5.11	2.31	2.67	296.42	305.28	-2.23	6.63
000594-56-9	2,3,3-Trimethyl-1-Butene	256.15	256.15	351.05	a	5.07	2.80	2.78	249.75	255.97	-6.40	-0.18
000594-82-1	2,2,3,3-Tetramethylbutane	281.00	278.00	379.55	a	5.14	3.00	2.59	261.99	273.44	-19.01	-7.56
000595-37-9	Neohexanoic Acid	352.15	352.15	459.15	a	5.07	2.69	2.77	343.11	353.73	-9.04	1.58
000598-03-8	Di-n-Propyl Sulfone	399.15	399.15	543.15	a	5.29	2.12	2.22	392.19	401.27	-6.96	2.12
000598-04-9	Di-n-Butyl Sulfone	416.15	416.15	564.15	a	5.47	1.95	1.74	423.47	411.77	7.32	-4.38
000598-75-4	3-Methyl-2-Butanol	299.15	299.15	385.15	a	4.96	2.47	3.07	310.63	307.90	11.48	8.75
000060-12-8	2-Phenylethanol	375.00	369.00	491.35	a	5.14	2.52	2.59	374.68	376.50	-0.32	1.50
000060-24-2	2-Mercaptoethanol	340.15	340.15	431.15	a	4.72	3.48	3.67	329.81	343.90	-10.34	3.75
000060-29-7	Diethyl Ether	228.15	228.15	307.65	a	4.89	2.95	3.25	236.06	232.77	7.91	4.62
006032-29-7	2-Pentanol	307.15	307.00	392.45	a	4.99	2.53	2.98	318.06	313.83	10.91	6.68
000606-20-2	2,6-Dinitrotoluene	433.15	417.00	573.15	a	5.25	2.77	2.32	415.92	422.26	-17.23	-10.89
006094-02-6	2-Methyl-1-Hexene	267.15	267.15	365.15	a	5.14	2.81	2.59	254.65	263.39	-12.50	-3.76

000611-14-3	o-Ethyltoluene	316.15	312.15	438.35	a	5.17	2.26	2.53	317.08	321.39	0.93	5.24
000611-15-4	o-Methylstyrene	320.15	320.15	442.95	a	5.14	2.25	2.59	324.20	326.69	4.05	6.54
000611-32-5	8-Methylquinoline	378.15		520.65	a	5.21	2.15	2.42	377.70	384.00	-0.45	5.85
006117-80-2	cis-2-Butene-1,4-Diol	401.15	401.15	508.15	a	4.90	2.95	3.23	391.76	406.84	-9.39	5.69
000615-60-1	4-Chloro-o-Xylene	340.15		467.15	a	5.18	2.35	2.50	337.92	343.30	-2.23	3.15
000616-02-4	Methyl Maleic Anhydride	374.15	374.15	486.65	a	4.92	3.26	3.16	372.03	371.97	-2.12	-2.18
000616-12-6	3-Methyl-trans-2-Pentene	246.15	246.15	343.55	a	5.01	2.66	2.94	240.91	250.76	-5.24	4.61
000616-21-7	1,2-Dichlorobutane	298.65	297.00	397.25	a	5.04	3.11	2.87	282.22	294.04	-16.43	-4.61
000616-23-9	2,3-Dichloro-1-Propanol	366.15	365.00	457.15	a	4.96	3.75	3.05	339.88	351.31	-26.27	-14.84
000616-38-6	Dimethyl Carbonate	289.85		363.65	a	4.83	3.94	3.39	271.49	279.61	-18.36	-10.24
000616-39-7	N,N-Diethylmethylamine	250.15	250.00	339.15	a	5.00	2.92	2.95	247.85	250.62	-2.30	0.47
000616-44-4	3-Methylthiophene	285.15	284.15	388.65	a	4.91	2.50	3.19	301.90	297.41	16.75	12.26
000616-45-5	2-Pyrrolidone	411.15	402.00	518.15	a	4.80	3.61	3.47	399.74	407.71	-11.41	-3.44
006163-66-2	Di-tert-Butyl Ether	275.65	270.00	380.35	a	5.24	2.19	2.34	284.96	278.09	9.31	2.44
000617-94-7	2-Phenyl-2-Propanol	360.15	360.15	475.15	a	5.21	2.33	2.43	369.18	361.91	9.03	1.76
000619-99-8	3-Ethylhexane	278.00	279.00	391.75	a	5.23	2.25	2.36	269.24	279.97	-8.76	1.97
000062-53-3	Aniline	344.15	343.15	457.25	a	4.91	2.67	3.18	355.89	354.35	11.74	10.20
000620-14-4	m-Ethyltoluene	311.15	311.15	434.45	a	5.19	2.10	2.46	315.58	317.90	4.43	6.75
000620-23-5	m-Tolualdehyde	351.15	351.15	472.15	a	5.10	2.69	2.69	347.99	351.05	-3.16	-0.10
000621-77-2	Triamylamine	370.15	376.00	515.65	a	5.85	0.73	0.76	380.65	370.60	10.50	0.45
000622-40-2	4-(2-Hydroxyethyl) Morpholine	380.15		500.15	a	5.13	2.98	2.63	366.30	372.59	-13.85	-7.56
000622-45-7	Cyclohexyl Acetate	331.15	330.15	446.15	a	5.25	2.38	2.32	340.78	330.12	9.63	-1.03
000622-96-8	p-Ethyltoluene	312.15	309.15	435.15	a	5.19	2.13	2.46	315.18	318.28	3.03	6.13
000622-97-9	p-Methylstyrene	320.65	319.00	445.95	a	5.16	2.16	2.54	324.38	327.90	3.73	7.25
000623-36-9	2-Methyl-2-Pentenal	304.15	304.15	409.65	a	5.04	2.86	2.85	297.84	303.83	-6.31	-0.32
000623-37-0	3-Hexanol	314.15		407.90	a	5.11	2.44	2.68	319.08	317.74	4.93	3.59
000623-42-7	Methyl n-Butyrate	287.00	287.00	375.95	a	5.04	3.10	2.86	275.69	282.80	-11.31	-4.20
000624-29-3	cis-1,4-Dimethylcyclohexane	284.26		397.55	a	5.14	2.27	2.59	285.50	289.82	1.24	5.56
000624-48-6	Dimethyl Maleate	368.15	386.15	475.15	a	5.20	2.96	2.45	364.98	357.95	-3.17	-10.20
000624-65-7	Propargyl Chloride	259.00		331.15	a	4.71	3.74	3.71	256.48	258.46	-2.52	-0.54
000624-89-5	Methyl Ethyl sulfide	258.15	258.15	339.85	a	4.83	3.31	3.41	259.12	259.87	0.97	1.72
000624-92-0	Dimethyl Disulfide	288.15	280.00	382.95	a	4.87	3.00	3.30	294.45	293.77	6.30	5.62
000625-69-4	2,4-Pentanediol	371.15	374.15	472.15	a	5.03	2.38	2.88	391.57	379.72	20.42	8.57
000625-80-9	Diisopropyl Sulfide	280.15		393.25	a	5.17	1.87	2.53	296.35	291.09	16.20	10.94
000626-67-5	N-Methylpiperidine	276.15		380.15	a	5.01	2.57	2.93	281.87	282.64	5.72	6.49
000626-93-7	2-Hexanol	318.15	319.26	409.15	a	5.12	2.50	2.65	320.91	320.43	2.76	2.28
000627-05-4	1-Nitrobutane	320.15	320.15	426.15	a	5.00	3.00	2.95	314.63	319.18	-5.52	-0.97
000627-21-4	2-Pentyne	243.00	243.00	329.25	a	4.88	3.09	3.26	239.11	245.79	-3.89	2.79
000627-30-5	1-Chloro-3-Propanol	346.15	346.15	438.15	a	4.84	3.14	3.36	342.78	350.14	-3.37	3.99
000627-58-7	2,5-Dimethyl-1,5-Hexadiene	280.00	280.00	387.45	a	5.21	2.52	2.42	270.41	278.29	-9.59	-1.71
000627-98-5	5-Methyl-1-Hexanol	338.15	340.00	443.15	a	5.22	2.07	2.39	342.67	343.15	4.52	5.00
000628-29-5	Methyl n-Butyl Sulfide	291.15	289.00	396.65	a	5.09	2.56	2.71	291.96	293.82	0.81	2.67

000628-32-0	Ethyl Propyl Ether	253.15	247.00	336.35	a	5.03	3.07	2.89	251.92	250.25	-1.23	-2.90
000628-41-1	1,4-Cyclohexadiene	267.15	262.15	358.65	a	4.85	2.99	3.34	275.13	273.37	7.98	6.22
000628-55-7	Diisobutyl Ether	287.65	281.15	396.15	a	5.33	2.22	2.12	292.55	285.90	4.90	-1.75
000628-63-7	n-Pentyl Acetate	310.15	296.15	422.35	a	5.28	2.14	2.24	324.13	311.81	13.98	1.66
000628-71-7	1-Heptyne	271.00	271.00	372.85	a	5.14	2.48	2.60	271.46	272.93	0.46	1.93
000628-73-9	Hexanenitrile	316.15	320.00	436.75	a	5.10	2.37	2.70	319.18	322.45	3.03	6.30
000628-92-2	Cycloheptene	280.65	267.15	388.15	a	4.99	2.55	2.98	284.78	288.51	4.13	7.86
000628-99-9	2-Nonanol	355.15	355.37	466.65	a	5.43	1.90	1.85	359.69	354.43	4.54	-0.72
000629-04-9	1-Bromoheptane	334.15	334.15	452.15	a	5.32	2.40	2.13	327.46	328.97	-6.69	-5.18
000629-05-0	1-Octyne	289.15	289.15	399.45	a	5.25	2.28	2.31	288.02	289.59	-1.13	0.44
000629-11-8	1,6-Hexanediol	420.15	372.00	523.15	a	5.19	2.87	2.46	406.36	412.46	-13.79	-7.69
000629-14-1	1,2-Diethoxyethane	295.00	300.15	392.55	a	5.22	2.58	2.38	297.29	291.75	2.29	-3.25
000629-19-6	Di-n-propyl Disulfide	339.15	339.15	466.65	a	5.31	2.36	2.17	319.62	335.27	-19.53	-3.88
000629-20-9	1,3,5,7-Cyclooctatetraene	299.26		413.65	a	5.02	2.10	2.92	323.04	313.77	23.78	14.51
000629-33-4	n-Hexyl Formate	320.00	317.00	428.65	a	5.28	2.62	2.25	313.20	313.15	-6.80	-6.85
000629-50-5	n-Tridecane	363.15	352.00	508.55	a	5.70	1.17	1.14	376.15	362.74	13.00	-0.41
000629-59-4	n-Tetradecane	382.45	373.15	526.65	a	5.77	1.50	0.98	367.07	372.55	-15.38	-9.90
000629-73-2	1-Hexadecene	402.15	405.15	558.05	a	5.87	1.05	0.71	392.68	395.58	-9.47	-6.57
000629-78-7	n-Heptadecane	421.15	421.15	575.15	a	5.94	1.20	0.53	405.11	408.38	-16.04	-12.77
000629-82-3	Di-n-Octyl Ether	412.00	385.15	556.15	a	5.92	1.31	0.58	405.87	398.67	-6.13	-13.33
000629-92-5	n-Nonadecane	441.00	441.00	603.05	a	6.04	0.87	0.27	427.57	429.66	-13.43	-11.34
000629-96-9	1-Eicosanol	468.15	467.00	645.15	a	6.11	0.09	0.09	472.32	468.18	4.17	0.03
000631-36-7	Tetraethyl Silane	305.15		427.85	a	5.36	2.59	2.02	270.61	294.13	-34.54	-11.02
000637-92-3	tert-Butyl Ethyl Ether	253.15	254.00	346.25	a	5.09	2.47	2.72	265.05	257.00	11.90	3.85
000638-02-8	2,5-Dimethylthiophene	297.04	296.15	409.65	a	5.04	2.36	2.85	305.72	306.02	8.68	8.98
000638-45-9	Hexyl Iodide	334.15	330.00	454.15	a	5.26	2.36	2.28	327.11	332.54	-7.04	-1.61
000638-49-3	Pentyl Formate	301.15	300.00	403.55	a	5.17	2.71	2.53	300.79	298.02	-0.36	-3.13
000064-17-5	Ethanol	286.15	286.00	351.35	a	4.49	3.41	4.27	304.81	299.39	18.66	13.24
000064-19-7	Acetic Acid	312.04		391.05	a	4.53	3.08	4.16	338.34	330.17	26.30	18.13
000644-49-5	Propyl Isobutyrate	300.15	302.00	408.55	a	5.26	2.26	2.28	309.01	300.52	8.86	0.37
006443-92-1	cis-2-Heptene	270.95	265.00	371.55	a	5.15	2.68	2.56	262.53	268.95	-8.42	-2.00
000645-62-5	2-Ethyl-2-Hexenal	329.65	341.15	468.15	a	5.26	2.05	2.29	319.58	334.36	-10.07	4.71
000646-04-8	trans-2-Pentene	228.00	225.00	309.45	a	4.91	3.11	3.20	223.51	229.39	-4.49	1.39
000065-85-0	Benzoic Acid	394.26	394.26	522.35	a	5.04	2.46	2.86	393.03	402.81	-1.23	8.55
000659-70-1	Isopentyl Isovalerate	333.15	345.00	463.55	a	5.50	1.59	1.66	342.57	334.47	9.42	1.32
000066-25-1	Hexanal	298.15	300.00	404.15	a	5.09	2.82	2.71	279.26	296.21	-18.89	-1.94
000067-56-1	Methanol	284.15	284.00	337.75	a	4.23	4.15	4.96	299.94	297.75	15.79	13.60
000067-63-0	Isopropanol	285.15		355.45	a	4.68	3.04	3.77	303.45	295.87	18.30	10.72
000067-64-1	Acetone	253.15	255.00	329.15	a	4.64	3.35	3.89	267.81	262.19	14.66	9.04
000067-68-5	Dimethyl Sulfoxide	361.00		462.15	a	4.73	3.50	3.66	359.22	364.79	-1.78	3.79
000674-82-8	Diketene	307.00	307.00	399.25	a	4.77	3.37	3.55	309.10	310.62	2.10	3.62
006795-87-5	Methyl sec-Butyl Ether	243.00		338.15	a	4.99	2.60	2.98	244.94	249.16	1.94	6.16

000068-12-2	N,N-Dimethylformamide	330.15	331.00	426.15	a	4.76	3.73	3.57	313.41	326.56	-16.74	-3.59
000681-84-5	Methyl Silicate	294.15		394.15	a	5.27	2.82	2.27	295.66	284.47	1.51	-9.68
000693-02-7	1-Hexyne	252.00	252.00	344.45	a	5.01	2.68	2.92	254.46	255.84	2.46	3.84
000693-65-2	Di-n-Pentyl Ether	330.15	330.15	463.15	a	5.53	1.53	1.58	331.27	331.02	1.12	0.87
000693-89-0	1-Methylcyclopentene	256.00	256.00	348.65	a	4.92	2.96	3.17	255.05	259.75	-0.95	3.75
000696-29-7	Isopropylcyclohexane	308.15	308.15	427.95	a	5.23	2.33	2.37	300.78	308.95	-7.37	0.80
006982-25-8	2,3-Butanediol	358.15		455.65	a	4.89	2.78	3.24	363.11	366.44	4.96	8.29
000700-12-9	Pentamethylbenzene	364.15	364.15	505.15	a	5.33	2.31	2.11	339.99	359.85	-24.16	-4.30
007058-01-7	sec-Butylcyclohexane	323.65	319.00	452.45	a	5.31	2.13	2.16	314.20	324.13	-9.45	0.48
000071-23-8	1-Propanol	297.59	291.00	370.35	a	4.69	3.14	3.74	308.73	306.94	11.14	9.35
000071-36-3	1-Butanol	310.50	306.00	390.85	a	4.86	2.95	3.31	315.21	316.16	4.71	5.66
000071-41-0	1-Pentanol	322.15	320.00	411.05	a	5.01	2.64	2.94	325.83	326.87	3.68	4.72
000071-43-2	Benzene	262.00	262.00	353.15	a	4.81	2.80	3.45	278.60	273.02	16.60	11.02
007146-60-3	2,3-Dimethyloctane	314.00	309.00	437.45	a	5.42	2.03	1.86	303.78	311.01	-10.22	-2.99
007154-79-2	2,2,3,3-Tetramethylpentane	294.65	289.00	413.35	a	5.23	2.39	2.36	277.69	294.13	-16.96	-0.52
007154-80-5	3,3,5-Trimethylheptane	304.00	301.00	428.85	a	5.37	2.00	2.00	293.11	303.91	-10.89	-0.09
000717-74-8	1,3,5-Triisopropylbenzene	359.82		511.15	a	5.65	1.04	1.28	367.67	364.18	7.85	4.36
007307-55-3	Undecylamine	365.15	365.15	515.15	a	5.61	1.25	1.37	359.99	367.32	-5.16	2.17
000074-96-4	Bromoethane	250.15	250.00	311.65	a	4.65	4.08	3.86	252.85	246.44	2.70	-3.71
007443-70-1	cis-2-Methylcyclohexanol	331.15		438.15	a	5.07	2.26	2.77	342.14	339.71	10.99	8.56
000075-00-3	Ethyl Chloride	223.15		285.45	a	4.60	3.74	3.99	231.67	227.05	8.52	3.90
000075-05-8	Acetonitrile	275.15	275.15	354.75	a	4.42	3.50	4.45	298.33	293.05	23.18	17.90
000075-07-0	Acetaldehyde	233.00	235.00	293.25	a	4.42	3.93	4.44	243.93	241.43	10.93	8.43
000075-12-7	Formamide	423.15		493.15	a	4.35	4.70	4.64	416.54	421.56	-6.61	-1.59
000075-15-0	Carbon Disulfide	243.15		319.15	a	4.60	4.09	3.98	229.18	241.05	-13.97	-2.10
000075-18-3	Dimethyl Sulfide	237.15	237.15	310.45	a	4.65	3.44	3.85	244.78	243.97	7.63	6.82
000075-29-6	Isopropyl Chloride	238.15	238.15	308.85	a	4.77	3.47	3.56	244.77	239.52	6.62	1.37
000075-30-9	Isopropyl Iodide	293.15		362.65	a	4.87	4.11	3.29	280.51	277.63	-12.64	-15.52
000075-31-0	Isopropylamine	236.15	236.15	304.85	a	4.72	2.79	3.68	252.67	247.62	16.52	11.47
000075-33-2	Isopropyl Mercaptan	239.00		325.75	a	4.81	2.62	3.46	255.71	251.98	16.71	12.98
000075-34-3	1,1-Dichloroethane	263.15	261.15	330.55	a	4.77	3.90	3.55	263.78	257.20	0.63	-5.95
000075-35-4	1,1-Dichloroethylene	248.15	251.15	304.75	a	4.73	4.45	3.66	231.10	234.38	-17.05	-13.77
000075-36-5	Acetyl Chloride	269.15	278.00	323.85	a	4.64	4.53	3.88	262.21	257.59	-6.94	-11.56
000075-52-5	Nitromethane	308.15	308.15	374.25	a	4.49	4.34	4.27	302.42	306.75	-5.73	-1.40
000075-54-7	Methyl Dichlorosilane	241.15		314.15	a	4.88	3.55	3.27	235.57	236.66	-5.58	-4.49
000075-55-8	Propyleneimine	263.15	263.15	340.15	a	4.65	3.43	3.85	259.20	270.16	-3.95	7.01
000075-56-9	1,2-Propylene Oxide	236.00	236.00	308.15	a	4.61	3.65	3.95	234.70	241.14	-1.30	5.14
000075-65-0	2-Methyl-2-Propanol	284.26	284.26	355.55	a	4.83	2.80	3.41	307.05	292.68	22.79	8.42
000075-77-4	Trimethylchlorosilane	245.00		333.15	a	5.02	2.98	2.91	238.42	243.93	-6.59	-1.07
000075-78-5	Dimethyldichlorosilane	264.15		343.45	a	5.01	3.40	2.93	260.71	256.28	-3.44	-7.87
000075-79-6	Methyl Trichlorosilane	276.15		338.75	a	5.00	4.29	2.95	253.77	252.42	-22.38	-23.73
000075-84-3	2,2-Dimethyl-1-Propanol	303.15	300.00	386.65	a	4.94	2.84	3.11	306.74	307.43	3.59	4.28

000075-85-4	2-Methyl-2-Butanol	292.15	293.15	375.55	a	4.95	2.45	3.08	307.87	301.23	15.72	9.08
000075-86-5	Acetone Cyanohydrin	347.15	336.15	444.15	a	4.87	2.78	3.29	366.93	356.28	19.78	9.13
000075-87-6	Trichloroacetaldehyde	348.00	323.00	370.95	a	4.93	6.14	3.14	280.49	281.81	-67.51	-66.19
000075-94-5	Vinyltrichlorosilane	283.15		364.65	a	5.09	3.57	2.73	265.72	268.04	-17.43	-15.11
000075-97-8	3,3-Dimethyl-2-Butanone	282.15	285.15	379.25	a	5.02	2.78	2.90	287.64	284.23	5.49	2.08
000075-98-9	Neopentanoic Acid	337.15	336.15	437.15	a	4.97	2.76	3.04	334.72	342.11	-2.43	4.96
007525-62-4	m-Ethylstyrene	335.65	333.00	463.15	a	5.26	2.20	2.28	333.89	337.24	-1.76	1.59
007564-63-8	o-Ethylstyrene	333.15	331.00	460.45	a	5.24	2.21	2.34	331.59	335.65	-1.56	2.50
000076-22-2	Camphor	338.70	338.70	477.15	a	5.23	1.79	2.36	352.49	349.93	13.79	11.23
000760-20-3	3-Methyl-1-Pentene	245.15	245.15	327.35	a	5.01	3.23	2.93	236.02	240.21	-9.13	-4.94
000760-21-4	2-Ethyl-1-Butene	247.15	247.15	337.85	a	5.00	2.87	2.96	243.08	248.61	-4.07	1.46
000760-23-6	3,4-Dichloro-1-Butene	301.15	301.15	389.15	a	5.02	3.30	2.91	297.61	294.17	-3.54	-6.98
000764-13-6	2,5-Dimethyl-2,4-Hexadiene	297.15	297.15	407.65	a	5.20	2.93	2.44	267.44	287.57	-29.71	-9.58
000764-35-2	2-Hexyne	262.15	262.15	357.65	a	5.02	2.85	2.89	256.97	262.89	-5.18	0.74
000764-93-2	1-Decyne	315.65	323.15	447.15	a	5.44	1.56	1.82	318.63	320.10	2.98	4.45
007642-04-8	cis-2-Octene	290.65	294.00	398.75	a	5.26	2.52	2.28	280.14	286.43	-10.51	-4.22
007642-15-1	cis-4-Octene	285.65	290.00	395.65	a	5.26	2.32	2.28	285.22	285.07	-0.43	-0.58
000765-30-0	Cyclopropylamine	248.15	245.00	323.65	a	4.65	2.92	3.86	260.99	261.78	12.84	13.63
000077-73-6	Dicyclopentadiene	318.15	305.37	443.15	a	5.14	2.25	2.60	320.27	325.10	2.12	6.95
000077-74-7	3-Methyl-3-Pentanol	297.15	297.15	395.55	a	5.05	2.01	2.83	318.04	309.31	20.89	12.16
000771-61-9	Pentafluorophenol	345.37		418.75	a	5.10	4.44	2.69	302.88	308.48	-42.49	-36.89
007731-28-4	cis-4-Methylcyclohexanol	343.15		446.15	a	5.08	2.37	2.74	352.12	349.40	8.97	6.25
007731-29-5	trans-4-Methylcyclohexanol	343.15		447.15	a	5.09	2.17	2.72	359.10	352.22	15.95	9.07
007778-85-0	1,2-Dimethoxypropane	273.15	273.71	369.15	a	5.08	2.85	2.76	267.47	271.66	-5.68	-1.49
000078-10-4	Tetraethoxysilane	324.82	324.82	441.95	a	5.62	1.74	1.35	339.14	318.53	14.32	-6.29
000078-40-0	Triethyl Phosphate	372.00	372.00	488.65	a	5.43	2.53	1.84	379.32	358.87	7.32	-13.13
000078-59-1	Isophorone	350.65	357.15	488.35	a	5.23	1.72	2.38	377.02	363.41	26.37	12.76
000078-76-2	2-Bromobutane	279.15	294.00	364.35	a	4.94	3.35	3.10	275.71	274.78	-3.44	-4.37
000078-79-5	Isoprene	225.00	219.26	307.15	a	4.83	2.90	3.38	228.58	232.32	3.58	7.32
000078-81-9	Isobutylamine	260.15	255.35	340.85	a	4.87	2.87	3.30	263.50	266.49	3.35	6.34
000078-82-0	Isobutyronitrile	281.48	281.48	377.05	a	4.81	3.10	3.46	287.20	288.17	5.72	6.69
000078-83-1	2-Methyl-1-Propanol	302.32	301.00	380.95	a	4.84	2.91	3.38	310.60	309.53	8.28	7.21
000078-84-2	2-Methylpropanal	254.15	266.00	337.65	a	4.80	3.27	3.48	254.06	257.89	-0.09	3.74
000078-85-3	Methacrolein	258.15	275.15	341.55	a	4.76	3.25	3.58	260.16	263.86	2.01	5.71
000078-86-4	sec-Butyl Chloride	258.15		341.15	a	4.91	3.24	3.19	256.93	257.35	-1.22	-0.80
000078-87-5	1,2-Dichloropropane	286.15	286.15	368.65	a	4.91	3.56	3.19	279.37	279.26	-6.78	-6.89
000078-88-6	2,3-Dichloropropene	288.15	283.15	367.15	a	4.88	3.73	3.26	277.52	279.31	-10.63	-8.84
000078-90-0	1,2-Propanediamine	306.15	306.15	392.65	a	4.83	3.08	3.40	305.68	311.54	-0.47	5.39
000078-92-2	2-Butanol	296.15	296.15	372.65	a	4.84	2.93	3.37	306.28	302.73	10.13	6.58
000078-93-3	Methyl Ethyl Ketone	264.15	267.00	352.65	a	4.81	2.98	3.45	273.64	272.12	9.49	7.97
000078-96-6	1-Amino-2-Propanol	347.04	347.04	433.15	a	4.79	3.53	3.49	341.86	346.23	-5.18	-0.81
000078-97-7	Lactonitrile	350.15	350.15	456.15	a	4.73	2.49	3.64	376.79	371.76	26.64	21.61

000078-99-9	1,1-Dichloropropane	280.00	280.00	361.25	a	4.91	3.50	3.19	276.54	273.15	-3.46	-6.85
000079-09-4	Propionic Acid	330.00	328.00	414.25	a	4.72	3.30	3.67	332.52	336.67	2.52	6.67
000079-10-7	Acrylic Acid	324.00		414.35	a	4.68	2.88	3.78	339.62	340.03	15.62	16.03
000079-16-3	N-Methylacetamide	381.15	381.15	478.15	a	4.77	3.57	3.55	374.19	380.58	-6.96	-0.57
000079-20-9	Methyl Acetate	260.15	263.15	329.95	a	4.74	3.65	3.62	265.53	259.65	5.38	-0.50
000079-21-0	Peracetic Acid	313.15		383.15	a	4.64	4.70	3.88	265.51	294.13	-47.64	-19.02
000079-22-1	Methyl Chloroformate	285.15	285.15	343.65	a	4.75	4.52	3.61	269.92	268.33	-15.23	-16.82
000079-24-3	Nitroethane	303.15	301.00	387.15	a	4.69	3.64	3.77	296.02	305.70	-7.13	2.55
000079-31-2	Isobutyric Acid	333.15	329.15	427.55	a	4.87	2.99	3.30	332.91	338.70	-0.24	5.55
000079-36-7	Dichloroacetyl Chloride	339.00	339.00	381.15	a	4.94	5.48	3.12	281.19	287.26	-57.81	-51.74
000079-41-4	Methacrylic Acid	340.00	340.00	436.15	a	4.83	3.03	3.40	336.10	346.91	-3.90	6.91
000079-46-9	2-Nitropropane	301.00	297.15	393.35	a	4.84	3.47	3.38	292.13	299.22	-8.87	-1.78
000079-92-5	Camphene	307.15	309.15	433.15	a	5.21	2.13	2.42	304.85	312.80	-2.30	5.65
000080-10-4	Diphenyldichlorosilane	415.15	415.37	578.15	a	5.58	1.31	1.47	422.55	418.43	7.40	3.28
000080-46-6	p-tert-Amylphenol	393.15	384.00	535.65	a	5.36	1.93	2.03	385.62	395.14	-7.53	1.99
000080-56-8	alpha-Pinene	305.00	303.15	429.05	a	5.22	2.01	2.39	309.31	312.07	4.31	7.07
000080-62-6	Methyl Methacrylate	284.15	284.15	373.65	a	4.99	3.15	2.99	281.01	281.30	-3.14	-2.85
000814-78-8	Methyl Isopropenyl Ketone	278.15	294.15	371.15	a	4.90	3.03	3.22	280.87	281.54	2.72	3.39
000818-61-1	2-Hydroxyethyl Acrylate	378.00	371.15	464.15	a	5.07	3.70	2.77	363.13	359.64	-14.87	-18.36
000821-55-6	2-Nonanone	345.50	337.15	468.45	a	5.41	2.21	1.91	343.33	339.91	-2.17	-5.59
000822-06-0	1,6-Hexamethylene Diisocyanate	408.15	396.00	528.15	a	5.44	3.19	1.83	374.78	377.10	-33.37	-31.05
000827-52-1	Cyclohexylbenzene	372.00	372.00	513.25	a	5.36	1.96	2.02	371.53	373.22	-0.47	1.22
000084-15-1	o-Terphenyl	436.00	436.00	605.15	a	5.60	1.09	1.41	453.47	442.74	17.47	6.74
000084-65-1	Anthraquinone	469.50	458.15	650.15	a	5.42	1.67	1.89	462.04	474.79	-7.46	5.29
000085-01-8	Phenanthrene	444.00	444.00	613.15	a	5.36	2.04	2.03	419.70	443.77	-24.30	-0.23
000085-44-9	Phthalic Anhydride	425.00	425.00	568.15	a	5.10	2.69	2.69	421.89	425.03	-3.11	0.03
000087-41-2	Phthalide	425.15		563.15	a	5.08	2.83	2.75	419.99	423.28	-5.16	-1.87
000087-61-6	1,2,3-Trichlorobenzene	386.00	386.00	491.65	a	5.16	3.50	2.53	354.39	363.93	-31.61	-22.07
000871-83-0	2-Methylnonane	314.00	314.00	440.25	a	5.46	1.82	1.77	307.61	313.22	-6.39	-0.78
000872-05-9	1-Decene	320.15	311.00	443.65	a	5.46	2.03	1.77	310.43	315.49	-9.72	-4.66
000872-50-4	N-Methyl-2-Pyrrolidone	359.15	359.15	475.15	a	4.95	3.16	3.10	353.03	357.72	-6.12	-1.43
000872-55-9	2-Ethylthiophene	300.15	297.00	407.15	a	5.04	2.53	2.87	309.65	306.25	9.50	6.10
000873-66-5	trans-1-Propenylbenzene	325.15	325.15	451.45	a	5.17	2.15	2.52	329.55	332.40	4.40	7.25
000877-44-1	1,2,4-Triethylbenzene	356.15	353.15	491.15	a	5.44	2.05	1.82	346.51	351.56	-9.64	-4.59
000088-09-5	2-Ethyl Butyric Acid	360.00	360.00	467.15	a	5.11	2.90	2.68	350.04	355.93	-9.96	-4.07
000088-73-3	o-Chloronitrobenzene	397.15	400.15	518.65	a	5.11	3.04	2.66	387.65	388.49	-9.50	-8.66
000088-74-4	o-Nitroaniline	441.15	441.15	557.15	a	5.07	3.36	2.77	429.40	426.89	-11.75	-14.26
000088-85-7	4,6-Dinitro-o-sec-Butylphenol	450.15		605.15	a	5.52	2.17	1.60	435.48	436.92	-14.67	-13.23
088917-22-0	Dipropylene Glycol Monomethyl Ether Acetate	359.00	359.00	473.15	a	5.54	2.16	1.57	371.29	348.84	12.29	-10.16
000089-78-1	l-Menthol	366.15		485.15	a	5.35	2.02	2.05	370.76	366.64	4.61	0.49
000089-83-8	Thymol	374.15	374.15	505.65	a	5.32	2.27	2.14	366.26	371.55	-7.89	-2.60
000089-95-2	o-Tolualcohol	377.15	377.15	497.15	a	5.12	2.55	2.66	371.89	379.29	-5.26	2.14

000090-00-6	o-Ethylphenol	358.15	351.15	477.65	a	5.12	2.58	2.64	355.72	359.48	-2.43	1.33
000090-02-8	Salicylaldehyde	349.15		470.15	a	5.02	2.79	2.92	328.89	351.89	-20.26	2.74
000090-05-1	Guaiacol	355.00	355.00	478.15	a	5.07	2.54	2.77	362.64	359.69	7.64	4.69
000090-12-0	1-Methylnaphthalene	367.15	355.15	517.85	a	5.22	1.84	2.38	367.77	378.77	0.62	11.62
000090-13-1	1-Chloronaphthalene	394.15	394.15	532.15	a	5.22	2.55	2.38	377.76	390.30	-16.39	-3.85
000091-20-3	Naphthalene	353.15	352.00	491.05	a	5.13	2.17	2.62	353.63	362.80	0.48	9.65
000091-22-5	Quinoline	374.00	374.00	510.25	a	5.11	2.30	2.68	379.61	382.25	5.61	8.25
000091-57-6	2-Methylnaphthalene	370.15	370.15	514.25	a	5.24	2.08	2.34	366.17	375.77	-3.98	5.62
000091-63-4	Quinaldine	383.15	352.59	519.65	a	5.22	2.28	2.39	386.45	385.48	3.30	2.33
000091-66-7	N,N-Diethylaniline	358.15	358.15	489.45	a	5.32	2.08	2.12	362.86	359.02	4.71	0.87
000092-06-8	m-Terphenyl	464.00	464.00	636.15	a	5.63	1.20	1.33	472.95	466.91	8.95	2.91
000092-51-3	Bicyclohexyl	358.15	347.15	511.15	a	5.41	1.44	1.91	359.00	367.58	0.85	9.43
000092-52-4	Biphenyl	383.15	386.00	529.25	a	5.30	1.90	2.18	386.66	389.13	3.51	5.98
000092-67-1	p-Aminodiphenyl	426.15	426.15	575.15	a	5.37	1.70	2.01	454.81	432.59	28.66	6.44
000092-94-4	p-Terphenyl	480.00	480.00	649.15	a	5.63	1.55	1.33	477.17	474.98	-2.83	-5.02
000922-62-3	3-Methyl-cis-2-Pentene	246.15	245.00	340.85	a	5.00	2.79	2.95	238.92	248.74	-7.23	2.59
000925-78-0	3-Nonanone	339.15	339.15	463.15	a	5.40	2.09	1.92	339.41	335.91	0.26	-3.24
000927-49-1	Diamyl Ketone	361.48	361.48	501.15	a	5.57	1.57	1.49	361.41	359.91	-0.07	-1.57
000927-62-8	N,N-Dimethyl-n-Butylamine	270.15	270.15	368.15	a	5.14	2.75	2.60	261.94	267.56	-8.21	-2.59
000093-53-8	2-Phenylpropionaldehyde	342.00	342.00	476.65	a	5.20	1.98	2.45	350.12	351.27	8.12	9.27
000093-54-9	1-Phenyl-1-Propanol	363.15	363.15	492.15	a	5.22	1.85	2.39	373.05	372.93	9.90	9.78
000093-58-3	Methyl Benzoate	352.50	355.15	472.15	a	5.17	2.53	2.53	357.45	352.37	4.95	-0.13
000093-89-0	Ethyl Benzoate	361.15	357.15	485.15	a	5.28	2.36	2.24	366.09	358.78	4.94	-2.37
000930-68-7	2-Cyclohexene-1-one	329.15	330.00	443.15	a	4.92	2.64	3.17	348.28	339.94	19.13	10.79
000939-27-5	2-Ethylnaphthalene	377.15	377.15	531.15	a	5.33	1.74	2.10	374.96	384.96	-2.19	7.81
000095-13-6	Indene	331.15		455.15	a	5.07	2.33	2.77	339.86	339.94	8.71	8.79
000095-15-8	Benzothiophene	364.15	383.15	494.15	a	5.09	2.46	2.72	365.18	369.80	1.03	5.65
000095-47-6	o-Xylene	305.15	290.00	417.65	a	5.06	2.56	2.80	306.28	309.69	1.13	4.54
000095-48-7	o-Cresol	354.00	354.00	464.15	a	5.01	2.88	2.93	351.98	355.15	-2.02	1.15
000095-49-8	o-Chlorotoluene	316.15	324.00	432.15	a	5.06	2.53	2.79	317.78	321.38	1.63	5.23
000095-50-1	o-Dichlorobenzene	339.00	339.00	453.15	a	5.07	2.82	2.79	333.22	338.34	-5.78	-0.66
000095-51-2	o-Chloroaniline	363.71	363.71	481.95	a	5.03	2.79	2.88	365.29	365.70	1.58	1.99
000095-53-4	o-Toluidine	358.15	358.15	473.45	a	5.03	2.76	2.88	359.20	360.59	1.05	2.44
000095-54-5	o-Phenylenediamine	409.00	429.15	530.15	a	5.00	3.09	2.97	398.58	406.16	-10.42	-2.84
000095-57-8	o-Chlorophenol	336.15		448.05	a	5.00	2.92	2.95	331.10	336.82	-5.05	0.67
000095-63-6	1,2,4-Trimethylbenzene	318.65	318.65	442.45	a	5.18	2.32	2.50	313.87	322.14	-4.78	3.49
000095-68-1	2,4-Dimethylaniline	363.15		487.15	a	5.15	2.59	2.57	357.67	362.90	-5.48	-0.25
000095-73-8	2,4-Dichlorotoluene	352.15	369.26	474.15	a	5.18	2.62	2.50	345.24	349.57	-6.91	-2.58
000095-76-1	3,4-Dichloroaniline	408.15	439.00	545.15	a	5.15	2.44	2.57	412.48	411.18	4.33	3.03
000095-87-4	2,5-Xylenol	368.15	360.00	484.25	a	5.13	2.85	2.62	356.51	363.43	-11.64	-4.72
000095-92-1	Diethyl Oxalate	348.15	339.25	458.85	a	5.26	2.71	2.29	337.66	340.10	-10.49	-8.05
000095-93-2	1,2,4,5-Tetramethylbenzene	346.15	328.00	469.95	a	5.26	2.62	2.28	327.61	338.99	-18.54	-7.16

000096-18-4	1,2,3-Trichloropropane	347.00	347.00	430.15	a	5.02	4.02	2.90	321.43	323.19	-25.57	-23.81
000096-22-0	3-Pentanone	280.15	286.00	375.05	a	4.95	2.94	3.08	282.42	282.51	2.27	2.36
000096-23-1	1,3-Dichloro-2-Propanol	358.15	358.15	449.15	a	4.96	3.79	3.06	334.40	342.50	-23.75	-15.65
000096-29-7	2-Butoxime	335.15		425.65	a	4.92	3.05	3.17	334.34	337.43	-0.81	2.28
000096-31-1	1,3-Dimethyl Urea	430.15		542.15	a	4.89	3.52	3.24	423.75	423.45	-6.40	-6.70
000096-33-3	Methyl Acrylate	270.00	270.00	353.35	a	4.86	3.09	3.31	278.49	273.69	8.49	3.69
000096-34-4	Methyl Chloroacetate	324.82	324.82	402.65	a	4.90	3.80	3.22	320.19	313.75	-4.63	-11.07
000096-48-0	gamma-Butyrolactone	367.15		477.15	a	4.77	3.46	3.55	363.55	369.20	-3.60	2.05
000096-49-1	Ethylene Carbonate	425.00		521.15	a	4.70	4.32	3.72	397.03	408.11	-27.97	-16.89
000096-54-8	N-Methylpyrrole	288.15	288.15	388.15	a	4.85	2.79	3.35	303.12	298.45	14.97	10.30
000097-00-7	1-Chloro-2,4-Dinitrobenzene	467.00	467.00	588.15	a	5.26	3.54	2.27	428.68	434.19	-38.32	-32.81
000097-62-1	Ethyl Isobutyrate	287.00	287.00	383.25	a	5.15	2.68	2.56	294.81	285.05	7.81	-1.95
000097-63-2	Ethyl Methacrylate	292.15	293.15	390.15	a	5.12	2.84	2.65	285.26	288.75	-6.89	-3.40
000097-64-3	Ethyl Lactate	331.00		427.15	a	5.09	3.31	2.72	320.41	319.58	-10.59	-11.42
000097-72-3	Isobutyric Anhydride	340.15		456.15	a	5.36	2.41	2.04	344.32	333.38	4.17	-6.77
000097-85-8	Isobutyl Isobutyrate	311.15	311.15	421.75	a	5.34	2.38	2.07	311.62	305.76	0.47	-5.39
000097-86-9	Isobutyl Methacrylate	314.15	314.15	428.15	a	5.31	2.29	2.15	315.82	311.60	1.67	-2.55
000097-88-1	n-Butyl Methacrylate	322.00	322.00	433.15	a	5.34	2.43	2.09	323.25	315.91	1.25	-6.09
000097-95-0	2-Ethyl-1-Butanol	326.15	330.00	420.15	a	5.08	2.67	2.76	323.13	327.60	-3.02	1.45
000097-99-4	Tetrahydrofurfuryl Alcohol	343.15	343.15	451.15	a	4.95	2.86	3.09	340.40	347.55	-2.75	4.40
000098-00-0	Furfuryl Alcohol	348.15	338.15	444.15	a	4.90	2.82	3.21	360.65	355.22	12.50	7.07
000098-01-1	Furfural	333.15	333.15	434.85	a	4.85	3.05	3.34	342.84	338.89	9.69	5.74
000098-06-6	tert-Butylbenzene	317.15	333.15	442.25	a	5.24	1.95	2.34	325.18	324.30	8.03	7.15
000098-07-7	Benzotrichloride	364.00	354.00	494.15	a	5.25	2.29	2.31	360.75	364.31	-3.25	0.31
000098-08-8	Benzotrifluoride	285.00	285.00	375.25	a	5.08	3.13	2.76	285.72	278.37	0.72	-6.63
000098-13-5	Phenyltrichlorosilane	364.15		474.15	a	5.33	2.98	2.10	347.69	346.38	-16.46	-17.77
000098-29-3	p-tert-Butylcatechol	425.00	403.00	558.15	a	5.33	2.58	2.11	410.57	414.86	-14.43	-10.14
000098-46-4	3-Nitrobenzotrifluoride	361.00	361.00	475.95	a	5.23	2.81	2.36	359.71	351.85	-1.29	-9.15
000098-54-4	p-tert-Butylphenol	386.00	386.00	510.15	a	5.29	2.46	2.21	377.81	381.10	-8.19	-4.90
000098-55-5	alpha-Terpineol	364.00	367.15	493.15	a	5.33	1.98	2.10	357.78	366.29	-6.22	2.29
000098-56-6	p-Chlorobenzotrifluoride	316.00	316.00	411.65	a	5.19	3.19	2.47	307.82	302.41	-8.18	-13.59
000098-82-8	Cumene	309.15	304.15	425.55	a	5.17	2.29	2.51	313.58	313.22	4.43	4.07
000098-83-9	alpha-Methylstyrene	315.65	313.15	438.55	a	5.14	2.12	2.59	323.07	324.41	7.42	8.76
000098-85-1	alpha-Methylbenzyl Alcohol	358.15		478.15	a	5.13	1.97	2.63	371.67	369.80	13.52	11.65
000098-86-2	Acetophenone	350.15	355.37	475.15	a	5.09	2.39	2.72	358.51	356.80	8.36	6.65
000098-87-3	Benzyl Dichloride	361.15	353.00	478.15	a	5.18	2.75	2.49	358.85	355.80	-2.30	-5.35
000098-88-4	Benzoyl Chloride	345.00	345.00	470.35	a	5.10	2.33	2.71	356.03	352.72	11.03	7.72
000098-95-3	Nitrobenzene	361.00	361.00	483.95	a	5.01	2.71	2.94	366.25	365.90	5.25	4.90
000099-08-1	m-Nitrotoluene	375.00	375.00	505.15	a	5.13	2.60	2.62	374.85	375.57	-0.15	0.57
000099-09-2	m-Nitroaniline	469.15	472.15	579.15	a	5.09	3.76	2.72	448.12	442.12	-21.03	-27.03
000099-54-7	1,2-Dichloro-4-Nitrobenzene	396.15	396.15	528.65	a	5.22	2.53	2.38	390.87	392.94	-5.28	-3.21
000099-62-7	m-Diisopropylbenzene	349.82	349.82	476.35	a	5.44	2.24	1.82	340.48	341.74	-9.34	-8.08

000099-63-8	Isophthaloyl Chloride	453.15	453.15	549.15	a	5.32	4.15	2.14	397.78	402.71	-55.37	-50.44
000099-65-0	m-Dinitrobenzene	423.15	423.15	564.15	a	5.17	2.62	2.51	420.21	420.50	-2.94	-2.65
000099-75-2	Methyl para-Toluate	363.71	363.71	493.15	a	5.27	2.23	2.26	370.21	364.35	6.50	0.64
000099-83-2	alpha-Phellandrene	322.00	322.00	445.15	a	5.28	2.16	2.22	320.08	323.12	-1.92	1.12
000099-85-4	gamma-Terpinene	325.65	324.15	456.15	a	5.30	2.00	2.19	323.37	329.29	-2.28	3.64
000099-86-5	alpha-Terpinene	319.15	319.15	448.15	a	5.30	2.03	2.19	316.03	322.20	-3.12	3.05
000099-87-6	p-Cymene	320.15	320.00	450.25	a	5.28	1.88	2.24	324.11	326.87	3.96	6.72
000099-99-0	p-Nitrotoluene	379.00	379.00	511.45	a	5.13	2.52	2.63	382.78	381.24	3.78	2.24
000994-05-8	Methyl tert-Pentyl Ether	262.15	262.15	359.45	a	5.06	2.71	2.81	260.02	263.75	-2.13	1.60
000999-97-3	Hexamethyldisilazane	284.15	281.15	398.15	a	5.43	2.38	1.86	265.29	275.11	-18.86	-9.04
000102-76-1	Glyceryl Triacetate	411.00	411.00			5.58	0.47	1.47	431.18	431.80	20.18	20.80
000107-52-8	Tetradecamethylhexasiloxane	375.15	375.15			6.26	-0.93	-0.30	384.54	385.62	9.39	10.47
000109-43-3	Dibutyl Sebacate	470.15	451.15			6.07	-0.93	0.20	491.72	492.79	21.57	22.64
000111-01-3	Squalane	490.00	490.00			6.41	-2.16	-0.67	515.17	516.45	25.17	26.45
000123-95-5	Butyl Stearate	433.15	433.15			6.21	-3.05	-0.16	481.80	482.90	48.65	49.75
002652-13-3	Eicosamethylnonasiloxane	432.04	432.04			6.60	-2.60	-1.18	454.75	456.17	22.71	24.13
027554-26-3	Diisooctyl Phthalate	505.15	504.00			6.21	-1.82	-0.16	537.40	538.67	32.25	33.52
000541-01-5	Hexadecamethylheptasiloxane	406.15	406.15			6.40	-1.00	-0.66	410.83	412.05	4.68	5.90
000556-68-3	Hexadecamethylcyclooctasiloxane	405.00	405.00			6.37	-2.89	-0.59	444.40	445.67	39.40	40.67
000084-66-2	Diethyl Phthalate	423.15	390.15			5.58	0.48	1.46	443.34	443.96	20.19	20.81
000084-69-5	Diisobutyl Phthalate	444.50	434.15			5.82	-0.07	0.83	462.51	463.41	18.01	18.91
000084-74-2	Di-n-Butyl Phthalate	444.26	430.15			5.84	-0.43	0.78	468.16	469.07	23.90	24.81
000100-01-6	p-Nitroaniline	486.15	472.15			5.09	2.11	2.72	501.88	501.99	15.73	15.84
000100-10-7	p-Dimethylaminobenzaldehyde	420.15	420.15			5.27	1.57	2.27	436.09	436.36	15.94	16.21
010075-38-4	1,3-Dichloro-trans-2-Butene	300.15	300.15			5.02	2.88	2.91	300.66	300.66	0.51	0.51
000101-68-8	Diphenylmethane-4,4'-Diisocyanate	472.00	474.15			5.67	1.74	1.23	459.69	460.43	-12.31	-11.57
000102-01-2	Acetoacetanilide	423.15	423.15			5.39	0.69	1.96	450.77	451.21	27.62	28.06
000102-36-3	3,4-Dichlorophenyl Isocyanate	383.15	386.00			5.26	2.96	2.28	368.44	368.68	-14.71	-14.47
010486-19-8	Tridecanal	386.00	390.00			5.72	1.22	1.11	383.26	383.90	-2.74	-2.10
000106-20-7	Di-2-Ethylhexylamine	401.15	405.00			5.88	1.14	0.70	392.12	392.91	-9.03	-8.24
000106-51-4	Quinone	350.15				4.92	2.55	3.16	363.00	362.89	12.85	12.74
010605-40-0	(3-Chloropropyl)Dimethylchlorosilane	313.15				5.33	1.99	2.11	315.08	315.38	1.93	2.23
001066-35-9	Dimethylchlorosilane	245.15				4.89	4.35	3.25	227.05	226.94	-18.10	-18.21
001067-53-4	Tris(2-Methoxyethoxy)Vinylsilane	388.15				5.85	-0.99	0.77	419.70	420.50	31.55	32.35
000107-89-1	Acetaldol	355.93	339.00			4.86	4.52	3.32	330.86	330.70	-25.07	-25.23
000107-96-0	3-Mercaptopropionic Acid	366.15				4.91	2.18	3.20	385.82	385.68	19.67	19.53
000108-29-2	gamma-Valerolactone	369.26				4.92	3.38	3.16	364.18	364.05	-5.08	-5.21
000108-57-6	m-Divinylbenzene	340.15	338.00			5.23	2.27	2.35	341.54	341.75	1.39	1.60
000110-06-5	Di-tert-Butyl Disulfide	335.15	337.15			5.40	1.38	1.93	344.77	345.13	9.62	9.98
000110-27-0	Isopropyl Myristate	424.50	423.00			5.97	-0.09	0.44	433.57	434.50	9.07	10.00
000110-33-8	Dihexyl Adipate	464.00	464.00			6.07	-0.60	0.20	478.52	479.57	14.52	15.57

000110-99-6	Diglycolic Acid	500.00	500.00			5.02	2.96	2.92	499.02	499.02	-0.98	-0.98
000111-20-6	Sebacic Acid	493.15	496.00			5.58	2.92	1.45	462.60	463.17	-30.55	-29.98
000112-44-7	Undecanal	366.00	369.15			5.57	1.74	1.48	360.42	360.94	-5.58	-5.06
000112-47-0	Decan-1,10-Diol	425.15	425.15			5.56	1.13	1.51	431.11	431.55	5.96	6.40
000112-54-9	Dodecanal	374.15	374.15			5.65	0.81	1.29	382.75	383.38	8.60	9.23
001123-85-9	2-Phenyl-1-Propanol	381.15	366.15			5.21	2.66	2.41	376.07	376.26	-5.08	-4.89
000115-77-5	Pentaerythritol	533.15	533.15			5.07	5.82	2.77	456.02	456.07	-77.13	-77.08
000117-84-0	Dioctyl Phthalate	489.00				6.23	-2.82	-0.21	538.16	539.44	49.16	50.44
001190-76-7	Cis-Crotonitrile	288.65	285.00			4.77	3.14	3.56	296.94	296.67	8.29	8.02
001195-14-8	2-Methyl Benzothiophene	386.15	386.15			5.21	2.92	2.42	374.95	375.16	-11.20	-10.99
000123-18-2	2,6,8-Trimethyl-4-Nonanone	364.15	356.00			5.58	1.80	1.45	357.04	357.59	-7.11	-6.56
000123-79-5	Dioctyl Adipate	500.15	500.15			6.24	-0.94	-0.24	512.67	513.88	12.52	13.73
000123-99-9	Azelaic Acid	488.15	492.00			5.51	2.30	1.65	473.45	473.96	-14.70	-14.19
000131-17-9	Diallyl Phthalate	431.15				5.70	0.08	1.16	452.73	453.47	21.58	22.32
000141-82-2	Malonic Acid	474.82	496.00			4.81	4.31	3.44	454.19	453.94	-20.63	-20.88
000143-07-7	Dodecanoic Acid	437.00	430.00			5.68	1.92	1.20	422.17	422.79	-14.83	-14.21
001446-61-3	Dehydroabietylamine	464.00				5.79	0.64	0.93	469.47	470.28	5.47	6.28
014814-09-6	[3-(mercapto)propyl]triethoxysilane	360.93	360.93			5.73	-0.36	1.08	385.65	386.30	24.72	25.37
148462-57-1	2-Propanol-1-Methoxy-Propanoate	327.15				5.32	1.76	2.13	333.82	334.06	6.67	6.91
000149-31-5	2-Methyl-1,3-Pentanediol	383.15	394.00			5.12	2.30	2.64	389.01	389.13	5.86	5.98
001559-35-9	Ethylene Glycol 2-Ethylhexyl Ether	371.15	383.15			5.54	2.39	1.57	355.40	355.86	-15.75	-15.29
015798-64-8	cis-Crotonaldehyde	285.93	281.15			4.76	3.27	3.56	291.48	291.23	5.55	5.30
001638-16-0	Tripropylene Glycol	413.15				5.48	2.79	1.71	388.92	389.42	-24.23	-23.73
017689-77-9	Ethylsilanetriol Triacetate	377.15				5.58	0.31	1.46	399.27	399.87	22.12	22.72
018328-90-0	N-Ethyl-2-Methylallylamine	280.15	280.15			5.12	2.89	2.65	276.04	276.09	-4.11	-4.06
018912-81-7	2-(2-Pentoxyethoxy)Ethanol	383.00	383.00			5.54	1.94	1.56	375.25	375.75	-7.75	-7.25
021282-97-3	2-Acetoacetoxy Ethyl Methacrylate	407.05	407.05			5.59	0.31	1.45	429.05	429.68	22.00	22.63
021460-36-6	Propylene Glycol Monoallyl Ether	327.55				5.16	2.98	2.56	319.58	319.68	-7.97	-7.87
002163-42-0	2-Methyl-1,3-Propanediol	393.50	386.00			4.89	3.65	3.24	385.79	385.65	-7.71	-7.85
002274-11-5	Ethylene Glycol Diacrylate	373.15	373.15			5.40	1.61	1.93	379.03	379.40	5.88	6.25
002425-74-3	tert-Butylformamide	355.15	368.15			5.00	2.58	2.96	362.74	362.73	7.59	7.58
002471-08-1	Hexacosamethyldodecasiloxane	471.00	471.00			6.88	-4.94	-1.88	519.92	521.60	48.92	50.60
025103-58-6	tert-Dodecyl Mercaptan	370.15	363.15			5.68	0.45	1.19	383.01	383.64	12.86	13.49
002530-83-8	[3-(2,3-Epoxyproxy)Propyl]Trimethoxy Silane	408.15				5.67	2.09	1.22	389.73	390.36	-18.42	-17.79
025360-10-5	tert-Nonyl Mercaptan	338.15	338.15			5.45	1.71	1.79	339.35	339.73	1.20	1.58
025498-49-1	Tripropylene Glycol Monomethyl Ether	394.15	384.00			5.55	1.89	1.54	386.30	386.82	-7.85	-7.33
026438-27-7	1-n-Decylnaphthalene	450.15	458.00			5.89	0.19	0.65	458.30	459.18	8.15	9.03
026472-00-4	Methylcyclopentadiene Dimer	326.15				5.33	1.11	2.11	344.44	344.74	18.29	18.59
002768-02-7	Vinyltrimethoxysilane	296.15	295.85			5.27	3.01	2.27	283.05	283.25	-13.10	-12.90
002935-90-2	Methyl-3-Mercaptopropionate	333.15				5.06	2.45	2.81	340.08	340.15	6.93	7.00

029911-27-1	Dipropylene Glycol n-Propyl Ether	361.15	370.93			5.47	1.58	1.74	363.84	364.26	2.69	3.11
029911-28-2	Dipropylene Glycol n-Butyl Ether	373.55				5.56	1.48	1.51	373.56	374.11	0.01	0.56
030025-38-8	Dipropylene Glycol Monoethyl Ether	364.00	364.00			5.38	2.36	1.96	355.70	356.06	-8.30	-7.94
030453-31-7	Ethyl Propyl Disulfide	325.65	324.00			5.23	2.77	2.35	317.66	317.84	-7.99	-7.81
003068-00-6	1,2,4-Butanetriol	461.00	440.00			4.93	4.93	3.15	419.91	419.83	-41.09	-41.17
003228-02-2	1-Methyl-3-Hydroxy-6-Isopropyl Benzene	392.00	378.00			5.30	2.83	2.17	378.70	378.97	-13.30	-13.03
003268-49-3	3-(Methylmercapto)Propanal	334.15	334.15			5.00	3.24	2.95	328.52	328.47	-5.63	-5.68
003377-92-2	Vinyl Pivalate	282.15	282.15			5.20	2.02	2.45	289.06	289.23	6.91	7.08
034885-03-5	4-Methyl-Cyclohexane-Methanol	354.00				5.20	2.01	2.45	361.41	361.56	7.41	7.56
037143-54-7	3-Methoxyisopropylamine	281.15	281.15			4.96	2.87	3.05	284.04	284.01	2.89	2.86
003913-02-8	2-Butyl-Octan-1-ol	382.15	382.15			5.64	1.18	1.29	383.49	384.00	1.34	1.85
004098-71-9	Isophorone Diisocyanate	428.15	383.15			5.56	2.84	1.50	398.24	398.83	-29.91	-29.32
004454-05-1	Methoxydihydropyran	299.15	289.15			5.03	2.19	2.87	311.69	311.71	12.54	12.56
004536-23-6	2-Methylhexanoic Acid	370.65	375.00			5.24	3.25	2.35	354.25	354.44	-16.40	-16.21
055505-26-5	8-Methyl-1-Nonanol	370.65	377.59			5.50	1.45	1.66	373.76	374.18	3.11	3.53
000556-52-5	2,3-Epoxy-1-Propanol	344.15	344.15			4.71	4.29	3.71	333.07	332.81	-11.08	-11.34
000556-69-4	Octadecamethyloctasiloxane	417.15	417.15			6.49	-1.70	-0.89	429.79	431.08	12.64	13.93
057018-52-7	Propylene Glycol 1-tert-Butyl Ether	318.15	317.15			5.24	1.80	2.33	327.52	327.74	9.37	9.59
000582-24-1	2-Hydroxyacetophenone	371.15				5.14	1.74	2.59	388.91	389.05	17.76	17.90
000589-35-5	3-Methyl-1-Pentanol	331.15	331.15			5.09	2.66	2.72	332.02	332.08	0.87	0.93
000589-82-2	3-Heptanol	327.15				5.23	2.12	2.37	330.88	331.02	3.73	3.87
000592-98-3	cis-3-Octene	290.00	290.00			5.26	3.09	2.28	275.75	275.96	-14.25	-14.04
000599-64-4	p-Cumylphenol	444.00	433.00			5.53	1.43	1.58	446.84	447.39	2.84	3.39
000603-35-0	Triphenylphosphine	453.15	453.15			5.69	0.53	1.17	466.38	467.13	13.23	13.98
006196-58-3	2-Pentoxyethanol	348.15	347.00			5.31	2.54	2.16	341.08	341.33	-7.07	-6.82
000624-22-6	2-Methyl-1-Hexanol	333.65	333.00			5.22	2.06	2.40	338.91	339.04	5.26	5.39
000068-11-1	Thioglycolic Acid	399.15	398.00			4.75	4.34	3.59	382.90	382.60	-16.25	-16.55
006846-50-0	2,2,4-Trimethyl-1,3-Pentanediol Diisobutyrate	394.00	394.00			5.85	-0.33	0.76	413.76	414.62	19.76	20.62
006881-94-3	Diethylene Glycol Monopropyl Ether	372.00	372.00			5.37	2.85	2.00	355.31	355.64	-16.69	-16.36
000069-72-7	Salicylic Acid	430.00	430.00			5.07	4.26	2.78	396.41	396.47	-33.59	-33.53
000693-23-2	Dodecanedioic Acid	503.00				5.73	1.79	1.09	487.53	488.24	-15.47	-14.76
000706-31-0	1,5,9-Cyclododecatriene	360.15	360.15			5.37	1.50	1.99	369.61	369.99	9.46	9.84
000075-91-2	t-Butyl Hydroperoxide	299.82				4.90	2.35	3.21	313.15	313.08	13.33	13.26
075899-69-3	Tripropylene Glycol Monoethyl Ether	405.00	405.00			5.64	1.60	1.31	398.41	399.00	-6.59	-6.00
000762-75-4	tert-Butyl Formate	264.15				4.99	2.57	2.97	270.82	270.80	6.67	6.65
000766-90-5	cis-1-Propenylbenzene	320.65	311.00			5.15	2.33	2.57	325.07	325.18	4.42	4.53
000077-79-2	Sulfolene	386.00				4.92	1.32	3.16	426.38	426.22	40.38	40.22
000078-01-3	1,1-Diethylcyclohexane	322.15	322.15			5.28	2.73	2.25	312.83	313.09	-9.32	-9.06
000080-05-7	Bisphenol A	500.15	480.15			5.57	1.73	1.49	493.96	494.55	-6.19	-5.60
000080-15-9	Cumene Hydroperoxide	356.15				5.25	1.40	2.31	373.05	373.25	16.90	17.10
000821-11-4	trans-2-Butene-1,4-Diol	401.15	401.15			4.90	2.96	3.21	405.93	405.83	4.78	4.68

000828-00-2	Acetomethoxane	356.15	325.15			5.37	0.30	2.00	388.59	388.97	32.44	32.82
000084-75-3	Di-n-Hexyl Phthalate	466.15	466.15			6.06	-1.66	0.23	502.20	503.28	36.05	37.13
000868-77-9	2-Hydroxyethyl Methacrylate	374.15	370.15			5.17	3.12	2.51	362.13	362.28	-12.02	-11.87
000919-31-3	3-(Triethoxysilyl)Propionitrile	373.15				5.66	0.47	1.26	387.63	388.26	14.48	15.11
000923-26-2	2-Hydroxypropyl Methacrylate	374.15	369.15			5.27	3.23	2.26	354.68	354.91	-19.47	-19.24
000093-96-9	Bis(alpha-Methylbenzyl) Ether	408.15				5.64	0.34	1.30	427.18	427.84	19.03	19.69
000094-28-0	Triethylene Glycol bis(2-Ethylhexanoate)	480.15				6.26	-3.36	-0.30	536.98	538.27	56.83	58.12
000096-05-9	Allyl Methacrylate	306.15	306.15			5.21	2.12	2.42	311.34	311.51	5.19	5.36
000099-93-4	4-Hydroxyacetophenone	447.00				5.15	2.45	2.58	449.50	449.62	2.50	2.62
000999-61-1	2-Hydroxypropyl Acrylate	372.15	372.15			5.18	3.21	2.48	357.82	357.95	-14.33	-14.20
000999-61-1	2-Hydroxypropyl Acrylate	372.15	372.15			5.18	3.21	2.48	357.82	357.95	-14.33	-14.20

a) PhysProp, b) http://www.chemicalbook.com, c) GESTIS-Stoffdatenbank http://www.dguv.de/ifa/Gefahrstoffdatenbanken/GESTIS-Stoffdatenbank/index.jsp, d) http://www.chemicalland21.com, e) http://www.inchem.org/, f) http://www.sigmaaldrich.com,
g) NIST, http://webbook.nist.gov/chemistry/

Table S4. Mixture data

octane / ethanol											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.00	1.000	286.15	no LLE	286.15	286.15	286.15	286.15	0.0	0.0	0.0	0.0
0.01	0.990	284.85	no LLE	283.85	283.85	283.85	283.35	-1.0	-1.0	-1.0	-1.5
0.02	0.980	282.65	no LLE	282.15	282.15	282.15	282.15	-0.5	-0.5	-0.5	-0.5
0.03	0.970	282.25	no LLE	281.25	280.75	280.75	280.75	-1.0	-1.5	-1.5	-1.5
0.05	0.950	280.65	no LLE	279.15	278.65	279.15	279.15	-1.5	-2.0	-1.5	-1.5
0.10	0.900	278.75	no LLE	277.25	276.75	276.75	276.75	-1.5	-2.0	-2.0	-2.0
0.20	0.800	277.95	no LLE	275.95	275.95	275.95	275.95	-2.0	-2.0	-2.0	-2.0
0.30	0.700	277.95	no LLE	275.95	275.95	275.95	275.95	-2.0	-2.0	-2.0	-2.0
0.40	0.600	277.95	no LLE	276.45	276.45	276.45	276.45	-1.5	-1.5	-1.5	-1.5
0.50	0.500	277.85	no LLE	276.35	276.35	276.35	276.35	-1.5	-1.5	-1.5	-1.5
0.60	0.400	277.95	no LLE	276.45	276.45	276.45	276.45	-1.5	-1.5	-1.5	-1.5
0.70	0.300	278.15	no LLE	276.15	276.15	276.15	276.15	-2.0	-2.0	-2.0	-2.0
0.80	0.200	278.35	no LLE	275.85	275.85	275.85	275.85	-2.5	-2.5	-2.5	-2.5
0.90	0.100	278.35	no LLE	275.85	275.85	275.85	275.85	-2.5	-2.5	-2.5	-2.5

0.95	0.050	279.05	no LLE	276.05	276.55	276.55	276.55	-3.0	-2.5	-2.5	-2.5
0.96	0.040	279.65	no LLE	276.65	277.15	277.15	277.15	-3.0	-2.5	-2.5	-2.5
0.97	0.030	280.75	no LLE	276.75	277.75	277.75	277.75	-4.0	-3.0	-3.0	-3.0
0.98	0.020	281.95	no LLE	277.45	278.45	278.95	278.45	-4.5	-3.5	-3.0	-3.5
0.99	0.010	283.45	no LLE	279.45	280.95	280.95	280.95	-4.0	-2.5	-2.5	-2.5
0.99	0.008	285.25	no LLE	280.25	281.75	281.75	281.75	-5.0	-3.5	-3.5	-3.5
0.99	0.006	285.75	no LLE	281.25	282.75	282.75	282.75	-4.5	-3.0	-3.0	-3.0
1.00	0.005	286.15	no LLE	281.65	283.15	283.15	283.15	-4.5	-3.0	-3.0	-3.0
1.00	0.000	287.65	no LLE	287.65	287.65	287.65	287.65	0.0	0.0	0.0	0.0

octane / heptane											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.00	1.000	267.95	no LLE	267.95	267.95	267.95	267.95	0.0	0.0	0.0	0.0
0.10	0.900	269.45	no LLE	268.95	268.95	268.95	268.95	-0.5	-0.5	-0.5	-0.5
0.20	0.800	270.65	no LLE	270.65	270.65	270.65	270.65	0.0	0.0	0.0	0.0
0.30	0.700	272.15	no LLE	271.65	271.65	271.65	271.65	-0.5	-0.5	-0.5	-0.5
0.40	0.600	273.45	no LLE	273.45	273.45	273.45	273.45	0.0	0.0	0.0	0.0
0.50	0.500	275.25	no LLE	275.25	275.25	275.25	275.25	0.0	0.0	0.0	0.0
0.60	0.400	277.15	no LLE	277.15	277.15	277.15	277.15	0.0	0.0	0.0	0.0
0.70	0.300	279.55	no LLE	279.05	279.05	279.05	279.05	-0.5	-0.5	-0.5	-0.5
0.80	0.200	281.55	no LLE	281.55	281.55	281.55	281.55	0.0	0.0	0.0	0.0
0.90	0.100	284.25	no LLE	284.25	284.25	284.25	284.25	0.0	0.0	0.0	0.0
1.00	0.000	287.65	no LLE	287.65	287.65	287.65	287.65	0.0	0.0	0.0	0.0

octane / 1-butanol											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.000	1.000	310.05	no LLE	310.05	310.05	310.05	310.05	0.0	0.0	0.0	0.0
0.025	0.975	304.65	no LLE	303.65	303.65	303.65	303.65	-1.0	-1.0	-1.0	-1.0
0.050	0.950	300.85	no LLE	299.85	299.35	299.35	299.35	-1.0	-1.5	-1.5	-1.5
0.100	0.900	295.95	no LLE	294.45	294.45	294.45	294.45	-1.5	-1.5	-1.5	-1.5

0.150	0.850	292.85	no LLE	291.35	291.35	291.35	291.35	-1.5	-1.5	-1.5	-1.5
0.200	0.800	290.95	no LLE	291.85	289.45	289.45	289.95	0.9	-1.5	-1.5	-1.0
0.300	0.700	288.75	no LLE	289.95	287.75	287.75	287.75	1.2	-1.0	-1.0	-1.0
0.400	0.600	287.65	no LLE	287.75	286.65	287.15	287.15	0.1	-1.0	-0.5	-0.5
0.500	0.500	287.25	no LLE	286.25	286.75	286.75	286.75	-1.0	-0.5	-0.5	-0.5
0.600	0.400	286.85	no LLE	286.35	286.35	286.35	286.35	-0.5	-0.5	-0.5	-0.5
0.700	0.300	286.65	no LLE	286.15	286.65	286.65	286.65	-0.5	0.0	0.0	0.0
0.800	0.200	286.75	no LLE	286.25	286.75	286.75	286.75	-0.5	0.0	0.0	0.0
0.900	0.100	286.95	no LLE	285.95	286.95	286.95	286.95	-1.0	0.0	0.0	0.0
0.950	0.050	286.65	no LLE	286.15	286.65	286.65	286.65	-0.5	0.0	0.0	0.0
1.000	0.000	287.65	no LLE	287.65	287.65	287.65	287.65	0.0	0.0	0.0	0.0

octane / 2-butanol											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.0000	1.000	295.15	no LLE	295.15	295.15	295.15	295.15	0.0	0.0	0.0	0.0
0.0200	0.980	293.65	no LLE	293.15	293.15	293.15	293.15	-0.5	-0.5	-0.5	-0.5
0.0300	0.970	292.15	no LLE	292.15	292.15	292.15	292.15	0.0	0.0	0.0	0.0
0.0500	0.950	291.05	no LLE	290.55	290.55	290.55	290.55	-0.5	-0.5	-0.5	-0.5
0.1000	0.900	288.35	no LLE	287.85	287.85	287.85	287.85	-0.5	-0.5	-0.5	-0.5
0.1200	0.880	287.75	no LLE	287.25	287.25	287.25	287.25	-0.5	-0.5	-0.5	-0.5
0.2000	0.800	286.15	no LLE	285.15	285.15	285.15	285.15	-1.0	-1.0	-1.0	-1.0
0.3000	0.700	285.05	no LLE	284.05	284.05	284.05	284.05	-1.0	-1.0	-1.0	-1.0
0.4000	0.600	284.25	no LLE	283.75	283.75	283.75	283.75	-0.5	-0.5	-0.5	-0.5
0.5000	0.500	284.15	no LLE	283.15	283.15	283.15	283.15	-1.0	-1.0	-1.0	-1.0
0.6000	0.400	283.85	no LLE	283.35	283.85	283.85	283.85	-0.5	0.0	0.0	0.0
0.7000	0.300	283.95	no LLE	282.95	283.95	283.95	283.95	-1.0	0.0	0.0	0.0
0.8000	0.200	283.95	no LLE	283.45	283.95	283.95	283.95	-0.5	0.0	0.0	0.0
0.9000	0.100	284.35	no LLE	283.35	284.35	284.35	284.35	-1.0	0.0	0.0	0.0
0.9500	0.050	284.15	no LLE	284.15	284.15	284.15	284.15	0.0	0.0	0.0	0.0
0.9800	0.020	285.25	no LLE	284.75	285.25	285.25	285.25	-0.5	0.0	0.0	0.0
0.9900	0.010	285.95	no LLE	285.95	285.95	285.95	285.95	0.0	0.0	0.0	0.0

1.0000	0.000	287.65	no LLE	287.65	287.65	287.65	287.65	0.0	0.0	0.0	0.0

octane / isopropanol											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	286.05	no LLE	286.05	286.05	286.05	286.05	0.0	0.0	0.0	0.0
0.020	0.980	284.85	no LLE	283.85	283.85	283.85	283.85	-1.0	-1.0	-1.0	-1.0
0.050	0.950	282.95	no LLE	281.95	281.45	281.95	281.45	-1.0	-1.5	-1.0	-1.5
0.100	0.900	281.15	no LLE	280.15	279.65	279.65	279.65	-1.0	-1.5	-1.5	-1.5
0.200	0.800	279.75	no LLE	278.25	278.25	278.25	278.25	-1.5	-1.5	-1.5	-1.5
0.300	0.700	279.55	no LLE	278.05	278.05	278.05	278.05	-1.5	-1.5	-1.5	-1.5
0.350	0.650	279.65	no LLE	278.15	277.65	278.15	277.65	-1.5	-2.0	-1.5	-2.0
0.400	0.600	279.45	no LLE	277.95	277.95	277.95	277.95	-1.5	-1.5	-1.5	-1.5
0.500	0.500	279.55	no LLE	278.05	278.05	278.05	278.05	-1.5	-1.5	-1.5	-1.5
0.600	0.400	279.85	no LLE	277.85	277.85	277.85	277.85	-2.0	-2.0	-2.0	-2.0
0.700	0.300	279.65	no LLE	277.65	279.65	279.65	279.65	-2.0	0.0	0.0	0.0
0.800	0.200	280.25	no LLE	277.75	280.25	280.25	280.25	-2.5	0.0	0.0	0.0
0.850	0.150	280.85	no LLE	277.85	280.85	280.85	280.85	-3.0	0.0	0.0	0.0
0.900	0.100	281.25	no LLE	278.25	281.25	281.25	281.25	-3.0	0.0	0.0	0.0
0.930	0.070	281.55	no LLE	278.55	281.55	281.55	281.55	-3.0	0.0	0.0	0.0
0.950	0.050	281.65	no LLE	278.65	281.65	281.65	281.65	-3.0	0.0	0.0	0.0
0.970	0.030	282.25	no LLE	279.75	282.25	282.25	282.25	-2.5	0.0	0.0	0.0
0.980	0.020	282.65	no LLE	280.65	282.65	282.65	282.65	-2.0	0.0	0.0	0.0
0.990	0.010	284.05	no LLE	282.05	284.05	284.05	284.05	-2.0	0.0	0.0	0.0
0.995	0.005	285.05	no LLE	284.05	285.05	285.05	285.05	-1.0	0.0	0.0	0.0
1.000	0.000	287.65	no LLE	287.65	287.65	287.65	287.65	0.0	0.0	0.0	0.0

methylacetate / methylacrylate											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	271	no LLE	271.05	271.05	271.05	271.05	0.0	0.0	0.0	0.0
0.100	0.900	270	no LLE	269.25	269.25	269.25	269.75	-1.0	-1.0	-1.0	-0.5

0.200	0.800	268	no LLE	267.75	267.75	267.75	268.25	-0.5	-0.5	-0.5	0.0
0.300	0.700	268	no LLE	266.55	266.55	266.55	266.55	-1.0	-1.0	-1.0	-1.0
0.400	0.600	265	no LLE	264.85	265.35	264.85	265.35	-0.5	0.0	-0.5	0.0
0.500	0.500	264	no LLE	263.85	263.85	263.85	264.35	-0.5	-0.5	-0.5	0.0
0.600	0.400	263	no LLE	262.65	262.65	262.65	263.15	0.0	0.0	0.0	0.5
0.700	0.300	262	no LLE	261.55	261.55	261.55	262.05	0.0	0.0	0.0	0.5
0.800	0.200	261	no LLE	260.75	260.75	260.75	260.75	-0.5	-0.5	-0.5	-0.5
0.900	0.100	260	no LLE	259.65	259.65	259.65	260.15	0.0	0.0	0.0	0.5
1.000	0.000	259	no LLE	258.75	258.75	258.75	258.75	0.0	0.0	0.0	0.0

methanol / methylacrylate											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.000	1.000	271.05	no LLE	271.05	271.05	271.05	271.05	0.0	0.0	0.0	0.0
0.100	0.900	270.55	no LLE	270.55	270.55	270.55	270.55	0.0	0.0	0.0	0.0
0.200	0.800	270.65	no LLE	270.15	270.65	270.65	270.65	-0.5	0.0	0.0	0.0
0.300	0.700	270.65	no LLE	270.65	270.65	270.65	270.65	0.0	0.0	0.0	0.0
0.400	0.600	270.55	no LLE	270.55	271.05	271.05	271.05	0.0	0.5	0.5	0.5
0.500	0.500	270.75	no LLE	271.25	271.75	271.75	271.75	0.5	1.0	1.0	1.0
0.600	0.400	271.25	no LLE	271.75	272.25	272.25	272.25	0.5	1.0	1.0	1.0
0.700	0.300	272.75	no LLE	272.75	273.25	273.25	273.25	0.0	0.5	0.5	0.5
0.800	0.200	273.95	no LLE	274.45	274.95	274.95	274.45	0.5	1.0	1.0	0.5
0.850	0.150	274.65	no LLE	275.15	275.65	276.15	275.65	0.5	1.0	1.5	1.0
0.900	0.100	276.15	no LLE	277.15	277.65	277.65	277.15	1.0	1.5	1.5	1.0
0.950	0.050	278.65	no LLE	279.15	279.65	279.65	279.15	0.5	1.0	1.0	0.5
1.000	0.000	283.15	no LLE	283.15	283.15	283.15	283.15	0.0	0.0	0.0	0.0

isoamylalcohol / isoamylacetate											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.000	1.000	311.95	no LLE	311.95	311.95	311.95	311.95	0.0	0.0	0.0	0.0
0.100	0.900	311.75	no LLE	311.75	311.75	311.75	311.75	0.0	0.0	0.0	0.0

0.200	0.800	311.55	no LLE	312.05	312.05	312.05	311.55	0.5	0.5	0.5	0.0
0.300	0.700	311.45	no LLE	311.95	312.45	312.45	311.95	0.5	1.0	1.0	0.5
0.400	0.600	311.75	no LLE	312.75	312.75	312.75	312.25	1.0	1.0	1.0	0.5
0.500	0.500	311.85	no LLE	312.85	313.35	313.35	312.85	1.0	1.5	1.5	1.0
0.600	0.400	312.15	no LLE	313.65	313.65	313.65	313.15	1.5	1.5	1.5	1.0
0.700	0.300	312.85	no LLE	314.35	314.35	314.35	313.85	1.5	1.5	1.5	1.0
0.800	0.200	313.55	no LLE	315.55	315.55	315.55	315.05	2.0	2.0	2.0	1.5
0.900	0.100	315.75	no LLE	316.75	316.75	316.75	316.25	1.0	1.0	1.0	0.5
1.000	0.000	318.05	no LLE	318.05	318.05	318.05	318.05	0.0	0.0	0.0	0.0

water / n-propanol											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.000	1.000	294.65	no LLE	294.65	294.65	294.65	294.65	0.0	0.0	0.0	0.0
0.100	0.900	296.15	no LLE	296.15	296.15	296.15	295.65	0.0	0.0	0.0	-0.5
0.200	0.800	297.15	no LLE	298.15	297.65	297.65	297.15	1.0	0.5	0.5	0.0
0.300	0.700	298.15	no LLE	300.15	299.65	299.15	298.65	2.0	1.5	1.0	0.5
0.400	0.600	299.15	no LLE	302.15	301.15	301.15	300.65	3.0	2.0	2.0	1.5
0.500	0.500	300.15	no LLE	304.15	302.65	302.65	302.15	4.0	2.5	2.5	2.0
0.600	0.400	301.15	no LLE	306.65	304.15	304.15	303.15	5.5	3.0	3.0	2.0
0.700	0.300	302.15	no LLE	308.65	305.15	305.15	304.15	6.5	3.0	3.0	2.0
0.800	0.200	303.15	no LLE	309.65	305.65	305.65	304.65	6.5	2.5	2.5	1.5
0.900	0.100	304.15	no LLE	310.15	306.15	306.15	305.15	6.0	2.0	2.0	1.0
0.950	0.050	307.15	no LLE	312.15	309.15	309.15	308.15	5.0	2.0	2.0	1.0
0.960	0.040	308.15	no LLE	313.65	311.15	310.65	309.65	5.5	3.0	2.5	1.5
0.970	0.030	313.15	no LLE	316.15	313.65	313.65	312.65	3.0	0.5	0.5	-0.5
0.980	0.020	319.15	no LLE	320.15	319.15	318.65	317.15	1.0	0.0	-0.5	-2.0
0.990	0.010	333.65	no LLE	329.65	330.15	329.65	327.65	-4.0	-3.5	-4.0	-6.0
0.992	0.008	337.15	no LLE	333.65	334.65	333.65	331.65	-3.5	-2.5	-3.5	-5.5
0.993	0.007	340.15	no LLE	336.15	337.15	336.15	334.65	-4.0	-3.0	-4.0	-5.5

iso-propanol

water / isopropanol											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	286.15	no LLE	286.15	286.15	286.15	286.15	0.0	0.0	0.0	0.0
0.100	0.900	287.65	no LLE	287.65	287.65	287.65	287.15	0.0	0.0	0.0	-0.5
0.200	0.800	288.65	no LLE	289.65	289.65	289.65	288.65	1.0	1.0	1.0	0.0
0.300	0.700	289.65	no LLE	291.65	291.65	291.65	291.15	2.0	2.0	2.0	1.5
0.400	0.600	290.65	no LLE	294.65	294.15	294.15	293.15	4.0	3.5	3.5	2.5
0.500	0.500	291.15	no LLE	297.65	297.15	296.65	296.15	6.5	6.0	5.5	5.0
0.600	0.400	291.65	no LLE	300.65	299.65	299.65	298.65	9.0	8.0	8.0	7.0
0.700	0.300	292.15	no LLE	304.15	302.65	302.15	301.15	12.0	10.5	10.0	9.0
0.800	0.200	293.15	no LLE	307.15	304.65	304.65	303.15	14.0	11.5	11.5	10.0
0.900	0.100	295.65	no LLE	309.65	307.15	307.15	305.65	14.0	11.5	11.5	10.0
0.950	0.050	302.15	no LLE	312.65	311.65	311.15	309.65	10.5	9.5	9.0	7.5
0.960	0.040	306.15	no LLE	314.15	313.65	313.15	311.65	8.0	7.5	7.0	5.5
0.970	0.030	308.15	no LLE	316.65	316.65	316.15	314.65	8.5	8.5	8.0	6.5
0.980	0.020	315.65	no LLE	321.15	322.15	321.65	319.65	5.5	6.5	6.0	4.0
0.990	0.010	326.15	no LLE	331.15	333.65	332.65	330.65	5.0	7.5	6.5	4.5
0.995	0.005	341.15	no LLE	344.15	348.15	347.15	344.65	3.0	7.0	6.0	3.5

methanol / octane											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	288.15	Phase 1	288.15	288.15	288.15	288.15	0.0	0.0	0.0	0.0
0.010	0.990	284.65	Phase 1	274.15	277.65	277.65	277.15	-10.5	-7.0	-7.0	-7.5
0.020	0.980	281.45	Phase 1	271.45	273.95	274.45	273.95	-10.0	-7.5	-7.0	-7.5
0.030	0.970	279.55	Phase 1	270.55	272.55	272.55	272.55	-9.0	-7.0	-7.0	-7.0
0.050	0.950	277.65	Phase 1	269.65	271.15	271.15	271.65	-8.0	-6.5	-6.5	-6.0
0.060	0.940	275.45	Phase 1	269.45	270.95	270.95	270.95	-6.0	-4.5	-4.5	-4.5
0.088	0.912	275.25	Phase 1	269.25	270.25	270.25	270.75	-6.0	-5.0	-5.0	-4.5
0.957	0.043	275.25	Phase 2	270.75	270.75	271.25	270.75	-4.5	-4.5	-4.0	-4.5
0.970	0.030	275.45	Phase 2	271.95	272.45	272.45	272.45	-3.5	-3.0	-3.0	-3.0
0.980	0.020	275.85	Phase 2	273.85	274.35	274.35	273.85	-2.0	-1.5	-1.5	-2.0
0.985	0.015	278.15	Phase 2	275.15	275.65	275.65	275.65	-3.0	-2.5	-2.5	-2.5
0.990	0.010	279.65	Phase 2	277.15	277.15	277.15	277.15	-2.5	-2.5	-2.5	-2.5

0.995	0.005	280.55	Phase 2	279.55	279.55	279.55	279.55	-1.0	-1.0	-1.0	-1.0
1.000	0.000	283.15	Phase 2	283.15	283.15	283.15	283.15	0.0	0.0	0.0	0.0

methanol / decane											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	324.95	Phase 1	324.95	324.95	324.95	324.95	0.0	0.0	0.0	0.0
0.010	0.990	305.45	Phase 1	283.95	294.95	294.95	293.95	-21.5	-10.5	-10.5	-11.5
0.020	0.980	291.65	Phase 1	277.65	285.15	285.15	284.65	-14.0	-6.5	-6.5	-7.0
0.030	0.970	288.15	Phase 1	275.15	281.15	281.15	281.15	-13.0	-7.0	-7.0	-7.0
0.040	0.960	285.65	Phase 1	274.15	279.15	279.15	279.65	-11.5	-6.5	-6.5	-6.0
0.050	0.950	284.15	Phase 1	273.65	277.65	277.65	278.15	-10.5	-6.5	-6.5	-6.0
0.990	0.010	282.15	Phase 2	282.15	283.65	283.65	283.15	0.0	1.5	1.5	1.0
1.000	0.000	283.15	Phase 2	283.15	283.15	283.15	283.15	0.0	0.0	0.0	0.0

acetone / decane											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	324.95	Phase 1	324.95	324.95	324.95	324.95	0.0	0.0	0.0	0.0
0.010	0.990	303.15	Phase 1	311.15	302.65	302.15	303.65	8.0	-0.5	-1.0	0.5
0.020	0.980	289.15	Phase 1	300.65	289.15	288.65	290.15	11.5	0.0	-0.5	1.0
0.030	0.970	277.15	Phase 1	292.65	280.65	280.65	281.15	15.5	3.5	3.5	4.0
0.050	0.950	271.15	Phase 1	282.15	270.65	270.65	270.65	11.0	-0.5	-0.5	-0.5
0.100	0.900	260.75	Phase 1	269.25	259.25	259.25	258.75	8.5	-1.5	-1.5	-2.0
0.120	0.880	257.65	Phase 1	266.15	256.65	256.65	256.15	8.5	-1.0	-1.0	-1.5
0.130	0.870	256.65	Phase 1	264.65	255.65	255.65	255.15	8.0	-1.0	-1.0	-1.5
0.980	0.020	253.25	Phase 2	254.75	254.75	254.75	253.25	1.5	1.5	1.5	0.0
0.990	0.010	253.95	Phase 2	254.45	254.45	254.45	253.45	0.5	0.5	0.5	-0.5
0.995	0.005	254.65	Phase 2	254.65	254.65	254.65	253.15	0.0	0.0	0.0	-1.5
1.000	0.000	254.55	Phase 2	254.55	254.55	254.55	254.55	0.0	0.0	0.0	0.0

methanol / 2,2,4-trimethylpentane											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	265	Phase 1	265.05	265.05	265.05	265.05	0.0	0.0	0.0	0.0
0.050	0.950	264	Phase 1	258.65	259.65	259.65	260.15	-5.5	-4.5	-4.5	-4.0
0.980	0.020	267	Phase 2	263.55	263.55	263.55	264.05	-3.0	-3.0	-3.0	-2.5
0.990	0.010	272	Phase 2	269.95	269.95	269.95	270.45	-2.0	-2.0	-2.0	-1.5
0.995	0.005	279	Phase 2	274.85	274.85	274.85	275.35	-4.0	-4.0	-4.0	-3.5

1.000	0.000	283	Phase 2	283.15	283.15	283.15	283.15	0.0	0.0	0.0	0.0

ethanol / tetradecane											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	383.55	Phase 1	383.55	383.55	383.55	383.55	0.0	0.0	0.0	0.0
0.010	0.990	313.65	Phase 1	298.65	309.15	308.65	306.15	-15.0	-4.5	-5.0	-7.5
0.020	0.980	302.55	Phase 1	289.05	294.05	294.05	293.55	-13.5	-8.5	-8.5	-9.0
0.050	0.950	297.45	Phase 1	282.95	284.45	284.45	284.45	-14.5	-13.0	-13.0	-13.0
0.100	0.900	293.15	Phase 1	281.15	281.15	281.65	281.65	-12.0	-12.0	-11.5	-11.5
0.150	0.850	290.75	Phase 1	280.75	280.75	280.75	280.75	-10.0	-10.0	-10.0	-10.0
0.900	0.100	286.15	Phase 2	286.65	286.65	286.65	286.15	0.5	0.5	0.5	0.0
0.950	0.050	286.15	Phase 2	286.65	286.65	286.65	286.15	0.5	0.5	0.5	0.0
0.970	0.030	286.55	Phase 2	286.55	286.55	286.55	286.05	0.0	0.0	0.0	-0.5
1.000	0.000	286.15	Phase 2	286.15	286.15	286.15	286.15	0.0	0.0	0.0	0.0

water / 1-butanol											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	310.05	Phase 1	310.05	310.05	310.05	310.05	0.0	0.0	0.0	0.0
0.100	0.900	311.45	Phase 1	311.45	311.45	311.45	311.45	0.0	0.0	0.0	0.0
0.200	0.800	313.45	Phase 1	313.45	313.45	312.95	312.95	0.0	0.0	-0.5	-0.5
0.300	0.700	314.75	Phase 1	315.25	314.75	314.75	314.25	0.5	0.0	0.0	-0.5
0.400	0.600	315.25	Phase 1	317.25	316.25	316.25	315.75	2.0	1.0	1.0	0.5
0.500	0.500	316.25	Phase 1	319.25	317.75	317.75	317.25	3.0	1.5	1.5	1.0
0.982	0.018	316.85	Phase 2	320.35	320.85	320.85	319.85	3.5	4.0	4.0	3.0
0.983	0.017	317	Phase 2	321.00	321.50	321.50	320.50	4.0	4.5	4.5	3.5
0.985	0.015	318.05	Phase 2	322.05	323.05	322.55	322.05	4.0	5.0	4.5	4.0
0.990	0.010	323.85	Phase 2	326.85	328.85	328.35	327.35	3.0	5.0	4.5	3.5
0.992	0.008	327.35	Phase 2	329.85	332.35	331.85	330.85	2.5	5.0	4.5	3.5
0.993	0.007	328.75	Phase 2	331.75	334.75	334.25	333.25	3.0	6.0	5.5	4.5
0.994	0.006	331.65	Phase 2	334.15	337.65	337.15	336.15	2.5	6.0	5.5	4.5
0.995	0.005	336.75	Phase 2	337.25	341.25	340.75	339.75	0.5	4.5	4.0	3.0
0.996	0.004	341.25	Phase 2	341.25	346.25	345.25	344.25	0.0	5.0	4.0	3.0

water / 2-butanol											
				Pred. FP				Deviation			
x1	x2	FP exp.	LLE	1401	1501	1501(T)	1501(T)P	1401	1501	1501(T)	1501(T)P
0.000	1.000	295.15	Phase 1	295.15	295.15	295.15	295.15	0.0	0.0	0.0	0.0

0.100	0.900	296.45	Phase 1	296.95	296.45	296.45	296.45	0.5	0.0	0.0	0.0
0.200	0.800	298.15	Phase 1	298.65	298.15	298.15	298.15	0.5	0.0	0.0	0.0
0.300	0.700	299.25	Phase 1	300.75	300.25	300.25	300.25	1.5	1.0	1.0	1.0
0.400	0.600	300.25	Phase 1	303.25	302.75	302.75	302.75	3.0	2.5	2.5	2.5
0.970	0.030	305.05	Phase 2	311.55	311.05	311.05	310.55	6.5	6.0	6.0	5.5
0.980	0.020	309.25	Phase 2	314.25	314.75	314.75	314.25	5.0	5.5	5.5	5.0
0.990	0.010	318.85	Phase 2	321.35	323.85	323.35	322.85	2.5	5.0	4.5	4.0
0.993	0.007	324.75	Phase 2	326.25	329.75	328.75	328.75	1.5	5.0	4.0	4.0
0.995	0.005	331.75	Phase 2	331.25	335.75	335.25	334.75	-0.5	4.0	3.5	3.0
0.996	0.004	337.85	Phase 2	335.35	340.35	339.35	338.85	-2.5	2.5	1.5	1.0

water / isobutanol											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.000	1.000	302	Phase 1	301.65	301.65	301.65	301.65	0.0	0.0	0.0	0.0
0.100	0.900	303	Phase 1	303.15	303.15	303.15	302.65	0.0	0.0	0.0	-0.5
0.200	0.800	305	Phase 1	304.75	304.25	304.25	304.25	0.0	-0.5	-0.5	-0.5
0.300	0.700	306	Phase 1	306.45	305.95	305.45	305.45	0.5	0.0	-0.5	-0.5
0.980	0.020	309	Phase 2	306.05	306.55	306.05	306.05	-2.5	-2.0	-2.5	-2.5
0.990	0.010	318	Phase 2	312.70	314.20	314.20	314.70	-5.5	-4.0	-4.0	-3.5
0.995	0.005	330	Phase 2	322.35	325.35	324.85	326.35	-7.5	-4.5	-5.0	-3.5
0.996	0.004	335	Phase 2	325.85	329.85	329.35	330.35	-9.0	-5.0	-5.5	-4.5
0.997	0.003	340	Phase 2	331.15	335.65	335.15	336.65	-8.5	-4.0	-4.5	-3.0

water / 1-pentanol											
				Pred. FP				**Deviation**			
x1	**x2**	**FP exp.**	**LLE**	**1401**	**1501**	**1501(T)**	**1501(T)P**	**1401**	**1501**	**1501(T)**	**1501(T)P**
0.000	1.000	323	Phase 1	322.65	322.65	322.65	322.65	0.0	0.0	0.0	0.0
0.100	0.900	324	Phase 1	324.25	324.25	324.25	323.75	0.0	0.0	0.0	-0.5
0.200	0.800	326	Phase 1	326.25	325.75	325.75	325.25	0.5	0.0	0.0	-0.5
0.300	0.700	328	Phase 1	328.05	327.05	327.05	327.05	0.5	-0.5	-0.5	-0.5
0.996	0.004	332	Phase 2	332.85	335.85	335.85	335.35	1.0	4.0	4.0	3.5
0.997	0.003	339	Phase 2	337.15	341.65	341.15	340.65	-1.5	3.0	2.5	2.0
0.998	0.002	348	Phase 2	345.05	350.55	350.05	349.55	-2.5	3.0	2.5	2.0