CORRELATION AND PREDICTION OF SOLUTE TRANSFER TO CHLOROALKANES FROM BOTH WATER AND THE GAS PHASE

Laura M. Sprunger^a, Sai S. Achi^a, William E. Acree, Jr.^{a*}, Michael H. Abraham^b, Albert J. Leo^c,
and David Hoekman^d

^a Department of Chemistry, 1155 Union Circle Drive #305070, University of North Texas,
Denton, TX 76203-5017 (USA)

^b Department of Chemistry, University College London, 20 Gordon Street,
London, WC1H 0AJ (UK)

^c BioByte Corp., 201 W. Fourth St., Claremont, CA 91711 (USA)

^d David Hoekman Consulting, Inc., 107 NW 82nd, Seattle, WA 97117 (USA)

Abstract

Data have been compiled from the published literature on the partition coefficients of solutes and vapors into chloroform, carbon tetrachloride, dichloromethane and 1-chlorobutane from both water and from the gas phase. The logarithms of the water-to-chloroalkane ($\log P$) and gas-to-chloroalkane partition coefficients ($\log K$) are correlated with the Abraham solvation parameter model. The derived correlations describe the observed $\log P$ and $\log K$ values within standard deviations of about 0.13 to 0.20 log units. For chloroform and carbon tetrachloride, the derived correlations were validated using training set and test set analyses.

KEY WORDS: carbon tetrachloride, chloroform, dichloromethane, 1-chlorobutane, partition coefficients, molecular solute descriptors

* Corresponding author, Tel: +1 940 565 3543; fax: +1 940 565 4318; e-mail address:

acree@unt.edu

1. Introduction

Solvent extraction provides a convenient means for separating and concentrating solutes from mixtures prior to chemical analysis. The method is based on the equilibrium distribution of the analyte(s) and unwanted impurities/interferences between the extraction solvent and sample that is to be analyzed. Large partition coefficients, P , defined as the ratio of the solute's molar concentration in the extraction solvent to that in the analytical sample

$$P = \frac{\text{molar concentration of solute in extraction solvent}}{\text{molar concentration of solute in analytical sample}} \quad (1)$$

favor solute transfer to the extraction solvent, whereas small partition coefficients would keep any unwanted impurities/interferences in the sample solution. Many of the biological and environmental samples involve aqueous solutions. The choice of organic solvent in water-to-solvent extractions is of ongoing importance.

The general solvation method of Abraham [1,2] is one of the more useful approaches for the analysis and prediction of free energies of partition in chemical and biological systems. The method relies on two linear free energy relationships (lfers), one for processes within condensed phases

$$SP = c + e \cdot \mathbf{E} + s \cdot \mathbf{S} + a \cdot \mathbf{A} + b \cdot \mathbf{B} + v \cdot \mathbf{V} \quad (2)$$

and one for processes involving gas-to-condensed phase transfer

$$SP = c + e \cdot \mathbf{E} + s \cdot \mathbf{S} + a \cdot \mathbf{A} + b \cdot \mathbf{B} + l \cdot \mathbf{L} \quad (3)$$

The dependent variable, SP, is some property of a series of solutes in a fixed phase, which in the present study will be the logarithm of solute partition coefficient between two immiscible (or partly miscible) phases. The independent variables, or descriptors, are solute properties as follows: **E** and **S** refer to the excess molar refraction and dipolarity/polarizability descriptors of the solute, respectively, **A** and **B** are measures of the solute hydrogen-bond acidity and basicity, **V** is the McGowan volume of the solute and **L** is the logarithm of the solute gas phase dimensionless Ostwald partition coefficient into hexadecane at 298 K. The first four descriptors can be regarded as measures of the tendency of the given solute to undergo various solute-solvent interactions. The latter two descriptors, **V** and **L**, are both measures of solute size, and so will be measures of the solvent cavity term that will accommodate the dissolved solute. General dispersion interactions are also related to solute size, hence, both **V** and **L** will also describe the general solute-solvent interactions. The regression coefficients and constants (*c*, *e*, *s*, *a*, *b*, *v*, and *l*) are obtained by regression analysis of experimental data for a specific process (*i.e.*, a given partitioning process, a given stationary phase and mobile phase combination, *etc.*). In the case of partition coefficients, where two solvent phases are involved, the *c*, *e*, *s*, *a*, *b*, *v* and *l* coefficients represent differences in solvent phase properties. For any fully characterized system/process (those with calculated values for the equation coefficients) further values of SP can be estimated for solutes with known values for the solute descriptors. This is the major advantage in using Eqns. 2 and 3 to correlate solute properties having environmental, pharmaceutical and chemical importance.

At present we are developing/updating correlations for additional/existing systems [3-13], and are developing new computation methodologies for calculating solute descriptors from available experimental data and/or structural information [2,14-18]. To date we have published

Abraham model correlations for describing both the water-to-organic solvent partition coefficient (see Eqn. 1) and the gas-to-solvent partition coefficient, K ,

$$K = \frac{\text{molar concentration of solute in extraction solvent}}{\text{molar concentration of solute in the gas phase}} \quad (4)$$

where K is the dimensionless gas-to-water partition coefficient (with concentrations in each phase defined in terms of mol dm^{-3}) for more than 50 different common organic solvents. For several solvents, the published correlations include both the “practical” log P correlation where the solute is distributed between the equilibrium organic phase saturated with water and the aqueous phase that has been saturated with the organic solvent, as well as the “hypothetical” log P correlation that is calculated as the molar solubility ratio of the solute in the anhydrous organic solvent divided by the solute’s molar solubility in water. Even though hypothetical, these latter log P correlations are still quite useful in that calculated log P values can be used to predict the solute’s infinite dilution activity coefficient or molar solubility in the anhydrous (dry) solvent for those solutes for which the solute descriptors are known.

The aim of the present work is to collect experimental data from the published literature on the partition coefficients from water and from air into chloroform, carbon tetrachloride, dichloromethane and 1-chlorobutane, and to derive log P and log K correlations. Abraham model correlations have been previously reported for several of the solvents based on much smaller databases. Abraham *et al.* [19] published correlations for water-to-chloroform

$$\text{Log } P_{\text{chl}} = 0.327 + 0.157 \text{ E} - 0.391 \text{ S} - 3.191 \text{ A} - 3.437 \text{ B} + 4.191 \text{ V} \quad (5)$$

$$(N = 335, \text{SD} = 0.25, R^2 = 0.971, F = 2223)$$

and for gas-to-chloroform partition coefficients

$$\text{Log } K_{\text{chl}} = 0.168 - 0.595 \text{ E} + 1.256 \text{ S} + 0.280 \text{ A} + 1.370 \text{ B} + 0.981 \text{ L} \quad (6)$$

$$(N = 150, \text{SD} = 0.23, R^2 = 0.985, F = 1919)$$

where N is the number of data points, SD denotes the standard deviation, R^2 gives the squared correlation coefficient and F corresponds to the Fisher's F statistic. The present study differs from that of Abraham *et al.* in that we are using much larger data bases (394 log P values and 384 log K values), and are using revised, updated values for the solute descriptors for several compounds. At the time that Eqns 5 and 6 were developed solute descriptors were calculated by regressing experimental water-to-organic solvent and gas-to-organic solvent partition coefficient data. We are now using our gas-to-water log K_w correlations to increase the number of equations used in the solute descriptor computations, and have updated numerical values of the solute descriptors of those compounds that have not been used by us since the earlier study was published. We have also reported the water-to-dichloromethane partition coefficient based on only 34 experimental log P values, [20]

$$\log P_{\text{dcm}} = 0.314 + 0.001 \text{ E} + 0.022 \text{ S} - 3.238 \text{ A} - 4.137 \text{ B} + 4.259 \text{ V} \quad (7)$$

$$(N = 38, \text{SD} = 0.141, R^2 = 0.991, F = 680)$$

the gas-to-carbon tetrachloride partition coefficient correlation based on 89 experimental log K values, [21]

$$\log K_{\text{ct}} = 0.23 - 0.20 \text{ E} + 0.35 \text{ S} + 0.07 \text{ A} + 0.27 \text{ B} + 1.041 \text{ L} \quad (8)$$

$$(N = 89, \text{SD} = 0.069, R^2 = 0.999, F = 11877)$$

and have tabulated revised equation coefficients for log P and log K correlations for chloroform, carbon tetrachloride and dichloromethane in several of our published solubility studies. [22-24] The solubility studies did not provide any statistical information concerning the partition coefficient correlations, nor have we published the experimental log P and log K databases used in deriving our most recent chloroform, carbon tetrachloride and dichloromethane partition coefficient correlations. The present study updates the Abraham model log P and log K correlations that we have obtained for chlorinated alkanes. The updated log P and log K correlations for 1,2-dichloroethane were recently reported elsewhere. [11]

2. Data Sets and Computation Methodology

Most of the experimental data that we were able to retrieve from the published literature [25-127] pertained either to the log P values for “practical” partition between chloroalkane-saturated water and water-saturated chloroalkanes, or to the Raoult’s law infinite dilution activity coefficient, $\gamma_{\text{solute}}^{\infty}$, or Henry’s law constants, K_{Henry} , for solutes dissolved in the four chloroalkane solvents. In order to apply the Abraham model the infinite dilution activity coefficients and Henry’s law constants needed to be converted to log K values through Eqns. 9 and 10

$$\log K = \log \left(\frac{RT}{\gamma_{\text{solute}}^{\infty} P_{\text{solute}}^o V_{\text{solvent}}} \right) \quad (9)$$

$$\log K = \log \left(\frac{RT}{K_{\text{Henry}} V_{\text{solvent}}} \right) \quad (10)$$

or log P values for partition from water to the anhydrous chloroalkane through Eqn. (11)

$$\text{Log } P = \log K - \log K_w \quad (11)$$

In equations 9 - 11 R is the universal gas constant, T is the system temperature, $P_{\text{solute}}^{\circ}$ is the vapor pressure of the solute at T, and V_{solvent} is the molar volume of the solvent. The calculation of log P requires knowledge of the solute's gas phase partition coefficient into water, K_w , which is available for most of the solutes being studied. Equation 11 was also used to convert the practical log P to log K(wet) values for solute transfer into each of the four chloroalkane solvent saturated with water. The experimental log K and log P values at 298.15 for chloroform, carbon tetrachloride, dichloromethane and 1-chlorobutane are listed in Tables 1-4. We have separated the “wet” and “dry” partition coefficient data for chloroform and carbon tetrachloride as we need to be sure that the solubilizing properties of the anhydrous chloroalkane solvent and water-saturated chloroalkane solvent are the same before combining values into a single data set. For chloroform and carbon tetrachloride there were sufficient experimental log P and log K values to treat the “wet” and “dry” experimental values separately.

Our experimental databases also contain measured solubility data for several crystalline solutes dissolved in both the anhydrous chloroalkanes and in water. The solubility data were taken largely from our previously published solubility studies. At the time that our solubility studies were performed we included solvents for which we planned to update and to derive correlation equations in the future. In the case of crystalline solutes, the partition coefficient between water and the anhydrous organic solvent is calculated as a solubility ratio

$$P = C_S/C_W \quad (12)$$

of the solute's molar solubilities in the organic solvent, C_S , and in water, C_W . Molar solubilities can also be used to calculate $\log K_S$ values, provided that the equilibrium vapor pressure of the solute above crystalline solute, P_{solute}^0 , at 298.15 K is also available. P_{solute}^0 can be transformed into the gas phase concentration, C_G , and the gas-to-water and gas-to-organic solvent partitions, K_W and K_S , can be obtained through the following equations

$$K_W = C_W/C_G \quad \text{or} \quad K_S = C_S/C_G \quad (13)$$

The vapor pressure and aqueous solubility data needed for these calculations are reported in our previous publications.

As noted in an earlier publication [17], three conditions must be met to calculate partition coefficients from solubility data. The conditions are as follows: (1) the same solid phase must be in equilibrium with the saturated solutions in the solvent and in water (in practice this means that there should be no solvate or hydrate formation); (ii) the secondary medium activity coefficient of the solid in the saturated solutions must be unity (or near unity); and (iii) for the solutes that are ionized in aqueous solution, C_W , must refer to the solubility of the neutral form. The second condition would restrict the method to those solutes that are sparingly soluble in water and in the organic solvent. Past applications [17,18, 23, 128, 129] have shown that the Abraham model does accurately describe the solubility of several fairly soluble solutes. For example, Eqns. 2 and 3 described the molar solubility of benzil in 24 organic solvents to within overall standard deviations of 0.124 and 0.109 log units, respectively. [23] Standard deviations for acetylsalicylic acid dissolved in 13 alcohols, 4 ethers and ethyl acetate were 0.123 and 0.138 log units. [128] Flanagan and coworkers [129] further showed that Eqs. 2 and 3 of the Abraham model predicted the experimental solubilities of 1,2,4,5-tetramethylbenzene in 25 different solvents to within an

overall standard deviation of 0.15 log units using numerical values of the solute descriptors that had been previously calculated from infinite dilution partition coefficient and chromatographic retention data. Benzil, acetylsalicylic acid and 1,2,4,5-tetramethylbenzene exhibited solubilities exceeding 1 Molar in many of the organic solvents.

Molecular descriptors for all of the compounds considered in the present study are tabulated in Table 5. The tabulated values either came from our solute descriptor database, or were re-evaluated as part of the present study as discussed above. Several of the compounds have not been used since the publication of our earlier chloroform log P and log K correlations (Eqns. 5 and 6), and the solute descriptors of these compounds were updated so as to include our log Kw correlations in the solute descriptor computations. The revised numerical values were obtained exactly as described before, using various types of experimental data, including water-to-solvent partitions, gas-to-solvent partitions, solubility and chromatographic data. [2,16].

3. Results and Discussion

As search of the published literature yielded experimental log $P_{\text{chl}}(\text{wet})$ data for 339 solutes partitioned directly into water-saturated chloroform from the equilibrated aqueous solution at or near 298 K and experimental activity coefficient and solubility data for 55 different solutes dissolved in anhydrous chloroform at 298 K that can be used to calculate log $P_{\text{chl}}(\text{dry})$ for the hypothetical solute transfer from water to “dry” chloroform. There were five compounds for which we had both log $P_{\text{chl}}(\text{wet})$ and log $P_{\text{chl}}(\text{dry})$. The “wet” and “dry” data sets were analyzed separately

$$\begin{aligned} \text{Log } P_{\text{chl}}(\text{wet}) = & 0.200(0.031) + 0.095(0.037) \mathbf{E} - 0.363(0.035) \mathbf{S} - 3.088(0.037) \mathbf{A} \\ & - 3.416(0.043) \mathbf{B} + 4.280(0.044) \mathbf{V} \end{aligned} \quad (14)$$

$$(N = 339, SD = 0.198, R^2 = 0.982, F = 3487)$$

and

$$\begin{aligned} \text{Log } P_{\text{chl}}(\text{dry}) = & 0.208(0.041) + 0.231(0.086) \mathbf{E} - 0.483(0.131) \mathbf{S} - 2.981(0.196) \mathbf{A} \\ & - 3.691(0.130) \mathbf{B} + 4.488(0.053) \mathbf{V} \end{aligned} \quad (15)$$

$$(N = 55, SD = 0.168, R^2 = 0.995, F = 1818)$$

to determine whether the dissolved water molecules present in the water-saturated chloroform affected the properties of the organic solvent. All regression analyses were performed using SPSS statistical software. 5-Methyl-2-hexanol was identified as an outlier in the preliminary regression analysis, and was eliminated from the $\log P_{\text{chl}}(\text{wet})$ data set prior to the final calculation. The statistics of both derived correlations are quite good as evidenced by the near unity values of the squared correlation coefficients and by the small deviations of $SD = 0.198$ and $SD = 0.168$ log units.

Examination of Eqns. 13 and 14 indicate that the equation coefficients are for all practical purposes identical, at least to within the coefficient's standard error, which is given in parenthesis after the coefficient. There is therefore very little (if any) difference in the solubilizing properties of anhydrous chloroform and a solution of chloroform that has been saturated with water. The $\log P_{\text{chl}}(\text{wet})$ and $\log P_{\text{chl}}(\text{dry})$ data sets are combined into a single $\log P_{\text{chl}}$ database to give

$$\begin{aligned} \text{Log } P_{\text{chl}}(\text{wet and dry}) = & 0.191(0.026) + 0.105(0.034) \mathbf{E} - 0.403(0.034) \mathbf{S} \\ & - 3.112(0.037) \mathbf{A} - 3.514(0.039) \mathbf{B} + 4.395(0.036) \mathbf{V} \end{aligned} \quad (16)$$

$$(N = 394, SD = 0.204, R^2 = 0.984, F = 4869)$$

There was no loss in descriptive ability by combining the two data sets into a single correlation model. This is in accord with our earlier observations which had shown that for solvents that are “almost” completely immiscible with water, such as alkanes, cyclohexanes and 1,2-dichloroethane and many nonpolar aromatic solvents, the indirect partition ($\log P(\text{dry})$) will be nearly identical to direct partition ($\log P(\text{wet})$). Comparable solubilizing properties of “wet” and “dry” chloroform is further supported by the experimental partition coefficient for 2-naphthol ($\log P_{\text{chl}}(\text{wet}) = 7.69$ versus $\log P_{\text{chl}}(\text{dry}) = 7.68$) and diuron ($\log P_{\text{chl}}(\text{wet}) = 2.54$ versus $\log P_{\text{chl}}(\text{dry}) = 2.60$). See Figure 1 for a plot of calculated water-to-chloroform $\log P_{\text{chl}}(\text{wet and dry})$ versus calculated values based on Eqn. 16 versus experimental values that cover a range of approximately 13.5 log units.

There are 394 experimental data points in the combined log P data set for chloroform. To validate the derived correlation we divided the experimental values into a training set and test set by allowing the SPSS software to randomly select half of the experimental data points. The selected data points became the training set and the compounds that were left served as the test set. Analysis of the experimental data in the training set gave

$$\begin{aligned} \text{Log } P_{\text{chl}}(\text{wet and dry}) = & 0.251(0.042) + 0.123(0.048) \mathbf{E} - 0.432(0.045) \mathbf{S} \\ & - 3.122(0.049) \mathbf{A} - 3.557(0.053) \mathbf{B} + 4.355(0.045) \mathbf{V} \end{aligned} \quad (17)$$

$$(N = 197, SD = 0.185, R^2 = 0.988, F = 3086)$$

There is very little difference in the equation coefficients for the full dataset and training dataset correlations, thus showing that the training set of compounds is a representative sample of the total data set. The training set equation was then used to predict the $\log P_{chl}$ values for the 197 data compounds in the test set. For the predicted and experimental values, we find that S.D. = 0.226, AAE(average absolute error) = 0.152, and AE(average error) = 0.002 log units. There is therefore very little bias in the predictions using Eqn. 17 with AE equal to 0.002 log units. The training set and test set analysis was performed two more times with very similar results.

For the solutes studied, we have experimental gas-to-water partition coefficient data (*e.g.* $\log K_W$ values) to convert 328 of the measured $\log P_{chl}(\text{wet})$ values to $\log K_{chl}(\text{wet})$. As before, the measured values are separated as $\log K_{chl}(\text{wet})$ and $\log K_{chl}(\text{dry})$, depending upon whether the organic solvent chloroform was saturated with water or was anhydrous. Analysis of the 328 $\log K_{chl}(\text{wet})$ and 56 $\log K_{chl}(\text{dry})$ values yielded the following correlation models

$$\begin{aligned} \text{Log } K_{chl}(\text{wet}) = & 0.170(0.034) - 0.517(0.048) \mathbf{E} + 1.303(0.039) \mathbf{S} + 0.380(0.041) \mathbf{A} \\ & + 1.393(0.045) \mathbf{B} + 0.948(0.014) \mathbf{L} \end{aligned} \quad (18)$$

$$(N = 328, SD = 0.204, R^2 = 0.992, F = 7821)$$

and

$$\begin{aligned} \text{Log } K_{chl}(\text{dry}) = & 0.177(0.025) - 0.454(0.065) \mathbf{E} + 0.992(0.097) \mathbf{S} + 0.623(0.144) \mathbf{A} \\ & + 1.294(0.095) \mathbf{B} + 1.005(0.010) \mathbf{L} \end{aligned} \quad (19)$$

$$(N = 56, SD = 0.123, R^2 = 0.999, F = 8029)$$

Both correlations provide a reasonably accurate mathematical description of the experimental gas-to-chloroform partition coefficient data. As expected the equation coefficients are sufficiently close so that one can combine the 384 experimental data points into a single correlation

$$\begin{aligned} \text{Log } K_{\text{chl}}(\text{wet and dry}) = & 0.157(0.025) - 0.560(0.039) \mathbf{E} + 1.259(0.035) \mathbf{S} \\ & + 0.374(0.038) \mathbf{A} + 1.333(0.038) \mathbf{B} + 0.976(0.010) \mathbf{L} \end{aligned} \quad (20)$$

$$(N = 384, SD = 0.196, R^2 = 0.995, F = 13711)$$

with no loss in predictive ability. The derived mathematical correlation describes the experimental log $K_{\text{chl}}(\text{wet and dry})$ values to within a standard deviation of $SD = 0.196$ log units (see Figure 2). The experimental log K data covers a range of approximately 22 log units.

In order to assess the predictive ability of Eqn. 20 we divided the 384 experimental data points into a training set and test set as before. Analysis of the experimental data in the training set gave

$$\begin{aligned} \text{Log } K_{\text{chl}}(\text{wet and dry}) = & 0.143(0.035) - 0.565(0.057) \mathbf{E} + 1.313(0.047) \mathbf{S} \\ & + 0.381(0.052) \mathbf{A} + 1.305(0.054) \mathbf{B} + 0.969(0.015) \mathbf{L} \end{aligned} \quad (21)$$

$$(N = 192, SD = 0.188, R^2 = 0.994, F = 6267)$$

The validation computation gave training set correlation equation not too different from that obtained from the parent 384 compound database. The training set equation was then used to predict log $K_{\text{chl}}(\text{wet and dry})$ values for the 192 compounds in the test set. Comparison of the

predicted and observed values gave SD = 0.206, AAE = 0.153 and AE = 0.022. There is very little bias in the predictions based on Eqn. 21 with AE = 0.022 log units.

The carbon tetrachloride data sets are the second largest of the chlorinated alkane solvents considered in the present study. Here, we were able to retrieve 176 experimental log P_{ct}(wet) and 129 log P_{ct}(dry) values. There are sufficient “wet” and “dry” partition coefficient data to perform separate regression analyses

$$\begin{aligned} \text{Log P}_{\text{ct}}(\text{wet}) = & 0.183(0.038) + 0.528(0.041) \mathbf{E} - 1.159(0.038) \mathbf{S} - 3.477(0.041) \mathbf{A} \\ & - 4.535(0.053) \mathbf{B} + 4.558(0.050) \mathbf{V} \end{aligned} \quad (22)$$

$$(N = 176, \text{SD} = 0.144, R^2 = 0.993, F = 5084)$$

and

$$\begin{aligned} \text{Log P}_{\text{ct}}(\text{dry}) = & 0.185(0.027) + 0.512(0.043) \mathbf{E} - 1.157(0.057) \mathbf{S} - 3.664(0.101) \mathbf{A} \\ & - 4.552(0.067) \mathbf{B} + 4.669(0.041) \mathbf{V} \end{aligned} \quad (23)$$

$$(N = 129, \text{SD} = 0.126, R^2 = 0.996, F = 5502)$$

Both correlations provide a reasonably accurate mathematical description of the experimental water-to-carbon tetrachloride partition coefficient data. As expected the equation coefficients are sufficiently close so that one can combine the 305 experimental data points into a single correlation

$$\begin{aligned} \text{Log P}_{\text{ct}}(\text{wet and dry}) = & 0.199(0.022) + 0.523(0.028) \mathbf{E} - 1.159(0.030) \mathbf{S} \\ & - 3.560(0.033) \mathbf{A} - 4.594(0.037) \mathbf{B} + 4.618(0.032) \mathbf{V} \end{aligned} \quad (24)$$

$$(N = 305, SD = 0.136, R^2 = 0.995, F = 12487)$$

There was no loss in descriptive ability by combining the two data sets into a single correlation model. Preliminary analysis of the “wet” and “dry” gas-to-carbon tetrachloride partition coefficient data showed that these two data sets could also be combined into a single correlation model

$$\begin{aligned} \text{Log } K_{ct}(\text{wet and dry}) = & 0.199(0.017) - 0.275(0.033) \mathbf{E} + 0.445(0.032) \mathbf{S} \\ & - 0.022(0.034) \mathbf{A} + 0.322(0.036) \mathbf{B} + 1.038(0.008) \mathbf{L} \end{aligned} \quad (25)$$

$$(N = 295, SD = 0.136, R^2 = 0.996, F = 15403)$$

$$\begin{aligned} \text{Log } K_{ct}(\text{wet and dry}) = & 0.217(0.019) - 0.435(0.031) \mathbf{E} + 0.554(0.033) \mathbf{S} \\ & + 1.069(0.008) \mathbf{L} \end{aligned} \quad (26)$$

$$(N = 295, SD = 0.156, R^2 = 0.996, F = 19700)$$

We have set the $a \cdot \mathbf{A}$ and $b \cdot \mathbf{B}$ terms equal to zero in Eqn 26 because carbon tetrachloride is not expected to possess any hydrogen-bonding character. To conserve journal space we have reported only the correlation equation for the combined 295 experimental log K_{ct} data points. Figures 3 and 4 give a graphical comparison of the observed log $P_{ct}(\text{wet and dry})$ and log $K_{ct}(\text{wet and dry})$ data versus calculated values based on Eqns. 24 and 26 for data sets that span 11.1 and 15.0 log units, respectively.

The robustness of each correlation was verified by a training set and test set analysis. The training set correlation for log P_{ct} predicted the 152 experimental values in the test set to within $SD = 0.145$, $AAE = 0.111$ and $AE = 0.021$ log units. The corresponding statistics for the

test predictions based on the log K_{ct} training set correlation were $SD = 0.145$, $AAE = 0.104$ and $AE = -0.006$ log units. The validation studies were reported three times with similar results obtained each time. Each time the built-in SPSS was used to randomly divide the parent database in half.

Experimental partition coefficient and activity coefficient data is more limited for both dichloromethane and 1-chlorobutane. Our search of the published literature yielded experimental values for 90 solutes dissolved in dichloromethane and 63 solutes dissolved in 1-chlorobutane. Analysis of experimental values yielded the following correlation models for dichloromethane

$$\begin{aligned} \text{Log } P_{\text{dcm}}(\text{wet and dry}) &= 0.319(0.034) + 0.102(0.051) \mathbf{E} - 0.187(0.064) \mathbf{S} \\ &\quad - 3.058(0.068) \mathbf{A} - 4.090(0.060) \mathbf{B} + 4.324(0.027) \mathbf{V} \end{aligned} \quad (27)$$

(N = 90, SD = 0.153, $R^2 = 0.997$, F = 6061)

$$\begin{aligned} \text{Log } K_{\text{dcm}}(\text{wet and dry}) &= 0.192(0.031) - 0.572(0.051) \mathbf{E} + 1.492(0.064) \mathbf{S} \\ &\quad + 0.460(0.068) \mathbf{A} + 0.847(0.060) \mathbf{B} + 0.965(0.027) \mathbf{L} \end{aligned} \quad (28)$$

(N = 83, SD = 0.154, $R^2 = 0.999$, F = 13338)

and for 1-chlorobutane

$$\begin{aligned} \text{Log } P_{\text{clbt}}(\text{wet and dry}) &= 0.222(0.035) + 0.273(0.049) \mathbf{E} - 0.569(0.066) \mathbf{S} \\ &\quad - 2.918(0.090) \mathbf{A} - 4.883(0.067) \mathbf{B} + 4.456(0.037) \mathbf{V} \end{aligned} \quad (29)$$

$$(N = 63, SD = 0.126, R^2 = 0.998, F = 4828)$$

$$\begin{aligned} \text{Log } K_{\text{clbt}}(\text{wet and dry}) = & 0.130(0.034) - 0.581(0.041) \mathbf{E} + 1.114(0.065) \mathbf{S} \\ & + 0.724(0.100) \mathbf{A} + 1.016(0.016) \mathbf{L} \end{aligned} \quad (30)$$

$$(N = 61, SD = 0.134, R^2 = 0.999, F = 11609)$$

There was not sufficient experimental data to develop separate “wet” and “dry” partition coefficient correlations, hence the retrieved experimental values were combined into a single database with the expectation that there would be very little (if any) difference in the solubilizing characteristics of the respective anhydrous chloroalkane and the chloroalkane saturated with water. The $b \cdot \mathbf{B}$ term was eliminated from the $\log K_{\text{clbt}}$ correlation because the b-coefficient was very small (*i.e.*, $b = 0.054$), and the standard error in the coefficient (*i.e.*, standard error = 0.078) was larger than the coefficient itself. The statistics of both correlations are quite good as evidenced by the near unity values of the squared correlation coefficients and by the small deviations, which are in the range of $SD = 0.13$ to $SD = 0.15$ log units.

The present study shows that the correlations derived from the Abraham solvation parameter model provide reasonably accurate mathematical descriptions of solute transfer from both water and from the gas phase into chloroform, carbon tetrachloride, dichloromethane and 1-chlorobutane. The derived correlations presented here do pertain to 298.15 K. Many manufacturing and separation processes take place at higher temperatures, and there is a growing need to determine partition properties into organic solvents at other temperatures. In this regard, we have recently published enthalpy of solvation correlations, ΔH_{solv} , for organic gases and

gaseous solutes into water [130], chloroform [131] and carbon tetrachloride [132]. The ΔH_{soln} correlations will allow one to extrapolate the predicted log P(wet and dry) and log K(wet and dry) based on Eqns. 16, 20, 24 and 25 to other temperatures not too far removed from 298.15 K.

References

- [1] M. H. Abraham, Chem. Soc. Reviews 22 (1993) 73-83.
- [2] M. H. Abraham, A. Ibrahim, A.M. Zissimos, J. Chromatogr. A 1037 (2004) 29-47.
- [3] M. H. Abraham, A. Ibrahim, J. Chem. Inf. Model. 46 (2006) 1735-1741.
- [4] M. H. Abraham, A. M. Zissimos, W. E. Acree Jr., New J. Chem. 27 (2003) 1041-1044.
- [5] M. H. Abraham, W. E. Acree Jr., New J. Chem. 28 (2004) 1538-1543.
- [6] M. H. Abraham, A. Ibrahim, W. E. Acree, Jr., Fluid Phase Equilibr. 251 (2007) 93-109.
- [7] L. Sprunger, W. E. Acree, Jr., M. H. Abraham, J. Chem. Inf. Model. 47 (2007) 1808-1817.
- [8] M. H. Abraham, A. Ibrahim, W. E. Acree, Jr. Chem. Res. Toxicol. 18 (2005) 904-911.
- [9] M. H. Abraham, A. Ibrahim, W. E. Acree, Jr. Eur. J. Med. Chem. 42 (2007) 743-751.
- [10] M. H. Abraham, A. Nasezadeh, W. E. Acree, Jr. Ind. Eng. Chem. Res. 47 (2008) 3990-3995.
- [11] L. M. Sprunger, J. Gibbs, W. E. Acree, Jr., M. H. Abraham, Fluid Phase Equilibr. 273 (2008) 78-86.
- [12] M. H. Abraham, W. E. Acree, Jr., A. J. Leo, D. Hoekman, New J. Chem. 33 (2009) 568-573.
- [13] L. M. Sprunger, A. Proctor, W. E. Acree, Jr., M. H. Abraham, N. Benjelloun-Dakhama, Fluid Phase Equilibr. 270 (2008) 30-44.
- [14] A. M. Zissimos, M. H. Abraham, C. M. Du, K. Valko, C. Bevan, D. Reynolds, J. Wood, K. Y. Tam, J. Chem. Soc., Perkin Trans. 2 (2002) 2001-2010.

- [15] A. M. Zissimos, M. H. Abraham, M. C. Barker, K. J. Box, K. Y. Tam, J. Chem. Soc., Perkin Trans. 2 (2002) 470-477.
- [16] C. E. Green, M. H. Abraham, W. E. Acree, Jr., K. M. De Fina, T. L. Sharp, Pest Manage. Sci. 56 (2000) 1043-1053.
- [17] M. H. Abraham, C. E. Green, W. E. Acree, Jr., C. E. Hernandez, L. E. Roy, J. Chem. Soc., Perkin Trans. 2 (1998) 2677-2682.
- [18] L. M. Sprunger, A. Proctor, W. E. Acree, Jr., M. H. Abraham, Phys. Chem. Liq. 46 (2008) 574-585.
- [19] M. H. Abraham, J. A. Platts, A. Hersey, A. J. Leo, R. W. Taft, J. Pharm. Sci. 88 (1999) 670-679.
- [20] M. H. Abraham, K. Takacs-Novak, R. C. Mitchell, J. Pharm. Sci. 86 (1997) 310-315.
- [21] M. H. Abraham, J. Andonian-Haftvan, J. P. Osei-Owusu, P. Sakellariou, J. S. Urieta, M. C. Lopez, R. Fuchs, J. Chem. Soc., Perkin Trans. 2 (1993) 299-304.
- [22] W. E. Acree, Jr., M. H. Abraham, Can. J. Chem. 79 (2001) 1466-1476.
- [23] W. E. Acree, Jr., M. H. Abraham, J. Solut. Chem. 31 (2002) 293-303.
- [24] W. E. Acree, Jr., M. H. Abraham, Fluid Phase Equilibr. 201 (2002) 245-258.
- [25] K. Shirono, T. Morimatsu, F. Takemura, J. Chem. Eng. Data 53 (2008) 1867-1871.
- [26] K. Shinoda, J. H. Hildebrand, J. Phys. Chem. 62 (1958) 295-296.
- [27] D. I. Eikens, Ph.D. Dissertation, University of Minnesota, Minneapolis, Minnesota 1993.
- [28] S. Endo, T. C. Schmidt, Fluid Phase Equilibr. 246 (2006) 143-152.

- [29] A. S. Goncalves, E. A. Macedo, *Fluid Phase Equilibr.* 85 (1993) 171-179.
- [30] A. J. Leo, *The MedChem database 2003*, Biobyte Corp. and Pomona College, Daylight Chemical Information Systems, 27401 Los Altos, #360 Mission Viejo, CA, USA.
- [31] V. Dwarakanath, G. A. Pope, *Environ. Sci. Technol.* 32 (1998) 1662-1666.
- [32] S. Pathare, V. R. Bhethanabotla, S. W. Campbell, *J. Chem. Eng. Data* 49 (2004) 510-513.
- [33] I. Kotula, B. Marciniak, *J. Chem. Eng. Data* 46 (2001) 783-787.
- [34] S. M. Leschev, A. V. Sin'kevich, *Russ. J. Appl. Chem.* 76 (2003) 1483-1488.
- [35] P. C. Ray, P. K. Das, *J. Phys. Chem.* 100 (1996) 15631-15633.
- [36] S. Azizian, A. H. Pour, *J. Chem. Res., Synopses* (2003) 402-404.
- [37] M. H. Abraham, J. Gil-Lostes, J. Enrique Cometto-Muniz, W. S. Cain, C. F. Poole, S. N. Atapattu, R. J. Abraham, P. Leonard, *New J. Chem.* 33 (2009) 76-81.
- [38] Y. Yoshimura, N. Suzuki, *Anal. Chim. Acta* 85 (1976) 383-391.
- [39] Y. Takeda, A. Tanaka, *Bull. Chem. Soc. Japan* 59 (1986) 733-735.
- [40] Y. Takeda, C. Takagi, *Bull. Chem. Soc.* 67 (1994) 56-60.
- [41] W. Robak, W. Apostoluk, P. Maciejewski, *Anal. Chim. Acta* 569 (2006) 119-131.
- [42] D. Cao, G. Zhao, W. Yan, *J. Chem. Eng. Data* 52 (2007) 1366-1368.
- [43] T. Wakabayashi, S. Oki, T. Omori, N. Suzuki, *J. Inorg. Nucl. Chem.* 26 (1994) 2255-2264.
- [44] W. Robak, W. Apostoluk, P. Maciejewski, *Anal. Chim. Acta* 569 (2006) 119-131.
- [45] Y. Takeda, H. Sato, S. Sato, *J. Solut. Chem.* 21 (1992) 1069-1080.
- [46] Y. Takeda, K. Endō, D. Yoshiyama, K. Watanabe, N. Fukada, S. Katsuta, *J. Mol. Liq.* 130 (2007) 21-28.

- [47] M. H. Abraham, N. Benjelloun-Dakhama, J. M. R. Gola, W. E. Acree, Jr., W. S. Cain, J. E. Cometto-Muniz, *New J. Chem.* 24 (2000) 825-829.
- [48] A. W. Shaw, A. J. Vosper, *J. Chem. Soc., Faraday Trans. 1* 73 (1977) 1239-1244.
- [49] P. Luhring, A. Schumpe, *J. Chem. Eng. Data* 34 (1989) 250-252.
- [50] S. A. Shchukarev, L. S. Lilich, A. B. Sheinin, *Dokl. Akad. Nauk USSR* 85 (1952) 1333-1335.
- [51] Y. Miyano, W. Hayduk, *Can. J. Chem. Eng.* 59 (1981) 746-751.
- [52] R. Garriga, P. Perez, M. Gracia, *Fluid Phase Equilibr.* 227 (2005) 71-78.
- [53] M. Gracia, *Int. DATA Ser., Sel. Data Mix.* (2001) 67.
- [54] M. Artal, J. M. Embid, S. Otin, I. Velasco, *Fluid Phase Equilibr.* 154 (1999) 223-239.
- [55] C. Berro, *Int. DATA Ser., Sel. Data Mix.* (2000) 3.
- [56] N. Asprion, H. Hasse, G. Maurer, *J. Chem. Eng. Data* 43 (1998) 74-80.
- [57] W. Chang, Ph.D. Dissertation, North Dakota State University, Fargo, North Dakota, 1969.
- [58] C. E. Hernandez, K. M. De Fina, L. E. Roy, T. L. Sharp, W. E. Acree, Jr., *Can. J. Chem.*, 77 (1999) 1465-1470.
- [59] M. H. Abraham, C. E. Green, W. E. Acree, Jr., C. E. Hernandez, L. E. Roy, *J. Chem. Soc., Perkin Trans. 2* (1998) 2677-2682.
- [60] C. I. Monarrez, D. M. Stovall, J. H. Woo, P. Taylor, W. E. Acree, Jr., *Phys. Chem. Liq.* 41 (2003) 73-80.
- [61] D. M. Stovall, W. E. Acree, Jr., M. H. Abraham, *Fluid Phase Equilibr.* 232 (2005) 113-121.

- [62] O. Jens, J. Chr. Gjaldbaek, *Acta Chem. Scand.* 28A (1974) 528.
- [63] S. Azizian, A. Haydarpour, *J. Chem. Eng. Data* 48 (2003) 1476-1478.
- [64] M. J. Cocero, F. Mato, I. Garcia, J. C. Cobas, *J. Chem. Eng. Data*, 34 (1989) 443-445.
- [65] M. J. Cocero, F. Mato, I. Garcia, J. C. Cobas, H. V. Kehiaian, *J. Chem. Eng. Data*, 34 (1989) 73-76.
- [66] M. H. Abraham, J. Gil-Lostes, W. E. Acree, Jr., J. E. Cometto-Muniz, W. S. Cain, J. *Environ. Monit.* 10 (2008) 435-442.
- [67] J. M. Berryman, E. L. Heric, *J. Chem. Eng. Data*, 12 (1967) 249-252.
- [68] M. H. Abraham, *Eur. J. Pharm. Sci.*, 21 (2004) 465-469.
- [69] R. G. Makitra, Ya. M. Vasyutyn, Ya. N. Pirig, G. G. Midyana, *Russ. J. Gen. Chem.* 67 (1997) 1376-1383.
- [70] R. G. Makitra, Ya. N. Pirig, Ya. M. Vasyutyn, *Russ. J. Gen. Chem.* 70 (2000) 672-677.
- [71] D. S. Abrams, J. M. Prausnitz, *J. Chem. Thermodyn.* 7 (1975) 61-72.
- [72] Ya. I. Korenman et al., *Zhur. Priklad. Khim.* 47 (1974) 2079-2083.
- [73] Ya. I. Korenman, *Zhur. Priklad. Khim.* 55 (1982) 399-402.
- [74] Ya. Korenman, *Zhur. Priklad. Khim.* 48 (1975) 1413-1415.
- [75] T. Wakabayashi, S. Oki, T. Omori, N. Suzuki, *J. Inorg. Nucl. Chem.* 26 (1964) 2255-2264.
- [76] Ya. I. Korenman, *Zhur. Priklad. Khim.* 50 (1977) 2736-2738.
- [77] A. S. Kertes, C. J. King, *Chem. Rev.* 87 (1987) 687-710.

- [78] Y. Marcus, *J. Org. Chem.* 55 (1990) 2224-2226.
- [79] A. E. Thal, Jr., R. C. Knox, D. A. Sabatini, *Ground, Water Monit. Remed.* 27 (2007) 135-142.
- [80] M. F. Hegazi, H. F. Al-Mudhaf, A. Abu-Shady, *J. Solut. Chem.* 36 (2007) 467-478.
- [81] W. Kemula, H. Buchowski, J. Teperek, *Bull. De L'Acad. Polonaise Scie., Ser. Sci. Chim.* 41 (1964) 343-345.
- [82] L. Lepori, E. Matteoli, M. R. Tine, *J. Solut. Chem.* 20 (1991) 57-70.
- [83] H. C. Van Ness, B. D. Smith, *Int. DATA Ser., Sel. Data Mix.* (1984) 28.
- [84] H. C. Van Ness, B. D. Smith, *Int. DATA Ser., Sel. Data Mix.* (1984) 26.
- [85] H. C. Van Ness, B. D. Smith, *Int. DATA Ser., Sel. Data Mix.* (1984) 24.
- [86] R. Srivastava, B. D. Smith, *J. Chem. Eng. Data*, 30 (1985) 313-318.
- [87] H. C. Van Ness, B. D. Smith, *Int. DATA Ser., Sel. Data Mix.* (1984) 30.
- [88] R. A. Granberg, A. C. Rasmuson, *J. Chem. Eng. Data* 44 (1999) 1391-1395.
- [89] R. Srivastava, B. D. Smith, *J. Chem. Eng. Data* 30 (1985) 313-318.
- [90] J. H. Park, A. Hussam, P. Couasnon, D. Fritz, P. W. Carr, *Anal. Chem.* 59 (1987) 1970-1976.
- [91] K. Shinoda, J. H. Hildebrand, *J. Phys. Chem.* 69 (1965) 605-608.
- [92] M.-C. Haulait-Pirson, G. Huys, E. Vanstraelen, *Ind. Eng. Chem. Res.* 26 (1987) 447-452.
- [93] J. Li, T. Zhu, G. D. Hawkins, P. Winget, D. A. Liotard, C. J. Cramer, D. G. Truhlar, *Theor. Chem. Acc.* 103 (1999) 9-63.

- [94] Y. Takeda, R. Taguchi, S. Katsuta, J. Mol. Liq. 115 (2004) 139-147.
- [95] I. M. Kolthoff, M. K. Chantooni, Jr., J. Chem. Eng. Data 42 (1997) 49-53.
- [96] R. Garriga, S. Martinez, P. Perez, M. Gracia, Fluid Phase Equilibr. 181 (2001) 203-214.
- [97] R. Garriga, S. Martinez, P. Perez, M. Gracia, J. Chem. Thermodyn. 33 (2001) 523-534.
- [98] E. R. Thomas, B. A. Newman, T. C. Long, D. A. Wood, C. A. Eckert, J. Chem. Eng. Data 27 (1982) 399-405.
- [99] E. R. Thomas, B. A. Newman, G. L. Nicolalde, C. A. Eckert, J. Chem. Eng. Data 27 (1982) 233-240.
- [100] K. M. De Fina, T. T. Van, W. E. Acree, Jr., Can. J. Chem. 78 (2000) 459-463.
- [101] S. A. Shchukarev, L. S. Lilich and A. B. Sheinin, Dokl. Akad. Nauk USSR, 85 (1952) 1333-1335.
- [102] H. C. Van Ness, F. Kohler, Int. DATA Ser., Sel. Data Mix. (1990) 261-262.
- [103] H. C. Van Ness, F. Kohler, Int. DATA Ser., Sel. Data Mix. (1990) 256-266.
- [104] H. C. Van Ness, B. D. Smith, Int. DATA Ser., Sel. Data Mix. (1983) 192-193.
- [105] H. C. Van Ness, B. D. Smith, Int. DATA Ser., Sel. Data Mix. (1983) 185-186.
- [106] H. C. Van Ness, B. D. Smith, Int. DATA Ser., Sel. Data Mix. (1983) 190-191.
- [107] H. C. Van Ness, B. D. Smith, Int. DATA Ser., Sel. Data Mix. (1983) 82.
- [108] H. C. Van Ness, B. D. Smith, Int. DATA Ser., Sel. Data Mix. (1983) 85-86.
- [109] H. C. Van Ness, B. D. Smith, Int. DATA Ser., Sel. Data Mix. (1983) 77-78.
- [110] H. C. Van Ness, P. Svejda, Int. DATA Ser., Sel. Data Mix (1990) 283-284.
- [111] H. C. Van Ness, P. Svejda, Int. DATA Ser., Sel. Data Mix (1990) 285-286.
- [112] J. Salas, M. Katz, J. Solut. Chem. 24 (1995) 357-367.

- [113] D. Dragoescu, M. Teodorescu, A. Barhali, J. Chem. Thermodyn. 39 (2007) 1452-1457.
- [114] S. Martinez, R. Garriga, P. Perez, M. Gracia, J. Chem. Eng. Data 46 (2001) 535-540.
- [115] R. Garriga, S. Martinez, P. Perez, M. Gracia, J. Chem. Thermodyn. 36 (2004) 59-69.
- [116] A. Reyes, M. Haro, I. Gascon, H. Artigas, C. Lafuente, J. Chem. Eng. Data 48 (2003) 887-891.
- [117] J. Munoz Embid, A. H. Roux, J.-P. E. Grolier, Int. DATA Ser., Sel. Data Mix (1990) 47.
- [118] O. Dahmani, I. Wichterle, A. Ait-Kaci, Fluid Phase Equilibr. 124 (1996) 135-146.
- [119] J. Munoz Embid, C. Berro, S. Otin, H. V. Kehiaian, J. Chem. Eng. Data, 35 (1990) 266-271.
- [120] J. Munoz Embid, C. Berro, S. Otin, Int. DATA Ser., Sel. Data Mix. (1991) 279.
- [121] S. M. Leschev, N. P. Novik, J. Struct. Chem. 40 (1999) 424-427.
- [122] L. E. Roy, C. E. Hernandez, W. E. Acree, Jr., Polycyclic Aromat. Compds. 13 (1999) 105-116.
- [123] K. M. De Fina, T. T. Van, K. A. Fletcher, W. E. Acree, Jr., Can. J. Chem. 78 (2000) 449-453.
- [124] K. M. De Fina, C. Ezell, W. E. Acree, Jr., Phys. Chem. Liq. 39 (2001) 699-710.
- [125] K. M. De Fina, T. L. Sharp, M. A. Spurgin, I. Chuca, W. E. Acree, Jr., C. E. Green, M. H. Abraham, Can. J. Chem. 78 (2000) 184-190.
- [126] L. E. Roy, C. E. Hernandez, W. E. Acree, Jr., Polycyclic Aromat. Compds. 13 (1999) 205-219.

- [127] K. A. Fletcher, S. Pandey, M. E. R. McHale, W. E. Acree, Jr., *Phys. Chem. Liq.* 33 (1997) 181-190.
- [128] A. K. Charlton, C. R. Daniels, W. E. Acree, Jr., M. H. Abraham, *J. Solut. Chem.* 32 (2003) 1087-1102.
- [129] K. B. Flanagan, K. R. Hoover, W. E. Acree, Jr., M. H. Abraham, *Phys. Chem. Liq.* 44 (2006) 173-182.
- [130] C. Mintz, M. Clark, W. E. Acree, Jr., M. H. Abraham, *J. Chem. Inf. Model.* 47 (2007) 115-121.
- [131] C. Mintz, K. Burton, W. E. Acree, Jr., M. H. Abraham, *Fluid Phase Equilibr.* 258 (2007) 191-198.
- [132] C. Mintz, M. Clark, K. Burton, W. E. Acree, Jr., M. H. Abraham, *J. Solution Chem.* 36 (2007) 947-966.

Table 1. Experimental Gas-to-Chloroform, K, and Water-to-Chloroform, P, Partition Coefficient

Data Measured at 298.15 K.

Solute	Log K _{obs}	Log P _{obs}	Phase	Ref
Helium	-1.54	0.48	Dry	25
Argon	-0.61	0.86	Dry	25
Krypton	0.01	1.22	Dry	19
Xenon	0.53	1.50	Dry	19
Radon	1.12	1.72	Dry	19
Hydrogen	-1.18	0.54	Dry	19
Nitrogen	-0.87	0.93	Dry	19
Oxygen	-0.71	0.81	Dry	25
Nitrous oxide	0.71	0.94	Dry	19
Carbon monoxide	-0.71	0.92	Dry	19
Carbon dioxide	0.45	0.53	Dry	25
Iodine	4.20	2.34	Dry	26
Pentane	2.36	4.06	Dry	27
Hexane	2.87	4.69	Dry	19
2-Methylpentane	2.71	4.55	Dry	27
Heptane	3.39	5.35	Dry	27
2,4-Dimethylpentane	3.04	5.12	Dry	27
Octane	3.90	6.01	Dry	19
2,5-Dimethylhexane	3.56	5.58	Dry	27
2,3,4-Trimethylpentane	3.63	5.51	Dry	27
Nonane	4.42	6.57	Dry	27
Cyclohexane	3.26	4.16	Wet	19
Ethylcyclohexane	3.99	5.57	Dry	27
Chloromethane	1.82	1.42	Dry	19
Dichloromethane	2.69	2.00	Dry	19
Trichloromethane	3.07	2.28	Dry	19
Tetrachloromethane	3.25	3.31	Dry	19
1,1-Dichloroethane	3.01	2.39	Dry	19
1,2-Dichloroethane	3.44	2.13	Dry	19
1,1,1-Trichloroethane	3.24	3.10	Dry	19
1,1,2-Trichloroethane	3.87	2.41	Dry	19
1-Chloropropane	2.65	2.46	Dry	19
Bromoethane	2.76	2.24	Dry	19
Iodomethane	2.78	2.13	Dry	19

1,1,2-Trifluorotrichloroethane	2.54	3.84	Dry	19
Diethyl ether	3.05	1.88	Wet	19
Diisopropyl ether	3.62	2.58	Dry	28
Methyl <i>tert</i> -butyl ether	3.58	1.99	Dry	28
Tetrahydrofuran	3.86	1.31	Wet	19
Tetrahydropyran	4.28	1.99	Wet	19
1,4-Dioxane	4.44	0.73	Dry	19
Propanone	3.29	0.50	Wet	19
Butanone	3.87	1.15	Wet	19
Propylene Carbonate	5.56	0.60	Wet	19
delta-pentanolactone	6.40	0.95	Wet	19
Ethyl formate	3.20	1.24	Dry	29
Methyl acetate	3.46	1.16	Wet	19
Ethyl acetate	3.98	1.82	Wet	19
Propyl acetate	4.61	2.56	Wet	19
Butyl acetate	4.99	3.05	Wet	19
Pentyl acetate	5.44	3.60	Wet	19
Methyl propanoate	4.02	1.87	Wet	19
Methyl pentanonate	4.89	3.01	Wet	19
Methyl hexanoate	5.31	3.48	Wet	19
Ethyl acetoacetate	5.79	1.49	Wet	19
Ethyl trifluoroacetate	3.04	2.00	Wet	19
Ethyl trichloroacetate	5.23	3.47	Wet	19
Acetonitrile	3.25	0.40	Dry	19
Ammonia	1.77	-1.38	Dry	19
Methylamine	2.32	-1.02	Dry	19
Ethylamine	2.95	-0.35	Wet	19
Propylamine	3.47	0.25	Wet	19
Butylamine	3.86	0.75	Wet	19
Dimethylamine	2.71	-0.44	Wet	19
Diethylamine	3.78	0.79	Wet	19
Diisopropylamine	3.97	1.61	Wet	19
Trimethylamine	2.86	0.51	Dry	19
Triethylamine	4.22	1.86	Dry	19
Nitromethane	3.39	0.44	Dry	19
Acetamide	5.57	-1.97	Wet	19
Propionamide	5.48	-1.40	Wet	19
N,N-Dimethylacetamide	5.91	-0.13	Wet	19

2,2,2-Trichloroacetamide	5.07	0.31	Wet	19
Ethyl carbamate	5.67	0.12	Wet	19
Formic acid	3.21	-2.12	Wet	19
Acetic acid	3.45	-1.46	Wet	19
Propanoic acid	3.68	-0.86	Wet	19
Butanoic acid	4.39	-0.27	Wet	19
2-Methylpropanoic acid	4.25	-0.26	Wet	19
Pentanoic acid	4.84	0.32	Wet	19
3-Methylbutanoic acid	4.66	0.19	Wet	19
Hexanoic acid	5.58	1.02	Wet	19
2-Methylpentanoic acid	5.12	0.90	Wet	19
Octanoic acid	6.61	2.17	Wet	19
Chloroacetic acid	4.91	-1.51	Wet	30
Succinic acid	7.31	-1.92	Wet	19
Water	1.54	-3.10	Wet	19
Methanol	2.41	-1.33	Wet	19
Methanol	2.51	-1.23	Dry	21
Ethanol	2.80	-0.87	Wet	19
Ethanol	2.94	-0.73	Dry	21
1-Propanol	3.26	-0.30	Wet	19
2-Propanol	3.13	-0.35	Wet	19
1-Butanol	3.88	0.42	Wet	19
2-Methyl-1-propanol	3.64	0.34	Wet	19
2-Butanol	3.69	0.30	Wet	19
2-Methyl-2-propanol	3.26	-0.02	Wet	19
1-Pentanol	4.40	1.05	Wet	19
1-Hexanol	4.92	1.69	Wet	19
1-Heptanol	5.50	2.41	Wet	19
2-Methyl-2-butanol	3.74	0.49	Wet	31
2-Methyl-1-pentanol	4.73	1.56	Wet	31
3-Methyl-1-pentanol	4.85	1.62	Wet	31
2-Methyl-2-pentanol	4.17	1.29	Wet	31
3-Methyl-2-pentanol	4.76	1.51	Wet	31
4-Methyl-1-pentanol	4.84	1.77	Wet	31
2-Methyl-3-pentanol	4.64	1.26	Wet	31
4-Methyl-2-pentanol	4.31	1.57	Wet	31
2,3-Dimethyl-2-butanol	4.48	1.22	Wet	31
3,3-Dimethyl-1-butanol	4.79	1.41	Wet	31

3-Methyl-3-hexanol	5.01	1.83	Wet	31
2-Methyl-3-hexanol	5.15	1.91	Wet	31
3-Methyl-2-hexanol	5.20	2.33	Wet	31
2-Methyl-2-hexanol	4.91	1.85	Wet	31
3-Ethyl-3-pentanol	5.18	2.00	Wet	31
4,4-Dimethyl-2-pentanol	5.17	2.18	Wet	31
2,3-Dimethyl-3-pentanol	5.03	1.91	Wet	31
2,2-Dimethyl-3-pentanol	4.88	2.47	Wet	31
Cyclohexanol	5.13	1.12	Wet	19
2-Propen-1-ol	3.18	-0.51	Wet	19
2-Chloroethanol	4.20	-0.40	Wet	19
3-Chloro-1-propanol	4.28	-0.03	Wet	19
1,3-Propanediol	5.13	-2.90	Wet	19
2-Ethoxyethanol	4.59	-0.32	Wet	32
Dimethyl sulfoxide	6.43	-0.98	Wet	30
Thiourea	5.31	-3.14	Wet	19
Tributylphosphine oxide	11.21	3.08	Wet	19
Trimethyl phosphate	6.97	0.76	Wet	19
Triethyl phosphate	7.81	2.28	Wet	19
Tripropyl phosphate	9.26	3.67	Wet	19
Benzene	3.39	2.76	Wet	19
Benzene	3.51	2.88	Dry	21
Toluene	4.06	3.41	Dry	19
Ethylbenzene	4.28	3.70	Wet	19
1,2-Dimethylbenzene	4.57	3.91	Wet	19
1,3-Dimethylbenzene	4.29	3.68	Wet	19
Biphenyl	6.62	4.67	Wet	19
Naphthalene	5.78	4.05	Wet	19
Acenaphthene	7.21	4.85	Dry	33
Anthracene	8.40	5.37	Dry	34
Pyrene	9.64	6.14	Dry	34
Fluoranthene	9.56	6.12	Dry	24
Fluorobenzene	3.44	2.85	Wet	30
Chlorobenzene	4.22	3.40	Wet	19
1,3-Dichlorobenzene	4.59	3.87	Wet	19
1,4-Dichlorobenzene	4.63	3.89	Wet	19
2-Chloronaphthalene	6.62	4.56	Wet	19
Bromobenzene	4.70	3.63	Wet	19

Iodobenzene	4.85	3.57	Wet	19
Anisole	4.92	3.12	Wet	19
Ethyl phenyl ether	5.25	3.62	Wet	19
Benzaldehyde	5.20	2.25	Wet	19
2-Methoxybenzaldehyde	6.93	2.53	Wet	19
Phenylacetaldehyde	5.32	2.07	Wet	19
Acetophenone	6.15	2.79	Wet	19
9-Fluorenone	8.15	3.95	Wet	19
Methyl benzoate	5.68	2.80	Wet	19
Phenyl acetate	6.24	2.33	Wet	19
Dimethyl phthalate	8.68	3.09	Wet	19
Diethyl phthalate	9.40	3.69	Wet	19
Benzonitrile	5.75	2.66	Wet	19
Phenylacetonitrile	5.95	2.25	Wet	19
1,2-Dicyanobenzene	8.20	2.60	Wet	19
1,3-Dicyanobenzene	7.64	2.12	Wet	19
1,4-Dicyanobenzene	8.30	2.60	Wet	19
Aniline	5.65	1.35	Wet	19
2-Methylaniline	6.02	1.96	Wet	19
4-Methylaniline	6.04	1.95	Wet	19
4-Ethylaniline	6.28	2.28	Wet	19
4-Propylaniline	6.97	2.99	Wet	19
4-Isopropylaniline	6.71	2.51	Wet	19
4-Butylaniline	7.22	3.37	Wet	19
4-Chloroaniline	6.42	2.09	Wet	19
2-Nitroaniline	7.24	1.83	Wet	19
3-Nitroaniline	8.09	1.60	Wet	19
4-Nitroaniline	8.80	1.26	Wet	19
3-Aminoacetophenone	8.13	1.73	Wet	19
4-Aminoacetophenone	8.14	2.13	Wet	19
2,4-Dimethylaniline	6.50	2.27	Wet	19
N-Methylaniline	5.84	2.40	Wet	19
N,N-Dimethylaniline	6.01	3.48	Wet	19
N,N-Diethylaniline	6.64	4.26	Wet	19
1-Naphthylamine	7.94	2.60	Wet	19
2-Naphthylamine	8.18	2.70	Wet	19
4-Aminobiphenyl	9.11	3.14	Wet	19
Benzylamine	5.83	1.18	Wet	19

1-Amino-2-phenylethane	7.06	1.37	Wet	19
Nitrobenzene	5.71	2.69	Wet	19
2-Nitrotoluene	6.02	3.39	Wet	19
3-Nitrotoluene	5.98	3.45	Wet	19
4-Nitrotoluene	6.16	3.31	Wet	19
4-Nitroanisole	7.23	3.18	Wet	19
1,2-Dinitrobenzene	7.74	2.64	Wet	19
1,3-Dinitrobenzene	7.82	2.63	Wet	19
1,4-Dinitrobenzene	7.79	2.62	Wet	19
Benzamide	8.19	0.12	Wet	19
N-Methylbenzamide	8.30	0.95	Wet	19
N-Ethylbenzamide	8.78	1.54	Wet	19
N,N-Dimethylbenzamide	8.53	1.75	Wet	19
Acetanilide	7.94	0.80	Wet	19
Phthalimide	8.95	1.37	Wet	30
Benzoic acid	5.70	0.60	Wet	19
2-Methylbenzoic acid	6.06	1.76	Wet	19
4-Methylbenzoic acid	6.66	1.36	Wet	19
4-Ethylbenzoic acid	6.75	1.85	Wet	19
4-Butylbenzoic acid	7.75	2.86	Wet	19
2-Chlorobenzoic acid	6.40	0.90	Wet	19
4-Chlorobenzoic acid	6.52	1.72	Wet	19
2-Bromobenzoic acid	7.09	0.91	Wet	19
3-Bromobenzoic acid	7.21	2.04	Wet	19
4-Bromobenzoic acid	6.35	1.49	Wet	35
2-Iodobenzoic acid	8.12	1.09	Wet	19
2-Methoxybenzoic acid	8.45	1.65	Wet	19
2-Nitrobenzoic acid	8.01	-0.08	Wet	19
3-Nitrobenzoic acid	7.33	0.48	Wet	19
4-Nitrobenzoic acid	7.78	0.88	Wet	35
4-Aminobenzoic acid	8.51	-0.92	Wet	19
Phenylacetic acid	6.70	0.49	Wet	19
3-Phenylpropanoic acid	7.80	1.20	Wet	19
4-Phenylbutanoic acid	8.00	1.78	Wet	19
Phenol	5.17	0.32	Wet	19
2-Methylphenol	5.54	1.23	Wet	19
3-Methylphenol	5.49	0.89	Wet	19
4-Methylphenol	5.56	1.06	Wet	19

2,4-Dimethylphenol	5.91	1.50	Wet	19
2,5-Dimethylphenol	5.93	1.59	Wet	19
3,5-Dimethylphenol	6.20	1.60	Wet	19
2-Ethylphenol	6.15	1.73	Wet	19
3-Ethylphenol	6.00	1.41	Wet	19
4-Ethylphenol	5.97	1.47	Wet	19
2-Isopropyl-5-methylphenol	7.06	2.80	Wet	19
2-Fluorophenol	4.45	0.57	Wet	19
3-Chlorophenol	5.87	1.02	Wet	19
4-Chlorophenol	6.23	1.07	Wet	19
2-Bromophenol	5.37	1.64	Wet	19
4-Bromophenol	6.30	1.07	Wet	19
2-Iodophenol	6.52	1.97	Wet	19
4-Iodophenol	7.14	1.56	Wet	19
2,4-Dichlorophenol	5.74	2.09	Wet	19
2-Methoxyphenol	5.79	1.70	Wet	19
3-Methoxyphenol	6.39	0.77	Wet	19
4-Methoxyphenol	6.61	0.46	Wet	19
2-Hydroxybenzaldehyde	5.69	2.21	Wet	19
4-Hydroxyacetophenone	8.10	0.08	Wet	19
2-Nitrophenol	5.89	2.53	Wet	19
3-Nitrophenol	7.56	0.50	Wet	19
4-Nitrophenol	8.01	0.20	Wet	19
2,4-Dinitrophenol	7.83	2.25	Wet	19
2-Hydroxybenzoic acid	5.97	0.58	Wet	19
Resorcinol	7.01	-1.34	Wet	19
Methyl 4-hydroxybenzoate	8.09	1.23	Wet	19
Ethyl 4-hydroxybenzoate	8.45	1.78	Wet	19
Methyl 2-hydroxybenzoate	6.12	3.15	Wet	19
Ethyl 2-hydroxybenzoate	6.71	3.91	Wet	19
2-Hydroxybenzamide	8.22	0.62	Wet	19
4-Hydroxy-3-methoxybenzaldehyde	7.84	1.42	Wet	19
4-Hydroxypropiophenone	8.51	0.71	Wet	19
4-Hydroxyacetanilide	9.30	-1.60	Wet	19
1-Naphthol	7.13	1.50	Wet	19
2-Naphthol	7.69	1.74	Wet	19
2-Naphthol	7.68	1.73	Dry	36
Benzyl alcohol	5.82	0.96	Wet	19

2-Hydroxybenzyl alcohol	6.96	-0.51	Wet	19
2-Phenylethanol	6.29	1.31	Wet	19
Ephedrine	8.02	1.10	Wet	19
Methyl phenyl sulfoxide	9.41	1.41	Wet	19
Diphenyl sulfoxide	10.73	3.36	Wet	19
Methyl phenyl sulfone	9.01	1.93	Wet	19
Phenylthiourea	8.12	0.56	Wet	19
Benzenesulfonamide	8.71	-0.24	Wet	19
N-Methylbenzenesulfonamide	8.82	1.31	Wet	19
N,N-Dimethylbenzenesulfonamide	9.16	2.69	Wet	19
3-Methylbenzenesulfonamide	9.15	0.32	Wet	19
4-Methylbenzenesulfonamide	9.18	0.33	Wet	19
Pyridine	4.73	1.29	Wet	19
2-Methylpyridine	5.12	1.72	Wet	19
3-Methylpyridine	5.39	1.89	Wet	19
4-Methylpyridine	5.50	1.88	Wet	19
2-Ethylpyridine	5.44	2.26	Wet	19
2-Chloropyridine	5.22	2.00	Wet	19
2-Bromopyridine	5.29	1.65	Wet	19
2-Methoxypyridine	4.94	2.21	Wet	19
2-Acetylpyridine	6.32	1.93	Wet	19
2-Cyanopyridine	6.24	1.42	Wet	19
3-Cyanopyridine	6.29	1.34	Wet	19
4-Cyanopyridine	5.71	1.29	Wet	19
4-Aminopyridine	5.40	-0.71	Wet	19
2-(N,N-Dimethylamino)pyridine	6.45	2.45	Wet	19
Nicotine	7.74	1.89	Wet	19
Piperidine	4.67	0.92	Wet	19
N-Methylpiperidine	4.21	1.44	Wet	19
Atropine	13.60	2.44	Wet	19
N-Methyl-2-pyridone	6.86	0.26	Wet	19
Quinoline	6.98	2.77	Wet	30
Isoquinoline	6.90	2.98	Wet	19
Pyrrole	4.12	0.91	Wet	19
Carbazole	9.15	3.75	Wet	19
N-Methylimidazole	5.25	0.29	Wet	19
Benzimidazole	7.62	-0.02	Wet	19
2-Cyanopyrazine	5.68	1.03	Wet	19

Pyrazine	4.58	0.59	Wet	19
2-Methylpyrazine	5.08	1.04	Wet	19
2,3-Dimethylpyrazine	5.64	1.46	Wet	19
2,5-Dimethylpyrazine	5.62	1.54	Wet	19
Trimethylpyrazine	6.18	1.93	Wet	19
Tetramethylpyrazine	6.77	2.32	Wet	19
2-Ethylpyrazine	5.66	1.66	Wet	19
2,3-Diethylpyrazine	6.73	2.47	Wet	19
2-Methyl-3-isobutylpyrazine	7.09	2.85	Wet	19
2-Fluoropyrazine	4.18	1.07	Wet	19
2-Chloropyrazine	5.02	1.59	Wet	19
2-Methoxypyrazine	5.26	1.71	Wet	19
2-Ethoxypyrazine	5.72	2.25	Wet	19
2-Propoxypyrazine	6.21	2.89	Wet	19
Methyl 2-pyrazinecarboxylate	7.76	1.36	Wet	19
Ethyl 2-pyrazinecarboxylate	8.18	1.88	Wet	19
2-(Dimethylamino)pyrimidine	6.39	1.99	Wet	19
5-(Dimethylamino)pyrimidine	6.56	1.33	Wet	19
2-Cyanopyrimidine	5.09	0.84	Wet	19
2-Thiomethoxypyrimidine	6.50	1.93	Wet	19
Pyrimidine	4.71	0.32	Wet	19
2-Methylpyrimidine	5.14	0.67	Wet	19
5-Methylpyrimidine	5.45	0.95	Wet	19
2-Fluoropyrimidine	4.15	0.85	Wet	19
5-Fluoropyrimidine	4.54	0.89	Wet	19
2-Chloropyrimidine	5.01	1.16	Wet	19
5-Chloropyrimidine	4.98	1.43	Wet	19
2-Bromopyrimidine	5.29	1.35	Wet	19
5-Bromopyrimidine	5.76	1.65	Wet	19
2-Methoxypyrimidine	5.95	1.28	Wet	19
2-Ethoxypyrimidine	6.34	1.77	Wet	19
5-Ethoxypyrimidine	6.14	1.59	Wet	19
Methyl 2-pyrimidinecarboxylate	8.09	0.73	Wet	19
Methyl 5-pyrimidinecarboxylate	7.78	1.55	Wet	19
Ethyl 2-pyrimidinecarboxylate	8.63	1.13	Wet	19
Antipyrine	11.19	1.45	Wet	19
N,N-Dimethylpiperazine	5.47	-0.20	Wet	19
1,2,4-Triazole	6.10	-2.42	Wet	19

Purine	7.50	-1.95	Wet	19
Adenine	8.56	-2.48	Wet	19
Morpholine	4.93	-0.33	Wet	19
N-Methylmorpholine	5.10	0.46	Wet	19
Scopolamine	13.96	1.64	Wet	19
Uracil	5.86	-1.70	Wet	19
1,3-Dimethyluracil	7.22	0.52	Wet	19
Caffeine	11.02	1.23	Wet	19
Guanine	9.39	-3.25	Wet	19
Codeine	14.97	2.20	Wet	19
Thiophene	4.03	3.00	Wet	30
Thiazole	4.33	1.01	Wet	19
Phenylurea	8.74	-0.68	Wet	19
1-Phenyl-3,3-dimethylurea	9.70	1.29	Wet	19
Barbituric acid	7.33	-2.10	Wet	19
5,5-Diethylbarbituric acid	8.50	-0.15	Wet	19
5-Ethyl-5-propylbarbituric acid	9.46	0.30	Wet	19
5-Ethyl-5-(2-pentyl)barbital	10.22	1.59	Wet	19
5-Allyl-5-ethylbarbital	10.31	0.64	Wet	19
5-Ethyl-5-phenylbarbital	11.97	0.65	Wet	19
Acetone oxime	4.16	-0.30	Wet	37
Cyclohexanone oxime	5.93	0.82	Wet	37
Diuron	10.60	2.60	Dry	16
Monuron	9.75	2.12	Dry	16
Diuron	10.54	2.54	Wet	30
Benzoylacetone	7.36	3.67	Wet	38
18 Crown 6	12.22	0.79	Wet	39
15 Crown 5	10.32	0.92	Wet	40
16 Crown 5	10.63	1.45	Wet	41
Betulin	20.82	10.43	Dry	42
Acetylacetone	4.91	1.37	Wet	43
Benzo 15 Crown 5	12.95	2.40	Wet	44
Benzo 18 crown 6	15.68	2.57	Wet	45
AC-B18C6 ^a	16.45	3.40	Wet	46
Germanium tetrabromide	5.19	0.49	Wet	30
Germanium tetrachloride	3.09	0.79	Wet	30
Methyl mercuric (II) chloride	5.76	1.04	Wet	30
Phenyl mercuric (II) chloride	8.81	2.45	Wet	30

Carbamazepine	13.09	1.96	Wet	30
Ibuprofen	8.73	3.03	Wet	30
Zidovudine	12.93	-0.31	Wet	30
Lactic acid	5.05	-2.00	Wet	30
Trichlorofluoromethane	2.07	2.52	Wet	30
Dichlorodifluoromethane	1.25	2.38	Wet	30
HCN	2.30	-0.67	Wet	30
Ferrocene	6.76*	4.84	Dry	47
2-Acetylpyrazine		1.42	Wet	19
Digitoxin		3.65	Wet	30
3-Methylindole		2.24	Wet	19
3-Bromopyridine		1.65	Wet	19
4-Hydroxybenzaldehyde	6.34*	-0.14	Wet	19
4-Methylbenzyl alcohol	7.05*	1.83	Wet	19
2-Chlorophenol	4.70*	1.36	Wet	19
4-Methoxybenzoic acid	7.89	1.19	Wet	19
Benzyl methyl ketone		3.53	Wet	19
Phenanthrene	7.86*	5.06	Wet	19
5-Methyl-2-hexanol		2.74*	Wet	31
Trichloroacetic acid		-1.11	Wet	19

*Not used in regression analysis.

^a 1,2-bis[2-(2-methoxyethoxy)ethoxy]benzene.

Table 2. Experimental Gas-to-Carbon Tetrachloride, K, and Water-to-Carbon Tetrachloride, P,
Partition Coefficient Data Measured at 298.15 K.

Solute	Log K _{obs}	log P _{obs}	Phase	Ref
Helium	-1.56	0.46	Dry	21
Neon	-1.37	0.56	Dry	21
Argon	-0.47	1.00	Dry	21
Krypton	0.12	1.33	Dry	21
Xenon	0.52	1.49	Dry	21
Hydrogen	-1.11	0.62	Dry	21
Oxygen	-0.52	0.99	Dry	21
Nitrogen	-0.79	1.01	Dry	21
Nitrous oxide	0.63	0.86	Dry	21
Nitric oxide	-0.45	0.89	Dry	48
Carbon monoxide	-0.66	0.96	Dry	21
Carbon dioxide	0.45	0.53	Dry	49
Iodine	3.85	1.99	Dry	50
Methane	-0.14	1.32	Dry	21
Tetrafluoromethane	-0.60	1.69	Dry	21
Sulfur hexafluoride	0.02	2.24	Dry	21
Ethane	0.73	2.07	Dry	21
Propane	1.34	2.78	Dry	21
Butane	1.96	3.48	Dry	21
2-Methylpropane	1.74	3.44	Dry	21
Pentane	2.36	4.06	Dry	21
Hexane	2.98	4.80	Dry	21
2-Methylpentane	2.81	4.65	Dry	27
Heptane	3.48	5.44	Dry	21
2,4-Dimethylpentane	3.13	5.21	Dry	27
Octane	4.05	6.16	Dry	21
2,5-Dimethylhexane	3.66	5.68	Dry	27
2,3,4-Trimethylpentane	3.72	5.60	Dry	27
Nonane	4.55	6.70	Dry	27
Hexadecane	8.36		Dry	21
Cyclohexane	3.22	4.12	Dry	21
Ethylcyclohexane	4.08	5.66	Dry	27
Ethene	0.57	1.51	Dry	21
Propene	1.35	2.32	Dry	21

1-Butene	1.83	2.84	Dry	21
Isobutene	1.79	2.65	Dry	21
2-Methyl-1,3-butadiene	2.56	3.06	Dry	21
Acetylene	0.48	0.48	Dry	51
Chloromethane	1.61	1.21	Dry	21
Chloropropane	2.71	2.47	Dry	21
2-Chloro-2-methylpropane	2.68	3.48	Dry	21
Dichloromethane	2.46	1.50	Dry	21
Trichloromethane	2.94	2.15	Dry	21
Carbon tetrachloride	3.24	3.43	Dry	21
1,1-Dichloroethane	2.77	2.15	Dry	21
1,2-Dichloroethane	3.15	1.88	Dry	21
1,1,1-Trichloroethane	3.11	2.99	Dry	21
1,1,2-Trichloroethane	3.71	2.25	Dry	21
1,1,2,2-Tetrachloroethane	4.35	2.54	Dry	52
1,2-Dichloropropane	3.41	2.44	Dry	21
1,3-Dichloropropane	3.81	2.42	Dry	21
1-Chlorobutane	3.16	3.04	Dry	21
Tetrachloroethene	4.02	4.09	Dry	52
Bromoethane	2.53	1.99	Dry	21
1-Bromopropane	3.06	2.59	Dry	21
2-Bromo-2-methylpropane	3.03	3.63	Dry	21
1-Bromobutane	3.48	3.19	Dry	21
1,2-Dibromoethane	3.91	2.20	Dry	53
Iodomethane	2.53	1.88	Dry	21
Iodoethane	3.06	2.52	Dry	21
1-Iodopropane	3.64	3.25	Dry	21
1-Iodobutane	4.08	3.90	Dry	21
Trifluorochloromethane	0.44	2.09	Dry	21
Difluorodichloromethane	1.41	2.55	Dry	21
1,1,2-Trifluorotrichloroethane	2.40	3.70	Dry	21
Bromochloromethane	2.87	1.68	Dry	54
Diethyl ether	2.58	1.29	Dry	21
Dipropyl ether	3.54	2.65	Dry	21
Diisopropyl ether	3.10	2.05	Dry	21
Dibutyl ether	4.60	3.91	Dry	21
Methyl butyl ether	3.22	2.09	Dry	21
Ethyl butyl ether	3.60	2.49	Dry	21

Dimethoxymethane	2.68	0.53	Dry	21
Diethoxymethane	3.64	1.60	Dry	21
1,2-Dimethoxyethane	3.40	-0.11	Dry	21
1-Methoxy-2-ethoxyethane	4.29		Dry	21
Tetrahydrofuran	3.13	0.58	Dry	21
1,4-Dioxane	3.64	-0.07	Dry	21
Methyl <i>tert</i> -butyl ether	2.89	1.30	Dry	55
Propanone	2.38	-0.45	Dry	21
Butanone	2.99	0.27	Dry	21
2-Hexanone	3.93	1.52	Dry	21
2-Octanone	4.91	2.75	Dry	21
Cyclopentanone	4.06	0.61	Dry	21
Cyclohexanone	4.57	0.97	Dry	21
Acetonitrile	2.22	-0.63	Dry	21
Propionitrile	2.77	-0.05	Dry	21
Methylamine	1.71	-1.63	Dry	21
Dimethylamine	2.11	-1.04	Dry	21
Trimethylamine	2.12	-0.23	Dry	21
Triethylamine	3.54	1.18	Dry	21
Nitromethane	2.54	-0.41	Dry	21
2-Nitropropane	3.35	1.05	Dry	21
Methanol	1.50	-2.24	Dry	21
Ethanol	2.06	-1.61	Dry	21
1-Propanol	2.59	-0.97	Dry	21
1-Butanol	3.26	-0.22	Dry	21
2-Methyl-2-propanol	2.58	-0.70	Dry	21
1-Hexanol	4.21	0.98	Dry	56
2-Ethoxyethanol	3.57	-1.34	Dry	32
Carbon disulfide	2.66	2.81	Dry	21
Tetramethyl tin	3.24		Dry	21
Benzene	3.24	2.61	Dry	21
Toluene	3.82	3.17	Dry	21
1,4-Dimethylbenzene	4.20	3.61	Dry	21
Naphthalene	5.59	3.86	Dry	21
Biphenyl	6.76	4.81	Dry	57
Phenanthrene	8.05	5.25	Dry	58
Anthracene	8.17	5.14	Dry	21
Pyrene	9.28	5.78	Dry	24

Acenaphthene	7.06	4.70	Dry	24
Fluoranthene	9.27	5.83	Dry	24
trans-Stilbene	8.18	5.40	Dry	59
Chlorobenzene	4.14	3.32	Dry	21
1,2-Dichlorobenzene	4.98	4.08	Dry	21
Bromobenzene	4.57	3.50	Dry	21
Iodobenzene	4.99	3.71	Dry	21
Benzil	8.81	3.94	Dry	23
9-Fluorenone	8.42	4.22	Dry	60
Xanthene	7.88	5.29	Dry	61
2-Naphthol	6.93	0.98	Dry	36
Diuron	9.13	1.13	Dry	16
Monuron	8.11	0.48	Dry	16
Ferrocene	6.24	4.31	Dry	62
Ethyl formate	2.44	0.48	Dry	29
Diethyl carbonate	4.24	1.59	Dry	64
Dimethyl carbonate	3.12		Dry	65
Mercury	1.87	1.41	Dry	66
1,4-Dibromobenzene	5.79	4.42	Dry	67
Thalidomide		-0.76	Dry	68
N-Methylthalidomide		1.25	Dry	68
N-Propylthalidomide		2.67	Dry	68
N-Pentylthalidomide		4.42	Dry	68
Benzophenone		3.73	Dry	63
Diethyl ether	2.59	1.30	Wet	69
Pentanoic acid	4.10	-0.42	Wet	70
Phenol	4.55	-0.30	Wet	71
2-Chlorophenol	4.53	1.19	Wet	72
3-Chlorophenol	5.34	0.49	Wet	72
4-Chlorophenol	5.56	0.40	Wet	30
1-Nitropropane	3.44	0.99	Wet	81
Benzoylacetone	6.43	2.74	Wet	38
15 Crown 5	8.20	-1.21	Wet	40
16 Crown 5	8.58	-0.60	Wet	41
Benzo 15 Crown 5	11.29	0.74	Wet	41
Benzo 18 crown 6	13.45	0.34	Wet	45
1-Naphthol	6.79	1.16	Wet	73
2-Naphthol	6.94	0.99	Wet	73

2-Hydroxybenzoic acid	5.39	0.00	Wet	74
3-Hydroxybenzoic acid	5.54	-1.46	Wet	74
4-Hydroxybenzoic acid	5.40	-1.38	Wet	74
Acetylacetone	4.05	0.51	Wet	75
1,4-Dioxane	3.58	-0.13	Wet	76
Benzyl alcohol	4.83	-0.04	Wet	30
2-Fluorophenol	3.83	-0.05	Wet	30
4-Fluorophenol	4.28	-0.26	Wet	30
4-Bromophenol	5.76	0.53	Wet	30
4-Iodophenol	6.12	0.94	Wet	30
4-Nitrophenol	6.82	-0.99	Wet	30
2,4-Dinitrophenol	6.76	1.18	Wet	76
Methanol	1.64	-2.10	Wet	77
Ethanol	1.93	-1.75	Wet	77
1-Propanol	2.64	-0.92	Wet	77
2-Propanol	2.12	-1.36	Wet	77
1-Butanol	3.17	-0.29	Wet	77
2-Methyl-1-propanol	2.89	-0.41	Wet	77
2-Butanol	2.85	-0.54	Wet	77
2-Methyl-2-propanol	2.43	-0.85	Wet	77
1-Pentanol	3.75	0.40	Wet	78
2-Pentanol	3.45	0.23	Wet	30
1-Hexanol	4.27	1.04	Wet	31
2-Methyl-2-butanol	3.20	-0.05	Wet	31
2-Methyl-2-pentanol	3.78	0.53	Wet	31
4-Methyl-1-pentanol	4.00	0.93	Wet	31
2-Methyl-3-pentanol	3.90	0.52	Wet	31
4-Methyl-2-pentanol	3.84	0.88	Wet	31
2,3-Dimethyl-2-butanol	3.78	0.52	Wet	31
3,3-Dimethyl-1-butanol	3.99	0.61	Wet	31
3-Methyl-3-hexanol	4.38	1.20	Wet	31
2-Methyl-3-hexanol	4.71	1.47	Wet	31
3-Methyl-2-hexanol	4.35	1.48	Wet	31
2-Methyl-2-hexanol	4.27	1.21	Wet	31
5-Methyl-2-hexanol	4.45	1.48	Wet	31
3-Ethyl-3-pentanol	4.41	1.23	Wet	31
4,4-Dimethyl-2-pentanol	4.38	1.39	Wet	31
2,3-Dimethyl-3-pentanol	4.37	1.25	Wet	31

2,2-Dimethyl-3-pentanol	4.00	1.59	Wet	31
1-Heptanol	4.66	1.65	Wet	30
1-Octanol	5.09	2.09	Wet	79
Formic acid	2.19	-3.06	Wet	30
Acetic acid	2.25	-2.66	Wet	80
Propanoic acid	2.92	-1.82	Wet	30
Butanoic acid	3.52	-1.14	Wet	30
3-Methylbutanoic acid	3.94	-0.53	Wet	30
Chlorine	1.39	1.21	Wet	30
Cyclohexene	3.36	3.63	Wet	30
Acetophenone	5.26	1.90	Wet	30
Acetone	2.49	-0.34	Wet	30
2-Pentanone	3.52	0.94	Wet	30
2-Hexanone	4.01	1.60	Wet	30
2-Heptanone	4.51	2.26	Wet	30
Germanium tetrabromide	5.21	0.51	Wet	30
Germanium tetrachloride	3.13	0.83	Wet	30
Chlorobenzene	4.16	3.34	Wet	30
1,3-Dichlorobenzene	4.55	3.83	Wet	30
1,4-Dichlorobenzene	4.60	3.86	Wet	30
Bromobenzene	4.65	3.58	Wet	30
Iodobenzene	5.15	3.87	Wet	30
1,5-Hexadiene	2.90	3.67	Wet	30
2,3-Dimethylbuta-1,3-diene	3.23	3.52	Wet	30
Isobutene	1.99	2.85	Wet	30
2-Methylbut-2-ene	2.38	3.34	Wet	30
1-Hexene	2.80	3.96	Wet	30
Methyl acetate	2.66	0.36	Wet	30
Ethyl acetate	3.11	0.95	Wet	30
Propyl acetate	3.64	1.59	Wet	30
Butyl acetate	4.17	2.23	Wet	30
Pentyl acetate	4.69	2.85	Wet	30
Methyl propanoate	3.25	1.10	Wet	30
Methyl pentanoate	4.18	2.30	Wet	30
Ammonia	0.79	-2.37	Wet	30
Methylamine	1.85	-1.49	Wet	30
Ethylamine	2.03	-1.27	Wet	30
Propylamine	2.63	-0.59	Wet	30

Butylamine	3.15	0.04	Wet	30
Dimethylamine	2.02	-1.13	Wet	30
Diethylamine	3.02	0.03	Wet	30
Trimethylamine	2.25	-0.10	Wet	30
Triethylamine	3.26	0.90	Wet	30
Tributylphosphine oxide	8.90	0.77	Wet	30
2-Methylphenol	4.98	0.67	Wet	30
4-Methylphenol	4.72	0.22	Wet	30
4-Ethylphenol	5.36	0.86	Wet	30
4-Propylphenol	5.85	1.52	Wet	30
2,3-Dimethylphenol	5.56	1.04	Wet	30
2,4-Dimethylphenol	5.19	0.78	Wet	30
2,5-Dimethylphenol	5.34	1.00	Wet	30
2,6-Dimethylphenol	5.11	1.25	Wet	30
3,5-Dimethylphenol	5.42	0.82	Wet	30
Benzene	3.29	2.66	Wet	30
Toluene	3.88	3.23	Wet	30
1,2-Dimethylbenzene	4.53	3.79	Wet	30
1,3-Dimethylbenzene	4.18	3.57	Wet	30
Biphenyl	6.46	4.51	Wet	30
Naphthalene	5.51	3.78	Wet	30
Phenanthrene	7.74	4.94	Wet	30
Pyridine	3.77	0.33	Wet	30
2-Methoxyphenol	5.07	0.98	Wet	30
4-Methoxyphenol	5.81	-0.34	Wet	30
Methoxybenzene	4.24	2.44	Wet	30
2-Chloroaniline	5.33	1.73	Wet	30
3-Chloroaniline	5.64	1.37	Wet	30
4-Chloroaniline	5.64	1.31	Wet	30
2-Methoxyaniline	5.71	1.22	Wet	30
2-Methylaniline	5.24	1.18	Wet	30
4-Methylaniline	5.21	1.12	Wet	30
2-Nitroaniline	6.49	1.08	Wet	30
3-Nitroaniline	6.93	0.44	Wet	30
4-Nitroaniline	7.41	-0.13	Wet	30
1-Naphthylamine	7.18	1.84	Wet	30
2-Naphthylamine	7.40	1.92	Wet	30
2-Nitrotoluene	5.49	2.86	Wet	30

4-Methylpyridine	4.46	0.84	Wet	30
Benzonitrile	4.85	1.76	Wet	30
Benzamide	6.77	-1.30	Wet	30
Cyclopentanone	3.87	0.42	Wet	30
Benzaldehyde	4.48	1.53	Wet	30
Nitrobenzene	5.26	2.24	Wet	30
2-Butanone	3.03	0.31	Wet	30
Methyl salicylate	5.41	2.44	Wet	30
Ethyl salicylate	6.06	3.26	Wet	30
Propyl salicylate	6.57	3.89	Wet	30
Butyl salicylate	7.13	4.56	Wet	30
Nicotine	6.79	0.94	Wet	30
Methyl benzoate	5.01	2.13	Wet	30
5-Methylfurfural	4.69	0.66	Wet	30
Caffeine	9.10	-0.69	Wet	30
4-Aminobenzoic acid	6.79	-2.64	Wet	30
2-Furaldehyde	4.06	0.23	Wet	30
Trichloroacetic acid	4.79	-2.00	Wet	30
Water	0.64	-4.00	Wet	30
5-Bromosalicylic acid	7.08	1.05	Wet	30
5-Nitrosalicylic acid	7.54	0.24	Wet	30
Allyl alcohol	2.60	-1.09	Wet	30
Hydrogen peroxide	1.69	-4.00	Wet	30
1,2,4-Triazole	4.02	-4.39	Wet	30
Methyl mercuric (II) chloride	4.73	0.01	Wet	30
4-Hydroxyacetophenone	6.72	-1.30	Wet	30
Nitromethane	2.55	-0.40	Wet	30
N-Methylaniline	4.84	1.40	Wet	30
5-Ethyl-5-phenylbarbital	10.69	-0.63	Wet	30
5-Ethyl-5-(2-pentyl)barbital	8.60	-0.03	Wet	30
4-Methyl-8-hydroxyquinoline	6.69	2.73	Wet	30
2,4,6-Trinitrophenol	9.49	0.36	Wet	30
2-Aminophenol	5.73	-1.72	Wet	30
3-Aminophenol	6.27	-2.39	Wet	30
4-Aminophenol	6.06	-2.64	Wet	30
Thiopental		1.10	Wet	30
2,4-Dichlorophenol		1.65	Wet	72
2-Bromophenol	5.20	1.49	Wet	30

2-Iodophenol		1.57	Wet	30
2-Chloronaphthalene		4.46	Wet	30
4-Nitrotoluene	5.56	2.71	Wet	30
Phenylacetonitrile	5.27	1.57	Wet	30
Thymol	6.65	2.39	Wet	30
4-Methoxybenzoic acid		0.56	Wet	30
Chloroacetic acid	3.88	-2.54	Wet	30
Dichloroacetic acid		-2.31	Wet	30
o-Vanillin	6.45	1.40	Wet	30
2-Methyl-8-hydroxyquinoline		2.64	Wet	30

Table 3. Experimental Gas-to-Dichloromethane, K, and Water-to-Dichloromethane, P,
Partition Coefficient Data Measured at 298.15 K.

Solute	log K _{obs}	Log P _{obs}	Phase	Ref
Helium	-1.49	0.53	Dry	25
Argon	-0.70	0.77	Dry	25
Hydrogen	-1.15	0.58	Dry	25
Nitrogen	-0.88	0.92	Dry	25
Oxygen	-0.66	0.85	Dry	25
Carbon dioxide	0.50	0.58	Dry	25
Pentane	2.24	3.94	Dry	27
Hexane	2.75	4.57	Dry	27
2-Methylpentane	2.59	4.43	Dry	27
Heptane	3.27	5.23	Dry	27
2,4-Dimethylpentane	2.92	5.00	Dry	27
Octane	3.72	5.83	Dry	27
2,5-Dimethylhexane	3.40	5.42	Dry	27
2,3,4-Trimethylpentane	3.47	5.35	Dry	27
Nonane	4.21	6.36	Dry	27
Cyclohexane	3.01	3.91	Dry	27
Ethylcyclohexane	3.82	5.40	Dry	27
Monuron	9.73	2.10	Dry	16
Diuron	10.39	2.42	Dry	16
Benzene	3.52	2.89	Dry	86
Naphthalene	5.94	4.21	Dry	57
Anthracene	8.62	5.59	Dry	122
Biphenyl	6.89	4.94	Dry	57
Chlorobenzene	4.33	3.51	Dry	89
Diethyl ether	2.87	1.58	Dry	82
Dipropyl ether	3.68	2.79	Dry	82
Methyl butyl ether	3.45	2.32	Dry	82
Diethoxymethane	4.01	1.97	Dry	82
1,2-Dimethoxyethane	4.27	0.76	Dry	82
Dichloromethane	2.83	1.87	Dry	Unity ^a
Ethyl acetate	3.83	1.67	Dry	83
Propanone	3.39	0.56	Dry	84
Methanol	2.29	-1.45	Dry	84
2-Ethoxyethanol	4.44	-0.47	Dry	32

Acetonitrile	3.45	0.60	Dry	87
Paracetamol	9.38		Dry	88
1,4-Dioxane	4.27	0.56	Dry	90
Butanone	3.86	1.14	Dry	90
Ethanol	2.72	-0.95	Dry	90
Toluene	4.02	3.37	Dry	90
Nitromethane	3.62	0.67	Dry	90
Iodine	4.12	2.26	Dry	91
Betulin	20.28	9.89	Dry	42
9-Fluorenone	8.79	4.59	Dry	60
Tetracosane	11.73	15.57	Dry	92
Octacosane	13.60	17.94	Dry	92
Dibenzo 24 Crown 8	21.78	4.46	Wet	94
Dibenzo 18 Crown 6	17.53	4.15	Wet	95
Benzoylacetone	7.17	3.48	Wet	38
4-Methylphenol	5.65	1.15	Wet	93
Thiophenol	5.21	3.34	Wet	30
4-Bromophenol	6.66	1.43	Wet	93
15 Crown 5	10.04	0.64	Wet	40
16 Crown 5	10.27	1.09	Wet	44
Benzo 18 Crown 6	15.63	2.52	Wet	45
Benzo 15 Crown 5	12.97	2.42	Wet	44
AC-B18C6 ^b	16.23	3.18	Wet	46
Acetylacetone	4.86	1.32	Wet	43
2-Chlorophenol	5.10	1.76	Wet	30
Ethanol	2.79	-0.88	Wet	30
Caffeine	10.42	0.63	Wet	30
Phenol	5.49	0.64	Wet	30
3-Chlorophenol	6.13	1.28	Wet	30
4-Iodophenol	7.32	1.74	Wet	30
3-Nitrophenol	7.86	0.80	Wet	30
2-Bromophenol	5.70	1.99	Wet	30
2-Nitrophenol	6.28	2.90	Wet	30
Tributylphosphine oxide	10.61	2.48	Wet	30
8-Hydroxyquinoline	7.02	2.58	Wet	30
Benzotriazole	7.75	0.04	Wet	30
Ephedrine	7.54	0.62	Wet	30
Procaine	11.29	2.11	Wet	30

Procaineamide	13.97	0.95	Wet	30
4-Aminobenzoic acid	8.63	-0.80	Wet	30
2-Hydroxybenzoic acid	6.08	0.69	Wet	30
o-Vanillin	7.77	2.72	Wet	30
Methyl mercuric chloride	6.04	1.32	Wet	30
2,4-Dibromophenol	6.85	2.68	Wet	30
Water	1.94	-2.70	Wet	30
5-Ethyl-5-(2-pentyl)barbital	10.14	1.51	Wet	30
4-Ethylphenol	6.16	1.66	Wet	30
8-Quinolinol	7.10	2.58	Wet	30
2,4-Dinitrophenol	8.18	2.60	Wet	30
Thiopental		2.35	Wet	30
2-Iodophenol	6.71*	2.16	Wet	30
2,6-Dichlorophenol		2.56	Wet	30
3,5-Dichlorophenol		1.79	Wet	30
Tributyl phosphate		4.50	Wet	30
Bromopheniramine		4.31	Wet	30
3-Bromophenol		1.46	Wet	30
2,4-Dichlorophenol	5.88	2.23	Wet	30

*Not used in regression analysis.

^a Activity coefficient is defined to be unity.

^b 1,2-bis[2-(2-methoxyethoxy)ethoxy]benzene.

Table 4. Experimental Gas-to-1-Chlorobutane, K, and Water-to-1-Chlorobutane, P,
Partition Coefficient Data Measured at 298.15 K.

Solute	Log Kobs	Log Pobs	Phase	Ref
Anthracene	8.21	5.17	Dry	122
Pyrene	9.40	5.90	Dry	126
Fluoranthene	9.38	5.94	Dry	126
Benzil	8.89	4.02	Dry	127
Ferrocene	6.14	4.22	Dry	124
Diphenyl sulfone	10.36	2.97	Dry	123
2-Butanol	3.06	-0.33	Dry	96
2-Methyl-1-propanol	3.23	-0.07	Dry	96
2-Methyl-2-propanol	2.80	-0.48	Dry	97
1-Butanol	3.38	-0.09	Dry	97
Chloroform	2.99	2.20	Dry	98
Dichloromethane	2.60	1.64	Dry	98
Methyl iodide	2.52	1.87	Dry	98
Nitromethane	2.98	0.03	Dry	98
Ethyl bromide	2.57	2.03	Dry	98
Ethyl iodide	3.01	2.47	Dry	98
Acetone	2.65	-0.18	Dry	98
1-Chloropropane	2.70	2.46	Dry	98
Cyclohexane	3.06	3.96	Dry	98
Hexane	2.83	4.65	Dry	98
Triethylamine	3.35	0.99	Dry	99
Cyclohexene	3.20	3.47	Dry	102
Benzene	3.27	2.64	Dry	103
1-Chlorobutane	3.24	3.12	Dry	Unity ^a
Aniline	4.89	0.59	Dry	104
Chlorobenzene	4.10	3.28	Dry	105
Ethyl acetate	3.17	1.01	Dry	106
Toluene	3.78	3.13	Dry	107
Acetonitrile	2.66	-0.19	Dry	108
Pentane	2.36	4.06	Dry	109
2,2,4-Trimethylpentane	3.35	5.47	Dry	110
2,2,4-Trimethyl-1-pentene	3.48		Dry	111
1,1,1-Trichloroethane	3.17	3.05	Dry	112
1-Hexanol	4.39	1.16	Dry	114

Ethanol	2.25	-1.42	Dry	114
1-Octanol	5.29	2.29	Dry	115
1,4-Dioxane	3.52	-0.19	Dry	116
Heptane	3.38	5.34	Dry	117
2-Chlorobutane	3.05	3.05	Dry	118
Cyclopentanone	4.00	0.55	Dry	113
1,2-Dichloroethane	3.24	1.97	Dry	119
Iodine	4.13	2.27	Dry	101
Hexachlorobenzene	7.79	6.24	Dry	100
Diuron	9.76	1.79	Dry	125
Diethyl ether	2.49	1.20	Dry	82
Dipropyl ether	3.43	2.54	Dry	82
Methyl butyl ether	3.12	1.99	Dry	82
Diethoxymethane	3.42	1.38	Dry	82
1,2-Dimethoxyethane	3.38	-0.13	Dry	82
Carbon tetrachloride	3.14	3.33	Dry	120
Dibenzo 24 Crown 8	19.78	2.46	Wet	94
Dibenzo 18 Crown 6	15.80	2.42	Wet	95
Benzo 15 Crown 5	11.17	0.62	Wet	41
Benzo 18 crown 6	13.48	0.37	Wet	45
15 Crown 5	8.20	-1.20	Wet	41
16 Crown 5	8.40	-0.78	Wet	41
AC-B18C6 ^b	14.10	1.05	Wet	46
Caffeine	8.84	-0.95	Wet	30
2-Hydroxybenzoic acid	5.55	0.16	Wet	30
5-Ethyl-5-(2-pentyl)barbital	9.12	0.49	Wet	30
Procaineamide	12.63	-0.39	Wet	30
Tetracosane		15.70	Dry	121
5-Ethyl-5-phenylbarbital		-0.44	Wet	30
Carbon disulfide		2.50	Dry	98

^a Activity coefficient is defined to be unity.

^b 1,2-bis[2-(2-methoxyethoxy)ethoxy]benzene.

Table 5. Numerical Values of Solute Descriptors for Compounds Studied.

Solute	E	S	A	B	L	V
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290
Radon	0.000	0.000	0.000	0.000	0.877	0.3840
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830
Nitrous oxide	0.068	0.350	0.000	0.100	0.164	0.2810
Nitric oxide	0.050	-0.150	0.000	0.040	-0.470	0.2026
Carbon monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809
Chlorine	0.360	0.320	0.100	0.000	1.193	0.3534
Iodine	1.398	0.670	0.280	0.000	3.681	0.6250
Mercury	0.850	0.430	0.000	0.040	1.721	0.3400
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643
Hydrogen peroxide	0.451	0.660	0.780	0.410	1.226	0.2260
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904
Propane	0.000	0.000	0.000	0.000	1.050	0.5313
Butane	0.000	0.000	0.000	0.000	1.615	0.6722
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949
Octane	0.000	0.000	0.000	0.000	3.677	1.2358
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.2358
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.3630
Tetracosane	0.000	0.000	0.000	0.000	11.758	3.4902
Octacosane	0.000	0.000	0.000	0.000	13.780	4.0538

Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.8454
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272
Ethene	0.110	0.100	0.000	0.070	0.289	0.3474
Propene	0.100	0.080	0.000	0.070	0.946	0.4883
1-Butene	0.100	0.080	0.000	0.070	1.529	0.6292
Isobutene	0.120	0.080	0.000	0.080	1.579	0.6292
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.9110
2-Methyl-1,3-butadiene	0.313	0.230	0.000	0.100	2.101	0.7271
cyclohexene	0.395	0.200	0.000	0.100	3.021	0.803
1,5-Hexadiene	0.191	0.150	0.000	0.100	2.450	0.8680
2,3-Dimethylbuta-1,3-diene	0.352	0.230	0.000	0.140	2.690	0.8680
2-Methylbut-2-ene	0.159	0.090	0.000	0.080	2.229	0.7701
2,2,4-Trimethyl-1-pentene	0.090	0.070	0.000	0.070	3.289	1.3337
Acetylene	0.190	0.600	0.060	0.040	0.140	0.3044
Chloromethane	0.250	0.430	0.000	0.080	1.163	0.3719
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943
Trichloromethane	0.430	0.490	0.150	0.020	2.480	0.6167
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.7391
1,1-Dichloroethane	0.320	0.490	0.100	0.100	2.316	0.6352
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352
1,1,1-Trichloroethane	0.370	0.410	0.000	0.090	2.733	0.7576
1,1,2-Trichloroethane	0.500	0.680	0.130	0.130	3.290	0.7576
1,1,2,2-Tetrachloroethane	0.600	0.760	0.160	0.120	3.803	0.8800
1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.6537
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946
1,2-Dichloropropane	0.370	0.630	0.000	0.170	2.836	0.7761
1,3-Dichloropropane	0.408	0.800	0.050	0.120	3.106	0.7761
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946
2-Chlorobutane	0.189	0.350	0.000	0.120	2.540	0.7946
Tetrachloroethene	0.640	0.440	0.000	0.000	3.584	0.8370
Bromoethane	0.366	0.400	0.000	0.120	2.120	0.5654
1-Bromopropane	0.366	0.400	0.000	0.120	2.620	0.7063
2-Bromo-2-methylpropane	0.305	0.290	0.000	0.070	2.609	0.8472
1-Bromobutane	0.360	0.400	0.000	0.120	3.105	0.8472
1,2-Dibromoethane	0.747	0.760	0.100	0.170	3.382	0.7404
Iodomethane	0.676	0.430	0.000	0.120	2.106	0.5077
Iodoethane	0.640	0.400	0.000	0.140	2.573	0.6486
1-Iodopropane	0.634	0.400	0.000	0.140	3.130	0.7895

1-Iodobutane	0.628	0.400	0.000	0.140	3.628	0.9304
1,1,2-Trifluorotrichloroethane	0.010	0.130	0.000	0.000	2.210	0.8107
Trifluorochloromethane	-0.250	-0.050	0.000	0.000	0.209	0.4250
Difluorodichloromethane	0.037	0.040	0.000	0.040	0.998	0.5297
Bromochloromethane	0.541	0.800	0.010	0.060	2.445	0.5469
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309
Dipropyl ether	0.008	0.250	0.000	0.450	2.954	1.0127
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.0127
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945
Methyl <i>tert</i> -butyl ether	0.024	0.220	0.000	0.550	2.372	0.8718
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223
Tetrahydropyran	0.296	0.500	0.000	0.470	3.017	0.7632
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810
Methyl butyl ether	0.045	0.250	0.000	0.440	2.658	0.8718
Ethyl butyl ether	0.013	0.250	0.000	0.450	2.989	1.0127
Dimethoxymethane	0.099	0.460	0.000	0.520	1.894	0.6487
Diethoxymethane	0.010	0.490	0.000	0.540	2.789	0.9305
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.7896
1-Methoxy-2-ethoxyethane	0.060	0.700	0.000	0.740	2.982	0.931
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829
2-Hexanone	0.136	0.680	0.000	0.510	3.286	0.9697
2-Heptanone	0.123	0.680	0.000	0.510	3.760	1.1106
2-Octanone	0.108	0.680	0.000	0.510	4.257	1.2515
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.7202
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8611
5-Methylfurfural	0.744	1.110	0.000	0.520	3.933	0.8339
2-Furaldehyde	0.690	1.130	0.000	0.450	3.318	0.6969
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.9462
Dimethyl carbonate	0.142	0.540	0.000	0.570	2.328	0.664
Propylene Carbonate	0.319	1.370	0.000	0.600	3.088	0.6967
delta-pentanolactone	0.441	1.520	0.000	0.630	3.680	0.7789
Ethyl formate	0.146	0.660	0.000	0.380	1.845	0.6057
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284

Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466
Methyl pentanonate	0.108	0.600	0.000	0.450	3.392	1.0284
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.1693
Ethyl acetoacetate	0.208	0.800	0.000	0.860	3.752	1.0441
Ethyl trifluoroacetate	-0.200	0.240	0.000	0.460	1.875	0.7997
Ethyl trichloroacetate	0.365	0.650	0.000	0.370	4.136	1.1138
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450
Ammonia	0.140	0.390	0.160	0.560	0.319	0.2084
Methylamine	0.250	0.350	0.160	0.580	1.300	0.3493
Ethylamine	0.236	0.350	0.160	0.610	1.677	0.4902
Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720
Dimethylamine	0.189	0.300	0.080	0.660	1.600	0.4902
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7720
Diisopropylamine	0.053	0.210	0.070	0.740	2.893	1.0538
Trimethylamine	0.140	0.200	0.000	0.670	1.620	0.6311
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237
1-Nitropropane	0.242	0.950	0.000	0.310	2.894	0.7055
2-Nitropropane	0.216	0.920	0.000	0.330	2.550	0.7055
Acetamide	0.460	1.300	0.550	0.690	2.990	0.5060
Propionamide	0.440	1.300	0.550	0.660	3.424	0.6468
N,N-Dimethylacetamide	0.363	1.380	0.000	0.800	3.639	0.7877
2,2,2-Trichloroacetamide	0.710	0.630	0.470	0.560	3.829	0.8731
Ethyl carbamate	0.290	1.380	0.330	0.460	3.234	0.7055
Formic acid	0.343	0.750	0.760	0.330	1.545	0.3239
Acetic acid	0.265	0.640	0.620	0.440	1.816	0.4648
Propanoic acid	0.233	0.650	0.610	0.440	2.276	0.6057
Butanoic acid	0.210	0.640	0.610	0.450	2.750	0.7466
2-Methylpropanoic acid	0.200	0.600	0.610	0.450	2.693	0.7466
Pentanoic acid	0.205	0.630	0.620	0.450	3.227	0.8875
3-Methylbutanoic acid	0.178	0.600	0.610	0.460	3.151	0.8875
Hexanoic acid	0.174	0.630	0.620	0.440	3.697	1.0284
2-Methylpentanoic acid	0.178	0.590	0.610	0.450	3.658	1.0284
Octanoic acid	0.150	0.650	0.620	0.450	4.680	1.3102
Chloroacetic acid	0.427	1.030	0.790	0.350	2.862	0.5872

Dichloroacetic acid	0.481	1.200	0.900	0.270		0.710
Trichloroacetic acid	0.524	1.210	1.010	0.260	4.102	0.8320
Succinic acid	0.370	1.320	1.030	0.710	3.951	0.8210
Carbon disulfide	0.876	0.260	0.000	0.030	2.370	0.4905
Water	0.000	0.450	0.820	0.350	0.260	0.1673
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.5900
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.7309
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.7309
2-Butanol	0.217	0.360	0.330	0.560	2.338	0.7309
2-Methyl-2-propanol	0.180	0.300	0.310	0.600	1.963	0.7309
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.8718
2-Pentanol	0.195	0.360	0.330	0.560	2.840	0.8718
1-Hexanol	0.210	0.420	0.370	0.480	3.610	1.0127
1-Heptanol	0.211	0.420	0.370	0.480	4.115	1.1536
1-Octanol	0.199	0.420	0.370	0.480	4.619	1.2945
2-Methyl-2-butanol	0.194	0.300	0.310	0.630	2.721	0.8718
2-Methyl-1-pentanol	0.211	0.390	0.310	0.560	3.471	1.0127
3-Methyl-1-pentanol	0.211	0.390	0.310	0.560	3.493	1.0127
2-Methyl-2-pentanol	0.169	0.300	0.310	0.640	3.240	1.0127
3-Methyl-2-pentanol	0.170	0.390	0.330	0.560	3.476	1.0127
4-Methyl-1-pentanol	0.196	0.390	0.330	0.530	3.439	1.0127
2-Methyl-3-pentanol	0.207	0.330	0.330	0.630	3.315	1.0127
4-Methyl-2-pentanol	0.167	0.330	0.330	0.550	3.263	1.0127
2,3-Dimethyl-2-butanol	0.208	0.270	0.310	0.650	3.223	1.0127
3,3-Dimethyl-1-butanol	0.188	0.360	0.310	0.610	3.332	1.0127
3-Methyl-3-hexanol	0.198	0.300	0.310	0.640	3.805	1.1536
2-Methyl-3-hexanol	0.200	0.330	0.330	0.620	3.839	1.1536
3-Methyl-2-hexanol	0.160	0.330	0.330	0.550	3.832	1.1536
2-Methyl-2-hexanol	0.163	0.300	0.310	0.630	3.686	1.1536
5-Methyl-2-hexanol	0.160	0.330	0.330	0.570	3.819	1.1536
3-Ethyl-3-pentanol	0.234	0.300	0.310	0.640	3.838	1.1536
4,4-Dimethyl-2-pentanol	0.190	0.330	0.330	0.570	3.858	1.1536
2,3-Dimethyl-3-pentanol	0.190	0.300	0.310	0.630	3.817	1.1536
2,2-Dimethyl-3-pentanol	0.227	0.300	0.300	0.550	3.856	1.1536
Cyclohexanol	0.460	0.540	0.320	0.570	3.758	0.9040

2-Propen-1-ol	0.342	0.460	0.380	0.480	1.951	0.5470
2-Chloroethanol	0.419	0.770	0.390	0.500	2.435	0.5715
3-Chloro-1-propanol	0.407	0.710	0.400	0.500	2.651	0.7124
1,3-Propanediol	0.397	0.890	0.770	0.870	2.863	0.6487
2-Ethoxyethanol	0.237	0.550	0.290	0.820	2.719	0.7896
Allyl alcohol	0.342	0.460	0.380	0.480	1.951	0.5470
Dimethyl sulfoxide	0.522	1.720	0.000	0.970	3.459	0.6126
Thiourea	0.840	0.790	0.820	0.900	3.262	0.5696
Tributylphosphine oxide	-0.009	1.150	0.000	1.640	7.505	2.0627
Trimethyl phosphate	0.113	1.360	0.000	0.930	3.850	0.9707
Triethyl phosphate	0.000	1.000	0.000	1.060	4.750	1.3934
Tripropyl phosphate	-0.050	1.070	0.000	1.130	6.341	1.8161
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982
1,2-Dimethylbenzene	0.663	0.560	0.000	0.160	3.939	0.9982
1,3-Dimethylbenzene	0.623	0.520	0.000	0.160	3.839	0.9982
1,4-Dimethylbenzene	0.613	0.520	0.000	0.160	3.839	0.9982
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544
Phenanthrene	2.055	1.290	0.000	0.290	7.632	1.4544
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5850
Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5850
<i>trans</i> -Stilbene	1.450	1.040	0.000	0.340	7.525	1.5630
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612
1,3-Dichlorobenzene	0.847	0.730	0.000	0.020	4.410	0.9612
1,4-Dichlorobenzene	0.825	0.750	0.000	0.020	4.435	0.9612
Hexachlorobenzene	1.490	0.990	0.000	0.000	7.624	1.4508
2-Chloronaphthalene	1.450	1.000	0.000	0.140	5.834	1.2078
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914
1,4-Dibromobenzene	1.150	0.860	0.000	0.040	5.324	1.0664
Iodobenzene	1.188	0.820	0.000	0.120	4.502	0.9746
Anisole	0.708	0.750	0.000	0.290	3.890	0.9160

Ethyl phenyl ether	0.681	0.700	0.000	0.320	4.242	1.0569
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730
2-Methoxybenzaldehyde	0.956	1.120	0.000	0.590	5.300	1.0726
Phenylacetaldehyde	0.811	1.020	0.000	0.430	4.426	1.0139
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.0139
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374
Benzophenone	1.447	1.500	0.000	0.500		1.4810
9-Fluorenone	1.600	1.490	0.000	0.350	7.474	1.3722
Methyl benzoate	0.733	0.850	0.000	0.460	4.704	1.0726
Phenyl acetate	0.661	1.130	0.000	0.540	4.414	1.0726
Dimethyl phthalate	0.780	1.260	0.000	0.860	6.051	1.4288
Diethyl phthalate	0.729	1.260	0.000	0.890	6.801	1.7106
Benzonitrile	0.742	1.110	0.000	0.330	4.039	0.8711
Phenylacetoneitrile	0.751	1.030	0.000	0.500	4.634	1.0120
1,2-Dicyanobenzene	0.874	1.960	0.000	0.410	5.595	1.0258
1,3-Dicyanobenzene	0.894	1.600	0.000	0.580	5.260	1.0258
1,4-Dicyanobenzene	0.874	1.980	0.000	0.420	5.634	1.0258
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571
4-Ethylaniline	0.942	0.910	0.230	0.450	4.859	1.0980
4-Propylaniline	0.922	0.900	0.230	0.480	5.514	1.2389
4-Isopropylaniline	0.922	0.870	0.230	0.540	5.386	1.2389
4-Butylaniline	0.914	0.880	0.210	0.500	5.771	1.3798
2-Chloroaniline	1.033	0.920	0.250	0.310	4.674	0.9390
3-Chloroaniline	1.053	1.100	0.300	0.300	4.909	0.9390
4-Chloroaniline	1.060	1.130	0.300	0.310	4.889	0.9390
2-Methoxyaniline	0.988	1.000	0.230	0.500	4.818	1.0160
2-Nitroaniline	1.180	1.370	0.300	0.360	5.627	0.9904
3-Nitroaniline	1.200	1.710	0.400	0.350	5.880	0.9904
4-Nitroaniline	1.220	1.920	0.460	0.350	6.042	0.9904
3-Aminoacetophenone	1.230	1.450	0.300	0.580	6.007	1.1137
4-Aminoacetophenone	1.190	1.470	0.320	0.480	6.111	1.1137
2,4-Dimethylaniline	0.950	0.950	0.200	0.500	4.983	1.0980
N-Methylaniline	0.948	0.900	0.170	0.430	4.478	0.9571
N,N-Dimethylaniline	0.957	0.810	0.000	0.410	4.701	1.0980
N,N-Diethylaniline	0.953	0.800	0.000	0.410	5.287	1.3798
1-Naphthylamine	1.670	1.270	0.190	0.510	6.490	1.1852

2-Napthylamine	1.670	1.300	0.180	0.510	6.540	1.1852
4-Aminobiphenyl	1.565	1.480	0.260	0.480	7.698	1.4240
Benzylamine	0.829	0.770	0.150	0.720	4.385	0.9571
1-Amino-2-phenylethane	0.824	1.010	0.290	0.720	5.064	1.0980
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906
2-Nitrotoluene	0.866	1.110	0.000	0.280	4.878	1.0315
3-Nitrotoluene	0.874	1.100	0.000	0.250	5.097	1.0315
4-Nitrotoluene	0.870	1.110	0.000	0.280	5.154	1.0315
4-Nitroanisole	0.980	1.440	0.000	0.360	5.450	1.0902
1,2-Dinitrobenzene	1.170	1.700	0.000	0.400	5.905	1.0648
1,3-Dinitrobenzene	1.150	1.600	0.000	0.470	5.903	1.0648
1,4-Dinitrobenzene	1.130	1.630	0.000	0.460	5.796	1.0648
Benzamide	0.990	1.500	0.490	0.670	5.767	0.9728
N-Methylbenzamide	0.950	1.490	0.400	0.710	5.773	1.1137
N-Ethylbenzamide	0.950	1.490	0.390	0.720	6.268	1.2546
N,N-Dimethylbenzamide	0.950	1.400	0.000	0.980	5.924	1.2546
Acetanilide	0.900	1.370	0.400	0.670	5.570	1.1137
Phthalimide	1.183	2.050	0.400	0.420	6.193	1.0208
Benzoic acid	0.730	0.900	0.590	0.400	4.657	0.9317
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726
4-Methylbenzoic acid	0.730	0.930	0.620	0.420	4.890	1.0726
4-Ethylbenzoic acid	0.730	0.900	0.610	0.390	5.355	1.2139
4-Butylbenzoic acid	0.730	0.900	0.630	0.420	6.363	1.4953
2-Chlorobenzoic acid	0.840	1.010	0.680	0.400	4.840	1.0541
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	4.947	1.0541
2-Bromobenzoic acid	1.000	1.000	0.640	0.530	5.454	1.1067
3-Bromobenzoic acid	1.000	1.100	0.640	0.270	5.526	1.1067
4-Bromobenzoic acid	1.000	1.010	0.630	0.260	5.399	1.1067
2-Iodobenzoic acid	1.310	1.270	0.740	0.460	6.364	1.1899
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.1313
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313
2-Nitrobenzoic acid	0.990	1.480	0.820	0.530	5.900	1.1059
3-Nitrobenzoic acid	0.990	1.130	0.730	0.530	5.535	1.1059
4-Nitrobenzoic acid	0.990	1.020	0.650	0.550	5.408	1.1059
4-Aminobenzoic acid	1.075	1.650	0.940	0.600	5.916	1.0315
Phenylacetic acid	0.730	1.080	0.660	0.570	4.962	1.0726
3-Phenylpropanoic acid	0.750	1.180	0.600	0.600	5.616	1.2135
4-Phenylbutanoic acid	0.760	1.290	0.610	0.570	6.204	1.3544

Phenol	0.805	0.890	0.600	0.300	3.766	0.7751
2-Methylphenol	0.840	0.860	0.520	0.300	4.218	0.9160
3-Methylphenol	0.822	0.880	0.570	0.340	4.310	0.9160
4-Methylphenol	0.820	0.870	0.570	0.310	4.312	0.9160
2,3-Dimethylphenol	0.850	0.820	0.510	0.370	4.495	1.0569
2,4-Dimethylphenol	0.843	0.790	0.520	0.400	4.770	1.0569
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569
2,6-Dimethylphenol	0.840	0.790	0.390	0.380	4.680	1.0569
3,5-Dimethylphenol	0.820	0.840	0.570	0.360	4.856	1.0569
2-Ethylphenol	0.831	0.840	0.520	0.370	4.612	1.0569
3-Ethylphenol	0.831	0.840	0.520	0.370	4.741	1.0569
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569
2-Isopropyl-5-methylphenol	0.822	0.840	0.440	0.430	5.801	1.3387
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928
4-Fluorophenol	0.670	0.970	0.630	0.230	3.844	0.7928
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501
4-Bromophenol	1.080	1.170	0.670	0.200	5.135	0.9501
2-Iodophenol	1.360	1.000	0.400	0.350	4.964	1.0333
4-Iodophenol	1.380	1.220	0.680	0.200	5.492	1.0333
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199
2,6-Dichlorophenol	0.900	0.900	0.380	0.240		1.0199
3,5-Dichlorophenol	1.020	1.000	0.910	0.000		1.0199
2,4-Dibromophenol	1.310	0.910	0.460	0.270	5.473	1.1251
2-Aminophenol	1.110	1.310	0.610	0.600	4.975	0.8749
3-Aminophenol	1.130	1.640	0.740	0.570	5.304	0.8749
4-Aminophenol	1.150	1.470	0.660	0.730	5.200	0.8749
2-Methoxyphenol	0.837	0.910	0.220	0.520	4.449	0.9747
3-Methoxyphenol	0.879	1.170	0.590	0.390	4.803	0.9747
4-Methoxyphenol	0.900	1.170	0.570	0.480	4.773	0.9747
2-Hydroxybenzaldehyde	0.962	1.050	0.120	0.330	4.570	0.9317
4-Hydroxyacetophenone	1.010	1.500	0.790	0.520	5.780	1.0726
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493
2,4-Dinitrophenol	1.200	1.490	0.090	0.560	5.981	1.1235

2,4,6-Trinitrophenol	1.430	2.660	0.460	0.420	8.128	1.298
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	4.732	0.9904
3-Hydroxybenzoic acid	0.910	0.880	0.860	0.580	4.860	0.9904
4-Hydroxybenzoic acid	0.930	0.900	0.810	0.560	4.867	0.9904
5-Bromosalicylic acid	1.497	1.070	0.620	0.430	6.346	1.1654
5-Nitrosalicylic acid	1.330	1.230	0.820	0.470	6.305	1.1646
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338
Methyl 4-hydroxybenzoate	0.900	1.370	0.690	0.450	5.716	1.1313
Ethyl 4-hydroxybenzoate	0.860	1.350	0.690	0.450	6.186	1.2722
Methyl 2-hydroxybenzoate	0.850	0.820	0.010	0.480	4.961	1.1313
Ethyl 2-hydroxybenzoate	0.802	0.860	0.010	0.460	5.246	1.2722
Propyl salicylate	0.793	0.900	0.020	0.430	5.955	1.4131
Butyl salicylate	0.784	0.850	0.150	0.350	6.541	1.5540
2-Hydroxybenzamide	1.160	1.580	0.610	0.510	5.820	1.0315
4-Hydroxy-3-methoxybenzaldehyde	0.990	1.300	0.310	0.680	5.727	1.1313
4-Hydroxypropiophenone	1.000	1.470	0.810	0.500	6.307	1.2135
4-Hydroxyacetanilide	1.060	1.630	1.040	0.860	6.430	1.1724
1-Naphthol	1.520	1.100	0.660	0.340	6.284	1.1441
2-Naphthol	1.520	1.080	0.610	0.400	6.200	1.1441
Benzyl alcohol	0.803	0.870	0.390	0.560	4.221	0.9160
2-Hydroxybenzyl alcohol	0.998	1.140	0.620	0.720	4.978	0.9747
2-Phenylethanol	0.811	0.860	0.310	0.650	4.628	1.0569
Ephedrine	0.916	0.740	0.210	1.210	6.150	1.4385
Methyl phenyl sulfoxide	1.104	1.750	0.000	0.880	6.545	1.0795
Diphenyl sulfoxide	1.500	1.640	0.000	0.960	7.972	1.5465
Diphenyl sulfone	1.570	2.150	0.000	0.700	8.902	1.6051
Methyl phenyl sulfone	1.080	1.850	0.000	0.760	6.234	1.1382
Phenylthiourea	1.250	1.690	0.480	0.790	5.376	1.1774
Benzenesulfonamide	1.130	1.550	0.550	0.800	5.977	1.0970
N-Methylbenzenesulfonamide	1.100	1.550	0.330	0.770	6.364	1.2380
N,N-Dimethylbenzenesulfonamide	1.100	1.580	0.000	0.820	6.594	1.3789
3-Methylbenzenesulfonamide	1.100	1.550	0.550	0.860	6.455	1.2380
4-Methylbenzenesulfonamide	1.100	1.550	0.550	0.870	6.469	1.2380
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.8162
3-Methylpyridine	0.631	0.810	0.000	0.540	3.631	0.8162
4-Methylpyridine	0.630	0.820	0.000	0.540	3.640	0.8162
2-Ethylpyridine	0.613	0.710	0.000	0.590	3.844	0.9571

2-Chloropyridine	0.738	1.040	0.000	0.370	3.875	0.7977
2-Bromopyridine	0.921	1.210	0.000	0.360	4.386	0.8503
2-Methoxypyridine	0.641	0.720	0.000	0.470	3.631	0.8749
2-Acetylpyridine	0.730	1.090	0.000	0.620	4.425	0.9728
2-Cyanopyridine	0.734	1.350	0.000	0.540	4.263	0.8300
3-Cyanopyridine	0.750	1.260	0.000	0.620	4.164	0.8300
4-Cyanopyridine	0.750	1.210	0.000	0.590	4.033	0.8300
4-Aminopyridine	0.980	0.920	0.430	0.670	4.079	0.7751
2-(N,N-Dimethylamino)pyridine	0.982	0.920	0.000	0.620	4.876	1.0569
Nicotine	0.865	0.880	0.000	1.090	5.880	1.3710
Piperidine	0.422	0.400	0.060	0.770	3.075	0.8043
N-Methylpiperidine	0.310	0.340	0.000	0.720	3.330	0.9452
Atropine	1.200	1.580	0.260	1.730	10.200	2.2820
N-Methyl-2-pyridone	0.914	1.100	0.000	1.040	4.334	0.8749
Quinoline	1.268	0.970	0.000	0.540	5.457	1.0443
Isoquinoline	1.211	1.000	0.000	0.540	5.595	1.0443
Pyrrole	0.613	0.910	0.220	0.250	2.792	0.5774
Carbazole	1.787	1.860	0.210	0.180	8.002	1.3154
N-Methylimidazole	0.589	0.950	0.000	0.800	3.805	0.6772
Benzimidazole	1.270	1.400	0.380	0.760	5.249	0.9053
2-Cyanopyrazine	0.761	1.070	0.000	0.650	3.795	0.7889
Pyrazine	0.629	0.820	0.000	0.640	2.875	0.6342
2-Methylpyrazine	0.629	0.850	0.000	0.660	3.333	0.7751
2,3-Dimethylpyrazine	0.657	0.800	0.000	0.740	3.826	0.9160
2,5-Dimethylpyrazine	0.686	0.740	0.000	0.740	3.851	0.9160
Trimethylpyrazine	0.659	0.740	0.000	0.810	4.277	1.0569
Tetramethylpyrazine	0.685	0.800	0.000	0.850	4.725	1.1978
2-Ethylpyrazine	0.616	0.840	0.000	0.670	3.887	0.9160
2,3-Diethylpyrazine	0.651	0.820	0.000	0.790	4.959	1.1978
2-Methyl-3-isobutylpyrazine	0.650	0.820	0.000	0.810	5.435	1.3387
2-Fluoropyrazine	0.496	0.760	0.000	0.510	2.714	0.6519
2-Chloropyrazine	0.727	0.940	0.000	0.450	3.627	0.7566
2-Methoxypyrazine	0.727	0.850	0.000	0.550	3.721	0.8338
2-Ethoxypyrazine	0.700	0.840	0.000	0.570	4.175	0.9747
2-Propoxypyrazine	0.695	0.820	0.000	0.570	4.675	1.1156
Methyl 2-pyrazinecarboxylate	0.752	1.640	0.000	0.750	5.028	0.9904
Ethyl 2-pyrazinecarboxylate	0.730	1.590	0.000	0.780	5.450	1.1313
2-(Dimethylamino)pyrimidine	0.940	0.900	0.000	0.720	4.685	1.0158

5-(Dimethylamino)pyrimidine	0.940	0.850	0.000	0.910	4.616	1.0158
2-Cyanopyrimidine	0.740	0.660	0.000	0.800	3.350	0.7889
2-Thiomethoxypyrimidine	1.060	1.160	0.000	0.580	4.780	0.9386
Pyrimidine	0.606	0.930	0.000	0.670	2.837	0.6342
2-Methylpyrimidine	0.600	0.850	0.000	0.750	3.373	0.7751
5-Methylpyrimidine	0.600	1.000	0.000	0.680	3.491	0.7751
2-Fluoropyrimidine	0.470	0.720	0.000	0.570	2.617	0.6519
5-Fluoropyrimidine	0.470	0.900	0.000	0.550	2.789	0.6519
2-Chloropyrimidine	0.720	0.860	0.000	0.600	3.395	0.7566
5-Chloropyrimidine	0.720	1.000	0.000	0.500	3.198	0.7566
2-Bromopyrimidine	0.880	0.890	0.000	0.610	3.631	0.8092
5-Bromopyrimidine	0.880	1.060	0.000	0.540	4.026	0.8092
2-Methoxypyrimidine	0.700	1.080	0.000	0.670	3.910	0.8338
2-Ethoxypyrimidine	0.680	1.070	0.000	0.680	4.337	0.9747
5-Ethoxypyrimidine	0.630	0.940	0.000	0.750	4.148	0.9747
Methyl 2-pyrimidinecarboxylate	0.730	1.680	0.000	0.930	5.012	0.9904
Methyl 5-pyrimidinecarboxylate	0.730	1.620	0.000	0.730	5.007	0.9904
Ethyl 2-pyrimidinecarboxylate	0.730	1.680	0.000	0.990	5.487	1.1313
Antipyrine	1.300	1.830	0.000	1.370	7.764	1.4846
N,N-Dimethylpiperazine	0.354	0.690	0.000	1.160	3.874	1.0450
1,2,4-Triazole	0.662	1.500	0.970	0.430	3.271	0.4952
Purine	1.320	1.250	0.780	0.880	5.128	0.8231
Adenine	1.680	1.590	0.900	0.930	6.068	0.9229
Morpholine	0.434	0.790	0.060	0.910	3.289	0.7221
N-Methylmorpholine	0.333	0.740	0.000	0.900	3.270	0.8630
Scopolamine	1.686	1.320	0.090	2.170	10.110	2.2321
Uracil	0.810	0.850	0.430	1.020	3.626	0.7516
1,3-Dimethyluracil	0.810	1.040	0.000	1.130	4.648	1.0334
Caffeine	1.500	1.820	0.080	1.250	7.838	1.3632
Guanine	1.800	1.460	0.970	1.250	6.566	0.9816
Codeine	1.960	1.950	0.220	1.790	11.040	2.2057
Thiophene	0.687	0.570	0.000	0.150	2.819	0.6411
Thiazole	0.706	0.930	0.000	0.430	2.877	0.6000
Phenylurea	1.110	1.330	0.790	0.790	6.332	1.0726
1-Phenyl-3,3-dimethylurea	1.050	1.590	0.410	0.900	6.812	1.3544
Barbituric acid	1.090	1.190	0.460	1.160	4.586	0.8103
5,5-Diethylbarbituric acid	1.030	1.000	0.580	1.120	6.368	1.3739
5-Ethyl-5-propylbarbituric acid	1.030	1.130	0.590	1.180	6.838	1.5148

5-Ethyl-5-(2-pentyl)barbital	1.030	1.170	0.620	1.190	8.064	1.7966
5-Allyl-5-ethylbarbital	1.160	1.200	0.600	1.220	7.010	1.4718
5-Ethyl-5-phenylbarbital	1.630	1.720	0.710	1.180	8.956	1.6999
Acetone oxime	0.390	0.660	0.370	0.560	2.557	0.6488
Cyclohexanone oxime	0.580	0.900	0.330	0.610	4.320	0.9609
Monuron	1.140	1.500	0.470	0.780	7.180	1.4768
Diuron	1.280	1.600	0.570	0.700	8.060	1.5992
Benzoylacetone	0.766	0.990	0.010	0.580	5.647	1.3114
18 Crown 6	0.400	1.470	0.000	2.100	8.228	2.0430
15 Crown 5	0.411	1.200	0.000	1.750	6.779	1.7025
16 Crown 5	0.410	1.170	0.000	1.760	7.276	1.8434
Betulin	1.790	2.120	0.700	1.140	17.470	3.8670
Acetylacetone	0.412	0.780	0.000	0.630	3.326	0.8445
Benzo 15 Crown 5	1.055	1.940	0.000	1.590	9.403	2.0285
Benzo 18 crown 6	1.045	2.470	0.000	1.900	11.076	2.3690
Dibenzo 18 Crown 6	1.690	2.730	0.000	1.780	13.384	2.6950
Dibenzo 24 Crown 8	1.680	3.400	0.000	2.340	16.414	3.3760
AC-B18C6 ^a	0.684	2.650	0.000	1.850	11.100	2.4776
Tetramethyltin	0.324	0.110	0.000	0.100	2.651	1.0431
Germanium tetrabromide	1.306	-0.050	0.850	0.570	4.902	1.0962
Germanium tetrachloride	0.463	-0.250	0.550	0.480	2.784	0.8858
Methyl mercuric (II) chloride	0.980	1.480	0.130	0.290	4.037	0.6463
Phenyl mercuric (II) chloride	1.650	1.820	0.170	0.430	6.841	1.1132
Carbamazepine	2.154	1.950	0.520	1.130	10.120	1.8106
Ibuprofen	0.730	0.695	0.565	0.790	7.184	1.7771
Zidovudine	1.830	1.500	0.510	1.850	9.249	1.8192
Lactic acid	0.350	0.860	0.720	0.720	2.874	0.6644
Trichlorofluoromethane	0.207	0.240	0.000	0.070	1.950	0.6344
Dichlorodifluoromethane	0.027	0.120	0.000	0.040	1.124	0.5297
HCN	0.213	0.890	0.400	0.060	1.010	0.2366
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209
2-Acetylpyrazine	0.837	1.310	0.000	0.730	4.636	0.9317
Digitoxin	3.460	5.560	1.670	4.350		5.6938
3-Methylindole	1.200	1.060	0.440	0.220	6.114	1.0870
3-Bromopyridine	0.906	1.010	0.000	0.340	4.185	0.8503
4-Hydroxybenzaldehyde	1.010	1.390	0.800	0.440	5.250	0.9317
4-Methylbenzyl alcohol	0.810	0.880	0.390	0.600	4.584	1.0569
Benzyl methyl ketone	0.748	0.900	0.000	0.700	4.726	1.1548

Thalidomide	1.920	2.810	0.360	1.190		1.7479
N-Methylthalidomide	1.982	2.430	0.000	1.280		1.8880
N-Propylthalidomide	1.894	2.450	0.000	1.280		2.1706
N-Pentylthalidomide	1.868	2.440	0.000	1.260		2.4524
4-Methyl-8-hydroxyquinoline	1.400	0.880	0.000	0.630	5.917	1.244
2-Methyl-8-hydroxyquinoline	1.400	0.950	0.000	0.620	6.136	1.244
Thiopental	1.480	1.360	0.550	1.040		1.9014
o-Vanillin	1.040	1.260	0.070	0.610	5.608	1.131
Procaineamide	1.268	2.160	0.570	1.500	9.860	2.0178
Paracetamol	1.060	1.630	1.040	0.860	6.430	1.1724
Thiophenol	1.000	0.800	0.120	0.170	4.110	0.8799
8-Hydroxyquinoline	1.450	1.010	0.020	0.590	5.790	1.1030
Benzotriazole	1.473	1.460	0.670	0.480	5.669	0.8642
Procaine	1.149	1.260	0.230	1.470	8.900	1.9767
8-Quinolinol	1.450	1.020	0.060	0.560	5.812	1.1030
Tributyl phosphate	-0.100	0.710	0.000	1.260	7.539	2.239
Bromopheniramine	1.600	1.530	0.000	1.360	10.543	2.262

^a 1,2-bis[2-(2-methoxyethoxy)ethoxy]benzene.

Figure 1. Comparison of calculated water-to-chloroform $\log P_{\text{chl}}$ (wet and dry) values based on Eqn. 16 versus experimental data.

Figure 2. Comparison of calculated gas-to-chloroform log K_{chl} (wet and dry) values based on Eqn. 20 versus experimental data.

Figure 3. Comparison of calculated water-to-carbon tetrachloride $\log P_{ct}$ (wet and dry) values based on Eqn. 24 versus experimental data.

Figure 4. Comparison of calculated gas-to-carbon tetrachloride $\log K_{ct}$ (wet and dry) values based on Eqn. 26 versus experimental data.