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Correlation of solute transfer into alkane solvents from water and from the gas phase with updated Abraham model equations

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Abstract

Literature data regarding partitioning of compounds from the gas phase to alkanes and from water to alkanes have been compiled and analyzed in accord with the Abraham solvation parameter model. Mathematical correlations have been developed for describing the partitioning behavior of organic solutes and gases into hexane, heptane, octane and decane. Derived mathematical expressions were found to predict the available partition coefficient data to within 0.15 log units or better.

Keywords: Alkane solvents; Partition coefficients; Gibbs energies of solvation; Activity coefficients

1. Introduction

Liquid-liquid extraction affords a convenient experimental method for removing trace impurities from organic solvents and chemical reagents, for pre-concentrating chemical analytes from aqueous samples prior to chemical analysis, and for isolating synthesized organic products from reaction solvent media. Extraction methods are based on the equilibrium solute partitioning in a biphasic liquid system containing two or more solvents having limited mutual solubility. Molecular interactions between the dissolved solute(s) and surrounding extraction solvents determine the solute's affinity for a given phase, which in turn affects both the solute recovery factor and chemical separation efficiency. Design of an effective extraction method requires complete (or nearly complete) solute recovery and large separation efficiency. Considerable attention has been given in recent years to developing predictive expressions to enable researchers to select the best biphasic partitioning system to achieve a desired chemical separation.

Of the proposed methods published in the chemical literature, the solvation parameter model of Abraham [1,2] is one of the more useful approaches for the analysis and prediction of Gibbs energies of partition in chemical and biological systems. The method has been successfully used to correlate both logarithms of the gas-to-organic solvent partition coefficients (log K) and logarithms of the water-to-organic solvent partition coefficients (log P) for more than 70 common organic solvents [3-8], as well as the partition coefficient data for solutes dissolved in 30 room temperature ionic liquids [9-15] and dissolved in nine alkane/polar organic solvent [16-22], in three diisopentyl ether/polar organic solvent [16, 17, 23] and in two 1,2-dichloroethane/polar organic solvent [16, 23] biphasic partitioning systems. The latter biphasic organic systems are needed for compounds that are not stable in an aqueous environment, or are too insoluble in water to enable an accurate determination of the water-to-organic solvent partition coefficient which might be used in calculating solute descriptors for future log P predictions.

The Abraham solvation parameter model relies on two linear free energy relationships, the first for transfer processes between two condensed phases:

$$-\Delta G_{trans}^{o}/RT = \log P = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \quad (1)$$

and the second process involving solute transfer from the gas phase:

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$$-\Delta G_{solv}^{o}/RT = \log K = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L} \quad (2)$$

The dependent variables in eqns. 1 and 2 are the logarithm of the water-to-organic solvent partition coefficient or alkane-to-polar organic solvent partition coefficient, log *P*, and the logarithm of the gas-to-organic solvent partition coefficient, log *K*, for a series of solutes. The partition coefficient when multiplied by the negative product of the universal gas constant times the system temperature equals the Gibbs energy for solute transfer between the two respective immiscible phases. In the case of solute transfer from the gas phase the property is referred to as the Gibbs energy of solvation, ΔG_{solv}^{o}.

The upper case letters in Eqns. 1 and 2 denote the solute descriptors as follows: **E** is the solute excess molar refraction in $cm^3\ mol^{-1}/10$, **S** is the solute dipolarity/polarizability, **A** is the overall solute hydrogen bond acidity, **B** is the overall solute hydrogen bond basicity, **V** is McGowan's characteristic molecular volume in $cm^3\ mol^{-1}/100$ and **L** is the logarithm of the gas-to-hexadecane partition coefficient measured at 298 K. The lower case regression coefficients and constants (c_p, e_p, s_p, a_p, b_p, v_p, c_k, e_k, s_k, a_k, b_k and l_k) in Eqns. 1 and 2 are obtained by multiple linear regression analysis of experimental partition coefficient data for a specific biphasic system. The regression coefficients and constants reflect the properties of the solubilizing media. The two terms, $e \cdot \mathbf{E}$ and $s \cdot \mathbf{S}$, describe the polar contributions to the partition process: capability of interacting with the solute's π- and nonbonding electrons (e_p and e_k), solvent/-process dipolarity/polarizability (s_p and s_k), solvent/process hydrogen-bond basicity (a_p and a_k) and the solvent/process hydrogen-bond acidity (b_p and b_k). Acidic solutes interact with the basic phase sites ($a_p \cdot \mathbf{A}$ and $a_k \cdot \mathbf{A}$ terms), while basic solutes interact with the acidic phase sites ($b_p \cdot \mathbf{B}$ and $b_k \cdot \mathbf{B}$ terms). The last term in Eqns. 1 and 2 is the hydrophobic contribution, and is a measure of the relative ease of forming a cavity in which the dissolved solute will reside for each phase. For any fully characterized partitioning system (those with calculated values for the equation coefficients), further values of log *P* and log *K* can be estimated with known values for the solute descriptors.

Currently, we are in the process of updating several of the older Abraham model correlations that were based on small datasets. Our existing equations for hexane, heptane, octane and decane are more than 12 years old [24], and were derived from 173 log *P* and 117 log *K* values for hexane, 183 log *P* and 107 log *K* values for heptane, 149 log *P* and 105 log *K* values for octane, and 62 log *P* and 60 log *K* values for decane. Standard deviations for the published log *P* correlations ranged from SD = 0.144 to SD = 0.254 log units, and from SD = 0.065 to SD = 0.102 log units for the published log *K* correlations. Moreover, the databases used in constructing these earlier Abraham model correlations were not published, and are thus not available for other research groups to use in developing new predictive methods. In fact, Lee *et al.* [25] noted in their study extending the applicability and predictability of their solvation free energy density (SFED) model that only 10 solvents could be studied due to the limited availability of experimental ΔG_{solv}^{o} data. Hexane and heptane were two of the ten solvents studied by the authors; however, the data sets used contained only 49 (hexane) and 54 (heptane) experimental values.

In the present study we have updated our existing Abraham model correlations for hexane, heptane, octane and decane based on larger databases containing a more chemical diverse set of solutes spanning a much wide range of solute descriptor values. Updated Abraham model log *P* and log *K* correlations have been derived for hexane based on 201 log *P* (SD = 0.158) and 196 log *K* (SD = 0.121) data points, for heptane based on 185 log *P* (SD = 0.143) and 186 log *K* (SD = 0.115) experimental values, for octane based on 174 log *P* (SD = 0.129) and 174 log *K* (SD = 0.115) values, and for decane based on 138 log *P* (SD = 0.138) and 138 log *K* (SD = 0.119) data points. The updated log *P* and log *K* correlations were validated through training set and test set analyses.

2. Data sets and computation methodology

Most of the experimental data [25-91] that we were able to retrieve from the published literature pertained either to the Raoult's law infinite dilution activity coefficient, γ_{solute}^{∞}, Henry's law constants (solute concentrations are in mole fraction), K_{Henry}, or solubilities for gaseous solutes dissolved in hexane, heptane, octane and decane. 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. 3 and 4

$$\log K = \log \left(\frac{RT}{\gamma_{solute}^{\infty} P_{solute}^{o} V_{solvent}} \right) \quad (3)$$

$$\log K = \log \left(\frac{RT}{K_{Henry} V_{solvent}} \right) \quad (4)$$

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or to log *P* values for partition from water to solvent through Eqn. 5 where K_w is the gas to water partition coefficient.

$$\log P = \log K - \log K_w \quad (5)$$

In Eqns. 3 and 4, R is the universal gas constant, *T* is the system temperature, P_{solute}^{o} 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.

Our experimental databases also contain measured solubility data [92-118] for several crystalline solutes dissolved in the four alkanes and in water. The solubility data were taken largely from our previously published solubility studies. In the case of crystalline solutes, the partition coefficient between water and the anhydrous organic solvent is calculated as a solubility ratio

$$P = C_{solute,organic\ solvent}/C_{solute,water} \quad (6)$$

of the solute's molar solubilities (in units of moles per liter) in the organic solvent, $C_{solute,organic\ solvent}$, and in water, $C_{solute,water}$. Molar solubilities can also be used to calculate log *K* values, provided that the equilibrium vapor pressure of the solute above crystalline solute, P_{solute}^{o}, at 298 K is also available. P_{solute}^{o} can be transformed into the gas phase concentration, $C_{solute,gas}$, and the gas-to-water and gas-to-organic solvent partitions, K_w and *K*, can be obtained through the following equations

$$K_w = C_{solute,water}/C_{solute,gas} \quad \text{or}$$
$$K = C_{solute,organic\ solvent}/C_{solute,gas} \quad (7)$$

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

Several published articles reporting experimental partition coefficient data for alcohols [119-123], alkyl esters [124], substituted phenols [125-133], substituted anilines [134, 135], substituted benzenediols [136] and a few miscellaneous organic compounds [121, 131, 137-146] were also found. These latter values pertain to practical partitioning studies where the aqueous and alkane phases were in direct contact with each other. Given the small mole fraction solubilities of water in the four alkane solvents at 298 K (x_{water} = 4.76 x 10^{-4} for hexane [147], x_{water} = 5.10 x 10^{-4} for heptane [90], x_{water} = 5.01 x 10^{-4} for octane [148] and x_{water} = 5.70 x 10^{-4} for decane [90], and the small mole fraction solubilities of the alkanes in water at 298 K (x_{hexane} = 2.57 x 10^{-6} [149], $x_{heptane}$ = 6.43 x 10^{-7} [149], x_{octane} = 1.74 x 10^{-7} [149] and x_{decane} = 6.27 x 10^{-9}) [150], we elected to combine the "dry" and "wet" data sets. Water and the linear alkane solvents are "almost" completely immiscible with each other at 298 K. The experimental log *K* and log *P* values at 298 K for hexane, heptane, octane and decane are listed in Tables 1-4 (see Appendix), respectively. Also included in the tables are the literature references pertaining to the log *K* and log *P* data, and the numerical values for the solute descriptors for all of the compounds considered in the present study. The tabulated values came from our solute descriptor database, and were obtained using various types of experimental data, including water-to-solvent partitions, gas-to-solvent partitions, solubility and chromatographic data [9-11, 15, 16].

3. Results and Discussion

We have assembled in Table 1 196 experimental log *K* and 201 experimental log *P* values for the partitioning of organic solutes and gases between the gas phase and hexane, and between water and hexane at 298 K. The solutes considered cover a reasonably wide range of compound type and descriptor values. Preliminary analysis of the experimental log *K* data yielded a correlation equation having very small s_k, a_k and b_k coefficients, as would be expected from the molecular structure considerations. Hexane is a nonpolar saturated hydrocarbon and does not have an acidic hydrogen or any basic sites for hydrogen-bond formation. The s_k, a_k and b_k-coefficients were set equal to zero, and the final regression analyses performed to give:

$$\log P = 0.333(0.032) + 0.560(0.014)\ \mathbf{E} - 1.710(0.053)\ \mathbf{S} - 3.578(0.051)\ \mathbf{A} - 4.939(0.065)\ \mathbf{B} + 4.463(0.037)\ \mathbf{V} \quad (8)$$
(N = 201, SD = 0.156, R^2 = 0.996, F = 8671)

and

$$\log K = 0.274(0.017) - 0.210(0.026)\ \mathbf{E} + 0.991(0.007)\ \mathbf{L} \quad (9)$$
(N = 196, SD = 0.120, R^2 = 0.997, F = 30750)

All regression analyses were performed using SPSS statistical software. The numerical values given in parenthesis denote the standard errors in the calculated equation coefficients. Here and elsewhere, N corresponds to the number of solutes, R denotes the correlation coefficient, SD is the standard deviation and F corresponds to the Fisher F-statistic. The statistics of both correlations are quite good as evidenced by the near unity values of the squared

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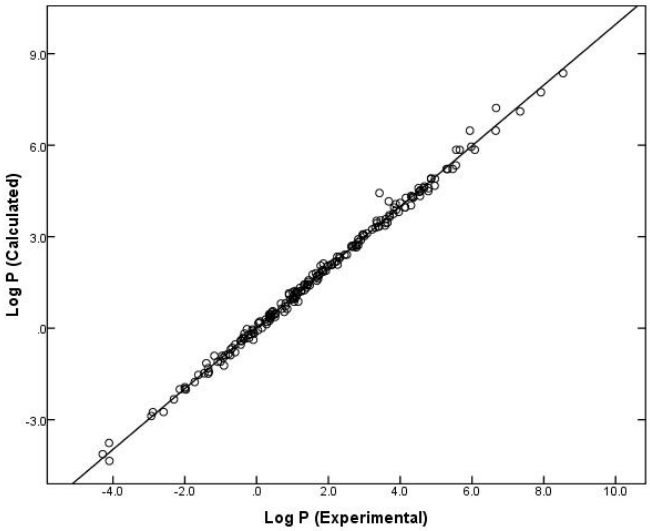

Figure 1. Comparison of experimental log *P* data versus calculated values based on Eqn. 8 for solutes dissolved in hexane.

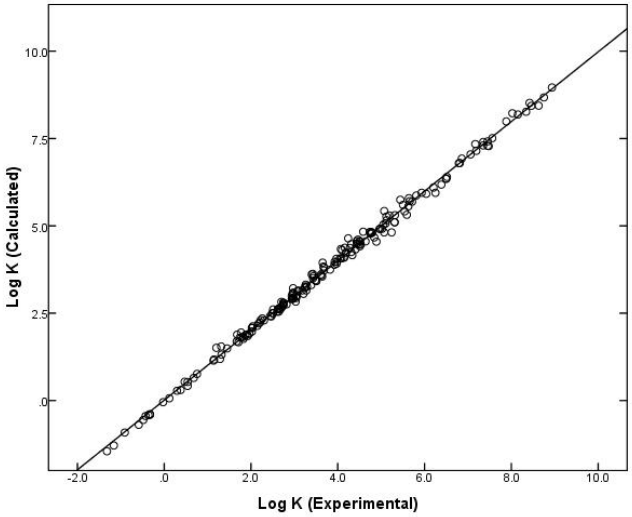

Figure 2. Comparison of experimental log *K* data versus calculated values based on Eqn. 9 for solutes dissolved in hexane.

correlation coefficients and by the small standard deviations of SD = 0.156 and SD = 0.120 log units. The statistics of the updated Abraham model correlations for hexane (Eqns. 8 and 9) are much better than our earlier published correlations based on much smaller data sets. The standard deviation of the earlier log *P* equation for hexane was SD = 0.207 [24]. See Figures 1 and 2 for plots of the calculated log *P* and log *K* values based on Eqns. 8 and 9 against observed data. The experimental log *P* and log *K* values cover ranges of about 12.8 and 10.3 log units, respectively.

In order to assess the predictive ability of Eqns. 8 and 9 we divided the data points into a training set and a test set by allowing the SPSS software to randomly select half of the experimental data points. The selected data points became the training sets and the remaining compounds that were left served as the test sets. Analysis of the experimental data in the log *P* and log *K* training sets gave:

log *P* = 0.322(0.043) + 0.491(0.059) **E** – 1.688(0.077) **S** – 3.479(0.075) **A** – 4.972(0.093) **B** + 4.482(0.050) **V** (10)
(N = 101, SD = 0.160, R^2 = 0.995, F = 3881)
and
log *K* = 0.270(0.020) – 0.216(0.030) **E** + 0.993(0.007) **L** (11)
(N = 98, SD = 0.109, R^2 = 0.998, F = 20960)

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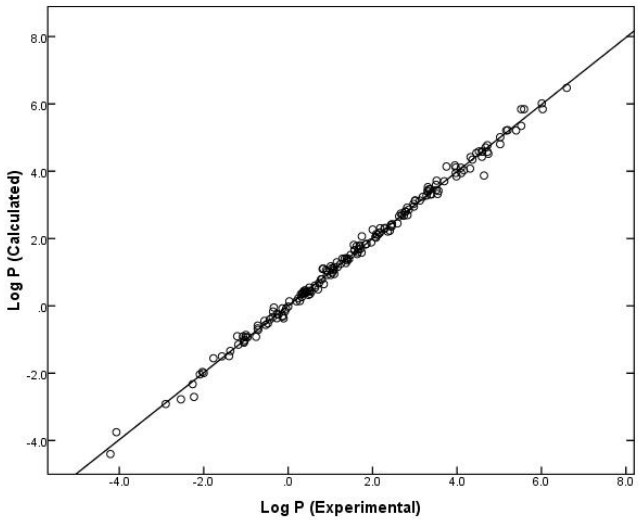

Figure 3. Comparison of experimental log *P* data versus calculated values based on Eqn. 12 for solutes dissolved in heptane.

There is very little difference in the equation coefficients for the full dataset and the training dataset correlations, thus showing that both training sets of compounds are representative samples of the total log *P* and log *K* data sets. The derived training set equations were then used to predict the respective partition coefficients for the compounds in the test sets. For the predicted and experimental values, we found SD = 0.160 (Eqn. 10) and SD = 0.131 (Eqn. 11), AAE (Average absolute error) = 0.114 (Eqn. 10) and AAE = 0.094 (Eqn. 11), and AE (Average error) = 0.029 (Eqn. 10) and AE = 0.003 (Eqn. 11). The numerical values of AAE and AE are using the calculated and experimental partition coefficient data as follows: AAE = (1/N) Σ |log P_{calc}(or K_{calc}) – log P_{exp}(or K_{exp})| and AE = (1/N) Σ (log P_{calc}(or K_{calc}) – log P_{exp}(or K_{exp})), with both summations extending over all of the data points in the two test sets. There is therefore very little bias in using Eqns. 10 and 11 with AE equal to 0.029 and 0.003 log units. The training and test set analyses were performed more than five times with similar results.

The heptane database is the second largest of the alkane data sets considered in the present study, and contains 185 experimental log *P* data points and 186 experimental log *K* values. Regression analysis of the tabulated experimental values in Table 2 gave the following two mathematical expressions:

log *P* = 0.297(0.029) + 0.634(0.039) **E** – 1.755(0.049) **S** – 3.571(0.050) **A** – 4.946(0.063) **B** + 4.488(0.040) **V** (12)
(N = 185, SD = 0.141, R^2 = 0.996, F = 7941)
and
log *K* = 0.251(0.016) – 0.155(0.027) **E** + 0.985(0.007) **L** (13)
(N = 186, SD = 0.114, R^2 = 0.997, F = 34477)

The s_k, a_k and b_k coefficients in the log *K* correlation were found to be negligible, and were removed from the final correlation. Both correlations provide a reasonably accurate mathematical description of the experimental water-to-heptane partition coefficient data (Eqn. 12) and gas-to-heptane partition coefficient data (Eqn. 13) for experimental values that cover ranges of about 10.8 and 10.8 log units, respectively. We note that the standard deviation in the updated log P correlation is significantly less than the standard deviation for our previously published heptane correlation equation, SD = 0.141 for Eqn. 12 versus a value of SD = 0.254 [24] for the earlier correlation. Comparisons of predicted values versus the observed data are given in Figures 3 and 4.

The predictive ability of Eqns. 12 and 13 was assessed as before by allowing the SPSS software to randomly divide the total data points into training and test sets as before. Analyses of the experimental data in the two training sets yielded:

log *P* = 0.308(0.045) + 0.638(0.060) **E** – 1.772(0.075) **S** – 3.563(0.085) **A** – 4.951(0.098) **B** + 4.485(0.062) **V** (14)
(N = 93, SD = 0.158, R^2 = 0.994, F = 2873)
and
log *K* = 0.251(0.021) – 0.163(0.038) **E** + 0.982(0.010) **L** (15)
(N = 93, SD = 0.116, R^2 = 0.998, F = 19133)

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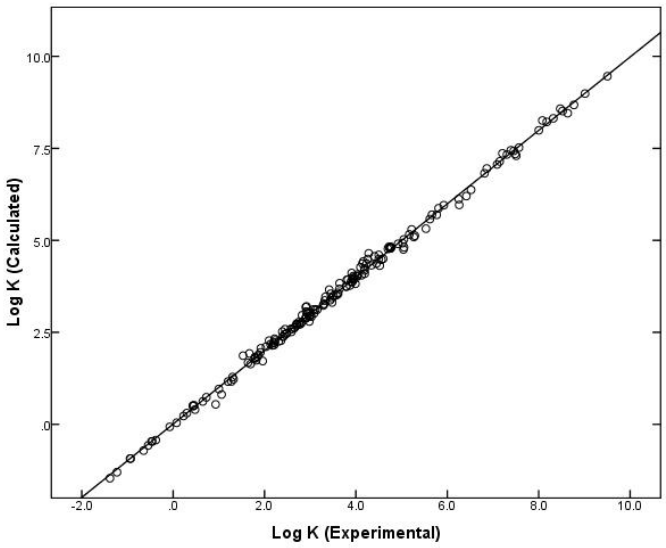

Figure 4. Comparison of experimental log *K* data versus calculated values based on Eqn. 13 for solutes dissolved in heptane.

Careful examination of Eqns. 12 versus 14, and Eqns. 13 versus 15 reveals that there is very little difference in the equation coefficients for the full dataset and the training dataset correlations. Both training sets of compounds are representative samples of the total log *P* and log *K* data sets. The derived training set equations were then used to predict the respective partition coefficients for the compounds in the test sets. For the predicted and experimental values, we found SD = 0.122 (Eqn. 14) and SD = 0.112 (Eqn. 15), AAE = 0.088 (Eqn. 14) and AAE = 0.082 (Eqn. 15), and AE = –0.001 (Eqn. 14) and AE = 0.029 (Eqn. 15). There is therefore very little bias in using Eqns. 14 and 15 with AE equal to –0.001 and 0.029 log units. The training and test set analyses were performed five more times with similar results.

The experimental log P and log K data in Tables 3 and 4 for octane and decane were analyzed in similar fashion to give the following Abraham model correlations:

$$\log P = 0.231(0.044) + 0.738(0.059)\ \mathbf{E} - 1.840(0.072)\ \mathbf{S} - 3.585(0.069)\ \mathbf{A} - 4.907(0.097)\ \mathbf{B} + 4.502(0.059)\ \mathbf{V} \quad (16)$$

(N = 174, SD = 0.206, R^2 = 0.990, F = 3485)

$$\log K = 0.188(0.016) - 0.122(0.026)\ \mathbf{E} + 0.987(0.007)\ \mathbf{L} \quad (17)$$

(N = 174, SD = 0.110, R^2 = 0.998, F = 37178)

and

$$\log P = 0.186(0.032) + 0.722(0.044)\ \mathbf{E} - 1.741(0.054)\ \mathbf{S} - 3.449(0.056)\ \mathbf{A} - 4.970(0.065)\ \mathbf{B} + 4.476(0.040)\ \mathbf{V} \quad (18)$$

(N = 139, SD = 0.134, R^2 = 0.996, F = 7113)

$$\log K = 0.141(0.019) - 0.064(0.029)\ \mathbf{E} + 0.986(0.008)\ \mathbf{L} \quad (19)$$

(N = 139, SD = 0.113, R^2 = 0.998, F = 30937)

Equations 16 and 17 pertain to solute transfer to octane, while Eqns. 18 and 19 describe the partition coefficient data for solutes dissolved in decane. Preliminary regression analysis showed the s_k, a_k and b_k term in Eqns. 17 and 19 to be negligible; thus the three terms were removed from the final set of log *K* equations. The derived Abraham model correlations provide a good mathematical description of the experimental partition coefficient data for solute transfer to both saturated alkane solvents from both water and the gas phase. As an informational note, the standard deviation of our previously reported log P correlation equation for octane, SD = 0.205 [24], was significantly larger. The robustness of each correlation was determined through a training set and test set analyses as before by splitting the large data set in half. To conserve journal space we give only the test results. The octane training set correlations predicted the experimental log *P* values in the test set to within SD = 0.113, AAE = 0.084 and AE = –0.006, and the experimental log *K* values in the test set to within SD = 0.116, AAE = 0.088 and AE = –0.039. Statistical information for the decane test analyses were: SD = 0.121 (Eqn. 18) and SD = 0.132 (Eqn. 19), AAE = 0.091 (Eqn. 18) and AAE = 0.085 (Eqn. 19), and AE = –0.005 (Eqn. 18) and AE = –0.009 (Eqn. 19). The training and test set analyses for each alkane solvent were performed five more times with similar results.

The present study shows that the correlations derived from the Abraham solvation

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Table 5. The coefficients in Equations for log P, together with C(N) the number of carbon atoms in the alkane solvents.

Solvent	C(N)	c	e	s	a	b	v
Hexane	6	0.333	0.560	-1.710	-3.578	-4.939	4.463
Heptane	7	0.297	0.634	-1.755	-3.571	-4.946	4.488
Octane	8	0.231	0.738	-1.840	-3.685	-4.907	4.502
Decane	10	0.186	0.722	-1.741	-3.449	-4.970	4.476
Undecane	11	0.058	0.603	-1.661	-3.421	-5.120	4.619
Dodecane	12	0.114	0.668	-1.644	-3.545	-5.006	4.459
Hexadecane	16	0.087	0.667	-1.617	-3.587	-4.869	4.433

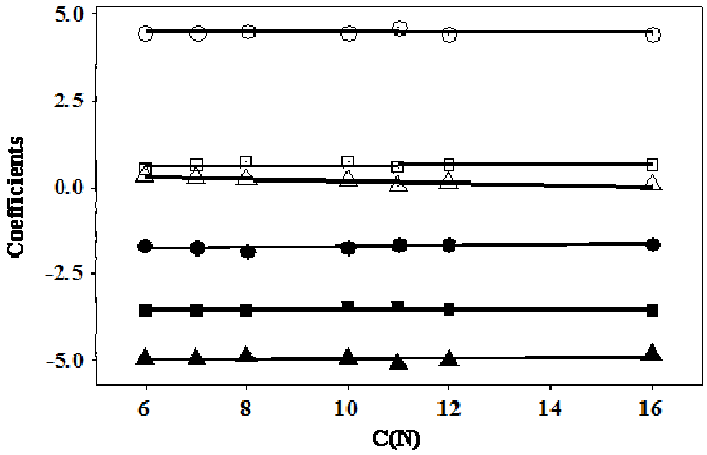

Figure 5. Plots of the coefficients in equations for log *P* against the number of carbon atoms in the alkane solvent: Δ c; □ e; ● s; ■ a; ▲b; ○ v.

parameter model provide reasonably accurate mathematical descriptions of solute transfer at 298 K from both water and from the gas phase into hexane, heptane, octane and decane. Derived mathematical expressions are expected to provide reasonable predictions of log *P* and log *K* for those solute molecules having known Abraham solute descriptor values, provided that the numerical values fall within the range of values used in deriving Eqns. 8 – 19. Numerical values of the solute descriptors covered by the data set range from: **E** = –0.060 to **E** = 2.808; **S** = 0.000 to **S** = 2.100; **A** = 0.000 to **A** = 1.090; **B** = 0.000 to **B** = 0.910; **V** = 0.068 to **V** = 1.864; and **L** = –1.741 to **L** = 9.603. The databases used in developing our earlier hexane, heptane, octane and decane correlations were never reported, and as a result one can only guess the predictive area of chemical space covered by the earlier expressions.

For informational purposes we note that the derived log P and log K correlations pertain to 298 K. Many commercial manufacturing and separation processes occur at higher temperatures, and there is a growing need to estimate partition properties into organic solvents at other temperatures. In this regard, we have published enthalpy of solvation correlations, ΔH_{solv}, for organic vapors and gaseous solutes into water [151] and into hexane [152] and heptane [153]. The ΔH_{solv} correlations will allow one to extrapolate the predicted log P and log K values based on Eqns. 8, 9, 12 and 13 to other temperatures not too far removed from 298 K. For octane and decane we have developed a generic alkane correlation [152] that can be used to estimate ΔH_{solv} values needed in the temperature extrapolation.

We now have updated coefficients in equations for partition from water into hexane, heptane, octane and decane. In addition, we have previously obtained coefficients in the corresponding equations for undecane and dodecane [4], and it is of some interest to compare coefficients along the alkane series. Details are in Table 5, together with C(N), the number of carbon atoms in the alkane. There are remarkable linear plots of the coefficients against C(N), as shown in Figure 5, showing that the various equations are quite consistent. The plots are so good that it should be possible to use them to obtain coefficients for log *P* equations for

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Table 6. The coefficients in Equations for log K together with C(N) the number of carbon atoms in the alkane solvents.

Solvent	C(N)	c	l
Hexane	6	0.320	0.945
Heptane	7	0.284	0.950
Octane	8	0.219	0.960
Decane	10	0.159	0.972
Undecane	11	0.113	0.971
Dodecane	12	0.017	0.989
Hexadecane	16	0.000	1.000

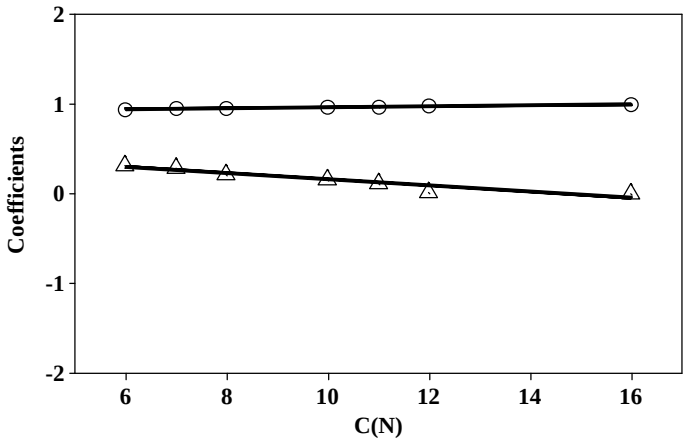

Figure 6. Plots of the coefficients for log *K* against the number of carbon atoms in the alkane solvents: Δ c; ○ l.

partition to nonane, tridecane, tetradecane and pentadecane provided that a number of experimental log *P* values are available as checks. Previously [4] we analyzed log *K* values from the gas phase to undecane and dodecane using only the **L**-descriptor. In order to compare the present work, we therefore determined corresponding equations for hexane, heptane, octane and decane as follows:

log *K*(Hexane) = 0.320(0.019) + 0.945(0.004) **L** (20)
(N = 196, SD = 0.139, R^2 = 0.996, F = 46263)

log *K*(Heptane) = 0.284(0.016) + 0.950(0.004) **L** (21)
(N = 186, SD = 0.124, R^2 = 0.997, F = 58927)

log *K*(Octane) = 0.219(0.016) + 0.960(0.004) **L** (22)
(N = 174, SD = 0.117, R^2 = 0.997, F = 66059)

log *K*(Decane) = 0.159(0.017) + 0.972(0.004) **L** (23)
(N = 139, SD = 0.115, R^2 = 0.998, F = 60149)

The values of SD in Eqns. 20-23 are a little higher than those in equations with the additional descriptor, but Eqns 20-23 are still excellent. The coefficients for all the alkane solvents are in Table 6, and plots of the coefficients against C(N) are shown in Figure 6. Note that the scale in Figure 6 is much larger than that in Figure 5. The equations with just the **L**-descriptor are remarkably consistent, and could be used to obtain coefficients for the missing alkane solvents.

4. Conclusions

The present study shows that the correlations derived from the Abraham solvation parameter model provide reasonably accurate mathematical descriptions of solute transfer at 298 K from both water and from the gas phase into hexane, heptane, octane and decane. The derived correlations should provide reasonably accurate predictions of the water-to-alkane and gas-to-alkane partition coefficients at 298 K for

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additional organic compounds and gases. The predicted partition coefficients can be converted to infinite dilution activity coefficients, γ_{solute}^{∞}, through the standard thermodynamic relationships given by Eqns. 3 – 5.

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Appendix

Table 1. Experimental log *P* and log *K* data for solutes dissolved in hexane at 298 K.

Solute	**E**	**S**	**A**	**B**	**L**	**V**	log *K*	log *P*	Ref
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	-1.320	0.700	85
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.161	0.799	85
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.328	1.142	85
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	0.118	1.328	85
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	0.680	1.650	28
Radon	0.000	0.000	0.000	0.000	0.877	0.3840	1.137	1.787	29
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-0.909	0.811	31
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.428	1.082	85
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-0.588	1.212	85
Nitrous Oxide	0.068	0.350	0.000	0.100	0.164	0.2810	0.540	0.770	60
Nitric oxide	0.370	0.020	0.000	0.090	-0.590	0.2026	-0.329	0.998	66
Carbon monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	-0.483	1.137	30
Iodine	1.398	0.670	0.280	0.000	3.681	0.6250	3.424	1.564	112
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.025	1.436	85
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	0.757	2.097	27
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.320	2.760	27
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.870	3.390	27
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.710	3.410	27
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	2.440	4.140	26
2,2-Dimethylpropane	0.000	0.000	0.000	0.000	1.820	0.8131	2.030	3.830	35
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.970	4.790	26

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2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540	2.820	4.660	26
2,2-Dimethylbutane	0.000	0.000	0.000	0.000	2.352	0.9540	2.670	4.510	35
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	3.500	5.460	26
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949	3.210	5.290	26
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.970	6.080	26
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.2358	3.640	5.660	26
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358	3.680	5.560	26
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	4.510	6.660	26
3,3-Diethylpentane	0.000	0.000	0.000	0.000	4.013	1.3767	4.310	5.940	35
Decane	0.000	0.000	0.000	0.000	4.686	1.5180	5.022	7.342	65
Undecane	0.000	0.000	0.000	0.000	5.191	1.6590	5.540	7.920	63
Dodecane	0.000	0.000	0.000	0.000	5.696	1.7990	6.038	8.538	64
Cyclopropane	0.408	0.230	0.000	0.000	1.314	0.4227	1.450	2.000	67
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.7045	2.710	3.590	35
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	3.100	4.000	26
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272	3.970	5.550	26
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	0.471	1.411	27
Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.286	2.256	27
1-Butene	0.100	0.080	0.000	0.070	1.529	0.6292	1.826	2.826	27
2-Methylpropene	0.120	0.080	0.000	0.080	1.579	0.6292	1.780	2.640	27
Ethyne	0.190	0.470	0.120	0.050	0.070	0.3044	0.380	0.380	86
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.364	1.926	85
Trichloromethane	0.430	0.490	0.150	0.020	2.480	0.6167	2.650	1.860	33
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.7391	3.030	3.220	33
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	1.908	1.448	32

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1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352	2.750	1.480	33
1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.6537	2.470	2.230	32
1,2-Dichloropropane	0.370	0.630	0.000	0.170	2.836	0.7761	3.055	2.085	48
1,3-Dichloropropane	0.408	0.800	0.050	0.120	3.106	0.7761	3.250	1.860	48
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946	2.950	2.830	33
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	2.510	3.310	33
1-Chloropentane	0.210	0.380	0.000	0.090	3.223	0.9355	3.506	3.456	32
Bromoethane	0.370	0.400	0.000	0.120	2.120	0.5654	2.302	1.762	32
2-Bromo-2-methylpropane	0.305	0.290	0.000	0.070	2.609	0.8472	2.750	3.350	32
Iodoethane	0.640	0.400	0.000	0.150	2.573	0.6486	2.709	2.169	32
1,2-Difluorotetrachloroethane	0.227	0.330	0.000	0.020	3.034	0.9154	3.250	3.890	61
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	1.313	-0.087	62
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945	4.334	3.644	70
Ethyl *tert*-butyl ether	-0.020	0.180	0.000	0.590	2.699	1.0127	2.980	1.710	49
Methyl *tert*-pentyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	3.275	1.680	71
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	2.700	0.150	33
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	2.980	-0.730	40
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	1.963	-0.867	91
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	2.490	-0.230	56
Hexan-2-one	0.136	0.680	0.000	0.510	3.286	0.9697	3.430	1.020	121
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.1106	3.929	1.679	121
3,3-Dimethylbutan-2-one	0.106	0.620	0.000	0.510	2.928	0.9697	3.181	0.901	121
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8611	3.650	0.050	33
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	2.146	-0.154	124
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	2.640	0.480	33

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Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	2.955	0.905	124
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	3.624	1.684	124
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	4.084	2.244	124
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	2.672	0.522	124
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	3.613	1.733	124
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.1693	4.139	2.309	124
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	1.770	-1.080	33
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450	2.225	-0.595	32
Butyronitrile	0.188	0.900	0.000	0.360	2.548	0.6860	2.748	0.078	32
Pentanonitrile	0.177	0.900	0.000	0.360	3.108	0.8269	3.260	0.680	32
Methylamine	0.250	0.350	0.160	0.580	1.300	0.3493	1.202	-2.138	32
Ethylamine	0.236	0.350	0.160	0.610	1.677	0.4902	1.680	-1.620	89
n-Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	2.260	-0.960	58
Isopropylamine	0.183	0.320	0.160	0.610	1.908	0.6311	2.040		58
Dimethylamine	0.189	0.300	0.080	0.660	1.600	0.4902	1.821	-1.329	32
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7720	2.620	-0.370	44
Trimethylamine	0.140	0.200	0.000	0.670	1.620	0.6311	1.926	-0.424	32
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	3.290	0.930	33
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	2.020	-0.930	33
Nitroethane	0.270	0.950	0.020	0.330	2.414	0.5646	2.510	-0.210	33
Nitropropane	0.242	0.950	0.000	0.310	2.894	0.7055	2.970	0.520	33
Nitrobutane	0.227	0.950	0.000	0.290	3.415	0.8464	3.401	1.131	121
Water	0.000	0.450	0.820	0.350	0.260	0.1673	0.540	-4.100	57
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	1.148	-2.592	32
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	1.672	-1.998	32

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Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.211	-1.349	32
Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.5900	2.020	-1.460	87
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	2.742	-0.718	32
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	2.607	-0.783	88
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	2.621	-0.679	119
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	3.387	0.037	122
3-Methylbutan-1-ol	0.192	0.390	0.370	0.480	3.011	0.8718	2.970	-0.270	119
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	3.678	0.448	34, 123
Heptan-1-ol	0.211	0.420	0.370	0.480	4.115	1.1536	4.099	1.009	123
Decan-1-ol	0.191	0.420	0.370	0.480	5.610	1.5763	5.640	2.970	34
Dodecan-1-ol	0.175	0.420	0.370	0.480	6.620	1.8581	6.790	4.350	34
2-Ethoxyethanol	0.237	0.520	0.310	0.810	2.792	0.7896	2.940	-1.970	51
Dimethyl sulphide	0.404	0.430	0.000	0.270	2.037	0.5539	2.175	1.035	69
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	0.295	2.515	85
Tetraethylsilicon	0.126	-0.120	0.000	0.000	4.348	1.4815	4.640	6.670	35
Tetramethyltin	0.324	0.110	0.000	0.100	2.651	1.0431	3.030	4.560	35
Mercury	0.850	0.430	0.000	0.040	1.721	0.3400	1.740	1.330	59
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	2.940	2.310	46
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.480	2.830	33
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	3.922	3.342	141
Propylbenene	0.604	0.500	0.000	0.150	4.230	1.1391	4.071	3.681	141
trans-Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	7.452	4.672	24
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.250	4.300	103
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.310	3.580	114, 115
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.495	4.135	104, 117

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Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5850	8.419	4.969	106, 107
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.452	3.422	99
Phenanthrene	2.055	1.290	0.000	0.290	7.632	1.4544	7.352	4.552	105, 99
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	8.461	4.961	106, 117
Fluorene	1.588	1.060	0.000	0.240	6.922	1.3565	6.812	4.362	110
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	3.820	3.000	142
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	4.500	3.600	142
1,3-Dichlorobenzene	0.847	0.730	0.000	0.020	4.410	0.9612	4.530	3.810	142
1,4-Dichlorobenzene	0.825	0.750	0.000	0.020	4.435	0.9612	4.440	3.700	142
1,2,3-Trichlorobenzene	1.030	0.860	0.000	0.000	5.419	1.0836	5.070	4.160	142
1,2,4-Trichlorobenzene	0.980	0.810	0.000	0.000	5.248	1.0836	5.120	4.300	142
1,3,5-Trichlorobenzene	0.980	0.730	0.000	0.000	5.045	1.0836	5.100	4.530	142
1,2,3,5-Tetrachlorobenzene	1.160	0.850	0.000	0.000		1.2060		4.860	142
1,2,4,5-Tetrachlorobenzene	1.160	0.860	0.000	0.000		1.2060		4.860	142
Pentachlorobenzene	1.330	0.920	0.060	0.000	6.630	1.3284		5.320	142
Hexachlorobenzene	1.490	0.990	0.000	0.000	7.390	1.4508	7.479	5.979	102, 117
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	4.148	3.078	121
1,4-Dibromobenzene	1.150	0.860	0.000	0.040	5.324	1.0660	5.316	3.876	113
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	3.042	2.452	121
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730	4.053	1.103	121
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.0139	4.434	1.074	121
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	4.464	1.444	121
Methyl-4-hydroxylbenzoate	0.900	1.370	0.690	0.450	5.716	1.1313	5.441	-1.399	116
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	3.070	-0.370	33
9-Fluorenone	1.600	1.490	0.000	0.350	7.474	1.3722	7.169	2.969	96

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Thianthrene	2.240	1.390	0.000	0.360	8.541	1.5426	8.340	4.340	96
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.059	4.559	96
1-Nitronaphthalene	1.600	1.590	0.000	0.290	7.056	1.2600	6.857	2.661	95
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	8.936	2.902	92
1,2,4,5-Tetramethylbenzene	0.739	0.600	0.000	0.190	5.029	1.2800	5.309	4.783	94
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	8.151	2.748	93
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	7.560	2.690	97
p-Chloro-1-phenyl-3,3-dimethylurea	1.140	1.500	0.470	0.780	7.180	1.4768	7.191	-0.440	100
2,4-Dichloro-1-phenyl-3,3-dimethylurea	1.280	1.600	0.570	0.700	8.060	1.5992	7.883	-0.120	100
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	5.625	3.705	98
2-Ethylanthraquinone	1.410	1.545	0.000	0.557	8.781	1.8106	8.750	3.957	118
4-Nitropyridine N-oxide	0.934	1.920	0.210	0.760	5.271	0.9082	5.187	-2.933	108
Diphenyl sulfone	1.570	2.100	0.000	0.720	8.577	1.6051	8.630	1.240	101
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	3.672	-1.178	132
m-Cresol	0.822	0.880	0.570	0.340	4.310	0.9160	4.280	-0.320	131
p-Cresol	0.820	0.870	0.570	0.310	4.312	0.9160	4.160	-0.340	131
2,3-Dimethylphenol	0.850	0.820	0.510	0.370	4.495	1.0569	4.890	0.380	131
2,4-Dimethylphenol	0.843	0.790	0.520	0.400	4.770	1.0569	4.772	0.362	125
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	4.738	0.398	125
3,4-Dimethylphenol	0.830	0.900	0.550	0.380	4.980	1.0569	5.049	0.279	125
3,5-Dimethylphenol	0.830	0.860	0.550	0.370	4.856	1.0569	4.962	0.362	125
2-Ethylphenol	0.831	0.840	0.520	0.370	4.612	1.0569	4.840	0.420	131
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	4.790	0.290	126
4-t-Butylphenol	0.810	0.890	0.560	0.410	5.264	1.3387	5.590	1.250	131
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	3.436	-0.444	130

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2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.191	0.851	130
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	4.779	-0.071	129
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	5.068	-0.092	129
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	4.982	1.332	129
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	4.782	1.072	130
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	4.751	1.391	128
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	5.713	-1.347	128
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	5.810	-2.000	128
2,4-Dinitrophenol	1.200	1.490	0.090	0.560	5.981	1.1235	5.932	0.352	133
1-Naphthol	1.520	1.100	0.660	0.340	6.284	1.1441	6.387	0.517	137
2-Naphthol	1.520	1.080	0.610	0.400	6.200	1.1441	6.205	0.255	137
2-Nitroaniline	1.180	1.370	0.300	0.360	5.627	0.9904	5.503	0.093	135
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	4.239	-4.111	136
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	3.980	-0.100	121
1-Naphthylamine	1.670	1.260	0.200	0.570	6.490	1.1852	6.501	1.161	139
2-Naphthylamine	1.670	1.280	0.220	0.550	6.540	1.1852	6.515	1.045	139
Catechol	0.970	1.100	0.880	0.470	4.450	0.8338	4.310	-2.890	136
Hydroquinone	1.063	1.270	1.060	0.570	4.827	0.8338	4.583	-4.287	136
1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	5.125	-2.305	136
Phenetole	0.681	0.700	0.000	0.320	4.242	1.0569	4.410	2.780	131
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	8.022	2.954	111
Acetone oxime	0.390	0.660	0.370	0.560	2.557	0.6499	2.739	-1.725	138
Cyclohexanone oxime	0.580	0.900	0.330	0.610	4.432	0.9609	4.516	-0.599	138
2,4-Dinitro-6-aminophenol	1.750	1.850	0.210	0.800	7.466	1.2233	7.350	-1.000	146
Benzoylacetone	0.766	0.990	0.010	0.580	5.647	1.3114	5.658	1.968	145

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4-Methoxyphenol	0.900	1.170	0.570	0.480	4.773	0.9747	5.240	-0.910	131
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	4.490	0.430	134
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	4.440	0.350	134
3-Chloroacetophenone	0.924	1.070	0.000	0.400		1.1370		1.860	131
4-Chloroacetophenone	0.955	1.090	0.000	0.440		1.1370		1.830	131
2-Propylphenol	0.822	0.860	0.520	0.370		1.1978		1.020	131

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Table 2. Experimental log *P* and log *K* data for solutes dissolved in heptane at 298 K.

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Log K	Log P	Ref
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	-1.384	0.636	85
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.229	0.731	85
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.379	1.091	85
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	0.076	1.286	85
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	0.650	1.620	28
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-0.943	0.777	31
Deuterium	0.000	0.000	0.000	0.000	-1.200	0.1100	-0.930	0.800	31
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.471	1.039	85
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-0.646	1.154	85
Nitrous Oxide	0.068	0.350	0.000	0.100	0.164	0.2810	0.480	0.710	60
Carbon monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	-0.547	1.073	30
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.300	0.380	42
Sulphur dioxide	0.370	0.660	0.280	0.100	0.778	0.3465	1.000	-0.530	60, 68
Iodine	1.398	0.670	0.280	0.000	3.681	0.6250	3.415	1.555	109
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.075	1.385	85
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	0.726	2.066	27
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.301	2.741	27
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.851	3.371	27
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.694	3.394	27
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	2.400	4.100	26
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.900	4.720	26
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540	2.760	4.600	26
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	3.440	5.400	26

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2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949	3.086	5.166	26
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.920	6.030	26
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.2358	3.570	5.590	26
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358	3.640	5.520	26
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	4.450	6.600	26
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	3.070	3.970	26
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	3.510	4.720	72
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272	3.940	5.520	26
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	0.457	1.397	27
Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.276	1.746	27
1-Butene	0.100	0.080	0.000	0.070	1.529	0.6292	1.817	2.827	27
2-Methylpropene	0.120	0.080	0.000	0.080	1.579	0.6292	1.789	2.629	27
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.7701	2.310	3.540	36
3-Methylbut-1-ene	0.063	0.060	0.000	0.050	1.933	0.7701	2.170	3.510	37
Hex-1-ene	0.080	0.080	0.000	0.070	2.572	0.9110	2.810	3.970	72
Hept-1-ene	0.092	0.080	0.000	0.070	3.063	1.0519	3.300	4.520	72
Oct-1-ene	0.090	0.080	0.000	0.070	3.568	1.1928	3.790	5.200	72
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	1.960	2.410	41
2-Methylbuta-1,3-diene	0.313	0.230	0.000	0.100	2.101	0.7271	2.360	2.860	36
Fluoroethane	0.050	0.350	0.000	0.100	0.576		1.060		55
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.456	1.834	85
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943	2.130	1.170	36
Trichloromethane	0.430	0.490	0.150	0.020	2.480	0.6167	2.650	1.860	36
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.7391	3.000	3.190	36
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352	2.710	1.440	36, 37

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1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.6537	2.410	2.170	36
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946	2.906	2.786	37
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	2.480	3.280	36
Bromoethane	0.370	0.400	0.000	0.120	2.120	0.5654	2.230	1.690	36
Iodomethane	0.676	0.430	0.000	0.120	2.106	0.5077	2.220	1.570	36
Iodoethane	0.640	0.400	0.000	0.150	2.573	0.6486	2.700	2.160	36
Difluorodichloromethane	0.037	0.040	0.000	0.040	0.998	0.5297	1.320	2.460	42
Trifluorochloromethane	-0.250	-0.050	0.000	0.000	0.209	0.4250	0.440	2.090	42
1,2-Difluorotetrachloroethane	0.227	0.330	0.000	0.020	3.034	0.9154	2.920	4.640	61
Ethyl *tert*-butyl ether	-0.020	0.180	0.000	0.590	2.699	1.0127	2.920	1.650	49
Methyl *tert*-butyl ether	0.024	0.220	0.000	0.590	2.380	0.8718	2.597	1.007	74
Methyl *tert*-pentyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	3.108	1.638	74
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	2.950	-0.760	40
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	1.870	-0.960	56
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	2.490	-0.230	40, 56
Pentan-2-one	0.143	0.680	0.000	0.510	2.755	0.8288	2.983	0.403	121
Hexan-2-one	0.136	0.680	0.000	0.510	3.286	0.9697	3.335	0.925	121
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.1106	3.826	1.576	121
Octan-2-one	0.108	0.680	0.000	0.510	4.257	1.2515	4.163	2.003	121
3,3-Dimethylbutan-2-one	0.106	0.620	0.000	0.510	2.928	0.9697	3.152	0.835	121
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.7202	3.320	-0.130	43
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8611	3.800	0.200	43
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	2.035	-0.265	124
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	2.590	0.430	36, 39
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	2.950	0.900	124

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Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	3.610	1.670	39
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	4.020	2.180	124
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	2.659	0.509	124
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	3.601	1.721	124
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.1693	4.127	2.297	124
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	1.670	-1.180	36
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450	2.100	-0.720	36, 39
Butyronitrile	0.188	0.900	0.000	0.360	2.548	0.6860	2.699	0.029	73
Ammonia	0.140	0.390	0.160	0.560	0.319	0.2084	0.930	-2.230	72
Ethylamine	0.236	0.350	0.160	0.610	1.677	0.4902	1.530	-1.770	140
n-Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	2.220	-1.000	140
n-Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	2.980	-0.130	48
n-Pentylamine	0.211	0.350	0.160	0.610	3.139	0.9129	3.480	0.480	48
n-Hexylamine	0.197	0.350	0.160	0.610	3.655	1.0538	3.990	1.090	48
n-Heptylamine	0.197	0.350	0.160	0.610	4.153	1.1947	4.520	1.740	48
n-Octylamine	0.187	0.350	0.160	0.610	4.600	1.3356	5.040	2.360	48
Trimethylamine	0.140	0.200	0.000	0.670	1.620	0.6311	1.790	-0.560	45
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	3.280	0.920	44
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	1.920	-1.030	36, 39
Nitroethane	0.270	0.950	0.020	0.330	2.414	0.5646	2.450	-0.270	36, 39
Nitropropane	0.242	0.950	0.000	0.310	2.894	0.7055	2.910	0.460	39
2-Nitropropane	0.216	0.920	0.000	0.330	2.550	0.7055	2.790	0.520	39
Water	0.000	0.450	0.820	0.350	0.260	0.1673	0.430	-4.210	90
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	1.200	-2.540	36, 38
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	1.640	-2.030	36

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Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.190	-1.370	38
Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.5900	1.910	-1.570	38
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	2.750	-0.710	38
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	2.580	-0.720	38
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	2.390	-1.000	38
2-Methylpropan-2-ol	0.180	0.300	0.310	0.600	1.963	0.7309	2.210	-1.070	38
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	3.300	-0.050	38
3-Methylbutan-1-ol	0.192	0.390	0.370	0.480	3.011	0.8718	2.903	-0.337	119
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	3.870	0.640	38
Heptan-1-ol	0.211	0.420	0.370	0.480	4.115	1.1536	4.099	1.009	123
Octan-1-ol	0.199	0.420	0.370	0.480	4.619	1.2945	4.700	1.700	56
2-Ethoxyethanol	0.237	0.520	0.310	0.810	2.792	0.7896	2.820	-2.090	51
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	0.227	2.447	85
Carbon disulfide	0.876	0.260	0.000	0.030	2.370	0.4905	2.440	2.590	36
Mercury	0.850	0.430	0.000	0.040	1.721	0.3400	1.800	1.340	59
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	2.910	2.280	46
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.470	2.820	40
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.9982	4.040	3.300	72
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.9982	3.950	3.340	72
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	3.950	3.360	72
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	3.890	3.310	72
n-Propylbenene	0.604	0.500	0.000	0.150	4.230	1.1391	4.340	3.950	121
Isopropylbenzene	0.602	0.490	0.000	0.160	4.084	1.1391	4.190	3.750	72
trans-Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	7.456	4.676	24
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.260	4.310	103

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Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.290	3.560	114
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.520	4.160	104, 117
Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5850	8.472	5.022	106, 107
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.487	4.457	99
Phenanthrene	2.055	1.290	0.000	0.290	7.632	1.4544	7.390	4.590	105, 99
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	8.522	5.022	106, 117
Fluorene	1.588	1.060	0.000	0.240	6.922	1.3565	6.814	4.364	110
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	3.790	2.970	53
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	4.405	3.505	121
1,4-Dichlorobenzene	0.825	0.750	0.000	0.020	4.435	0.9612	4.258	3.518	121
Hexachlorobenzene	1.490	0.990	0.000	0.000	7.390	1.4508	7.508	6.008	102, 99
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	4.192	3.122	121
1,4-Dibromobenzene	1.150	0.860	0.000	0.040	5.324	1.0660	5.533	4.093	121
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	3.027	2.437	121
Iodobenzene	1.188	0.820	0.000	0.120	4.502	0.9746	4.595	3.315	121
Anisole	0.708	0.750	0.000	0.290	3.890	0.9160	3.921	2.121	121
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730	4.031	1.081	121
Benzonitrile	0.742	1.110	0.000	0.330	4.039	0.8711	3.907	0.817	121
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.8906	4.500	1.480	121
Thiophene	0.687	0.560	0.000	0.150	2.943	0.6410	2.998	1.968	121
9-Fluorenone	1.600	1.490	0.000	0.350	7.474	1.3722	7.206	3.006	96
Thianthrene	2.240	1.390	0.000	0.360	8.541	1.5426	8.320	4.320	96
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.090	4.590	96
1-Nitronaphthalene	1.600	1.590	0.000	0.290	7.056	1.2600	6.865	2.669	95
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	9.013	2.979	92

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1,2,4,5-Tetramethylbenzene	0.739	0.600	0.000	0.190	5.029	1.2800	5.267	4.741	94
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	8.177	2.774	93
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	7.570	2.700	97
p-Chloro-1-phenyl-3,3-dimethylurea	1.140	1.500	0.470	0.780	7.180	1.4768	7.147	-0.480	100
2,4-dichloro-1-phenyl-3,3-dimethylurea	1.280	1.600	0.570	0.700	8.060	1.5992	8.003	0.000	100
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	5.618	3.698	98
2-Ethylanthraquinone	1.410	1.545	0.000	0.557	8.781	1.8106	8.771	3.987	118
4-Nitropyridine N-oxide	0.934	1.920	0.210	0.760	5.271	0.9082	5.220	-2.900	108
Diphenyl sulfone	1.570	2.100	0.000	0.720	8.577	1.6051	8.634	1.244	101
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	3.643	-1.207	132
m-Cresol	0.822	0.880	0.570	0.340	4.310	0.9160	4.233	-0.367	127
p-Cresol	0.820	0.870	0.570	0.310	4.312	0.9160	4.142	-0.358	127
2,4-Dimethylphenol	0.843	0.790	0.520	0.400	4.770	1.0569	4.752	0.342	125
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	4.720	0.380	125
3,4-Dimethylphenol	0.830	0.900	0.550	0.380	4.980	1.0569	5.049	0.279	125
3,5-Dimethylphenol	0.830	0.860	0.550	0.370	4.856	1.0569	4.922	0.322	125
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	4.740	0.240	126
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	3.448	-0.432	130
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.185	0.845	130
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	4.774	-0.076	129
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	5.052	-0.108	129
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	5.019	1.369	129
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	4.755	1.045	130
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	4.761	1.401	128
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	5.662	-1.398	128

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4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	5.810	-2.000	128
2,4-Dinitrophenol	1.200	1.490	0.090	0.560	5.981	1.1235	5.922	0.342	133
1-Naphthol	1.520	1.100	0.660	0.340	6.284	1.1441	6.417	0.547	137
2-Naphthol	1.520	1.080	0.610	0.400	6.200	1.1441	6.251	0.301	137
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	3.943	-0.137	131
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	4.281	-4.069	136
1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	5.168	-2.262	136
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	9.504	-1.046	143
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	8.079	3.011	111
2,4-Dinitro-6-aminophenol	1.750	1.850	0.210	0.800	7.466	1.2233	7.304	-1.046	146
Benzoylacetone	0.766	0.990	0.010	0.580	5.647	1.3114	5.769	2.079	145
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	4.560	0.500	134
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	4.500	0.410	134

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Table 3. Experimental log *P* and log *K* data for solutes dissolved in octane at 298 K.

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Log *K*	Log *P*	Ref
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	-1.453	0.567	85
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.265	0.695	85
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.437	1.033	85
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	0.024	1.234	85
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	0.620	1.590	28
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-0.990	0.730	31
Deuterium	0.000	0.000	0.000	0.000	-1.200	0.1100	-0.980	0.750	31
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.513	0.997	85
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-0.709	1.091	85
Nitrous Oxide	0.068	0.350	0.000	0.100	0.164	0.2810	0.440	0.670	60
Carbon monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	-0.587	1.033	30
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.260	0.340	60, 79
Sulphur dioxide	0.370	0.660	0.280	0.100	0.3465	0.7780	0.737	-0.793	60, 68
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.116	1.344	85
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	0.702	2.042	27
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.280	2.720	27
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.831	3.351	27
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.683	3.383	27
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	2.350	4.050	26
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.860	4.680	26
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540	2.720	4.560	26
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	3.370	5.330	26
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949	3.030	5.110	26
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.910	6.010	26

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2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.2358	3.540	5.560	46
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	3.270	5.390	47
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358	3.600	5.480	46
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	4.390	6.540	46
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	3.050	3.950	46
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272	3.940	5.520	46
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	0.440	1.380	27
Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.256	2.226	27
1-Butene	0.100	0.080	0.000	0.070	1.529	0.6292	1.796	2.806	27
2-Methylpropene	0.120	0.080	0.000	0.080	1.579	0.6292	1.770	2.630	27
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.7701	2.270	3.500	36
3-Methylbut-1-ene	0.063	0.060	0.000	0.050	1.933	0.7701	2.140	3.480	36
2-Methylbuta-1,3-diene	0.313	0.230	0.000	0.100	2.101	0.7271	2.330	2.830	36
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.531	1.759	85
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943	2.100	1.140	36
Trichloromethane	0.430	0.490	0.150	0.020	2.480	0.6167	2.580	1.790	36
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.7391	2.920	3.110	80, 81
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352	2.710	1.440	36
1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.6537	2.360	2.120	36
Bromoethane	0.370	0.400	0.000	0.120	2.120	0.5654	2.190	1.650	36
Iodomethane	0.676	0.430	0.000	0.120	2.106	0.5077	2.190	1.540	36
Iodoethane	0.640	0.400	0.000	0.150	2.573	0.6486	2.680	2.140	36
Difluorodichloromethane	0.037	0.040	0.000	0.040	0.998	0.5297	1.290	2.430	42
Trifluorochloromethane	-0.250	-0.050	0.000	0.000	0.209	0.4250	0.390	2.040	42
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	2.235	0.945	75
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.0127	2.812	1.762	75

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Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945	4.240	3.550	70
Methyl *tert*-butyl ether	0.024	0.220	0.000	0.590	2.380	0.8718	2.572	0.982	75
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	2.680	0.130	36
Propanal	0.196	0.650	0.000	0.450	1.815	0.5470	1.860	-0.660	47
Butanal	0.187	0.650	0.000	0.450	2.270	0.6879	2.370	0.040	47
Pentanal	0.163	0.650	0.000	0.450	2.851	0.8288	2.910	0.690	47
Hexanal	0.146	0.650	0.000	0.450	3.357	0.9697	3.490	1.430	47
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	1.850	-0.980	47
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	2.370	-0.350	47
Pentan-2-one	0.143	0.680	0.000	0.510	2.755	0.8288	2.840	0.260	47
4-Methylpentan-2-one	0.111	0.650	0.000	0.510	3.089	0.9697	3.180	0.940	47
Hexan-2-one	0.136	0.680	0.000	0.510	3.286	0.9697	3.372	0.962	121
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.1106	3.848	1.598	121
3,3-Dimethylbutan-2-one	0.106	0.620	0.000	0.510	2.928	0.9697	3.086	0.806	121
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	2.111	-0.189	124
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	2.490	0.330	47
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	2.946	0.896	124
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	3.591	1.651	124
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	3.972	2.132	124
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	2.619	0.469	124
Ethyl propanoate	0.087	0.580	0.000	0.450	2.807	0.8875	3.010	1.040	47
Ethyl butanoate	0.068	0.580	0.000	0.450	3.271	1.0284	3.440	1.610	47
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	3.558	1.678	124
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.1693	4.065	2.235	124
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	1.590	-1.260	36
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450	2.080	-0.740	36

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Ethylamine	0.236	0.350	0.160	0.610	1.677	0.4902	1.504	-1.796	140
n-Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	2.198	-1.022	140
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	2.525	-0.585	140
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	1.920	-1.030	36
Nitroethane	0.270	0.950	0.020	0.330	2.414	0.5646	2.470	-0.250	36
Nitropropane	0.242	0.950	0.000	0.310	2.894	0.7055	2.895	0.445	121
Water	0.000	0.450	0.820	0.350	0.260	0.1673	0.500	-4.140	90
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	1.060	-2.680	36
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	1.600	-2.070	36
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.130	-1.430	82
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	2.650	-0.810	82
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	2.442	-0.858	119
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	2.388	-1.002	119
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	3.128	-0.222	120
3-Methylbutan-1-ol	0.192	0.390	0.370	0.480	3.011	0.8718	2.920	-0.320	119
2-Methyl-2-butanol	0.194	0.300	0.310	0.630	2.721	0.8718	2.922	-0.328	120
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	3.661	0.431	120
2-Methyl-1-pentanol	0.211	0.390	0.310	0.560	3.471	1.0127	3.585	0.415	120
3-Methyl-1-pentanol	0.211	0.390	0.310	0.560	3.493	1.0127	3.531	0.301	120
2-Methyl-2-pentanol	0.169	0.300	0.310	0.640	3.240	1.0127	3.364	0.114	120
3-Methyl-2-pentanol	0.170	0.390	0.330	0.560	3.476	1.0127	3.572	0.322	120
4-Methyl-1-pentanol	0.196	0.390	0.330	0.530	3.439	1.0127	3.547	0.477	120
2-Methyl-3-pentanol	0.207	0.330	0.330	0.630	3.315	1.0127	3.459	0.079	120
4-Methyl-2-pentanol	0.167	0.330	0.330	0.550	3.263	1.0127	3.391	0.431	120
2,3-Dimethyl-2-butanol	0.208	0.270	0.310	0.650	3.223	1.0127	3.374	0.114	120
3,3-Dimethyl-1-butanol	0.188	0.360	0.310	0.610	3.332	1.0127	3.556	0.176	120

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3-Methyl-3-hexanol	0.198	0.300	0.310	0.640	3.805	1.1536	3.958	0.778	120
2-Methyl-3-hexanol	0.200	0.330	0.330	0.620	3.839	1.1536	3.912	0.672	120
3-Methyl-2-hexanol	0.160	0.330	0.330	0.550	3.832	1.1536	3.891	1.021	120
2-Methyl-2-hexanol	0.163	0.300	0.310	0.630	3.686	1.1536	3.880	0.820	120
5-Methyl-2-hexanol	0.160	0.330	0.330	0.570	3.819	1.1536	3.904	0.934	120
3-Ethyl-3-pentanol	0.234	0.300	0.310	0.640	3.838	1.1536	3.972	0.792	120
4,4-Dimethyl-2-pentanol	0.190	0.330	0.330	0.570	3.858	1.1536	3.968	0.978	120
2,3-Dimethyl-3-pentanol	0.190	0.300	0.310	0.630	3.817	1.1536	3.959	0.839	120
2,2-Dimethyl-3-pentanol	0.227	0.300	0.300	0.550	3.856	1.1536	3.617	1.207	120
Decan-1-ol	0.191	0.420	0.370	0.480	5.610	1.5763	5.770	3.100	50
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	0.161	2.381	85
Carbon disulfide	0.876	0.260	0.000	0.030	2.370	0.4905	2.410	2.560	36
Mercury	0.850	0.430	0.000	0.040	1.721	0.3400	1.800	1.340	59
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	2.900	2.270	46
trans-Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	7.470	4.690	24
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.250	4.300	103
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.525	4.165	104, 117
Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5850	8.511	5.061	106, 107
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.514	4.484	99
Phenanthrene	2.055	1.290	0.000	0.290	7.632	1.4544	7.405	4.605	105, 99
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	8.576	5.076	106, 117
Fluorene	1.588	1.060	0.000	0.240	6.922	1.3565	6.812	4.362	110
Hexachlorobenzene	1.490	0.990	0.000	0.000	7.390	1.4508	7.536	6.036	102, 99
9-Fluorenone	1.600	1.490	0.000	0.350	7.474	1.3722	7.227	3.027	96
Thianthrene	2.240	1.390	0.000	0.360	8.541	1.5426	8.330	4.330	96
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.097	4.597	96

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1-Nitronaphthalene	1.600	1.590	0.000	0.290	7.056	1.2600	6.874	2.678	95
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	9.042	3.008	92
1,2,4,5-Tetramethylbenzene	0.739	0.600	0.000	0.190	5.029	1.2800	5.235	4.709	94
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	8.223	2.820	93
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	7.570	2.710	97
p-Chloro-1-phenyl-3,3-dimethylurea	1.140	1.500	0.470	0.780	7.180	1.4768	7.174	-0.460	100
2,4-dichloro-1-phenyl-3,3-dimethylurea	1.280	1.600	0.570	0.700	8.060	1.5992	7.994	-0.010	100
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	5.593	3.673	98
2-Ethylanthraquinone	1.410	1.545	0.000	0.557	8.781	1.8106	8.801	3.987	118
4-Nitropyridine N-oxide	0.934	1.920	0.210	0.760	5.271	0.9082	5.229	-2.891	108
Diphenyl sulfone	1.570	2.100	0.000	0.720	8.577	1.6051	8.644	1.254	101
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	3.633	-1.217	132
m-Cresol	0.822	0.880	0.570	0.340	4.310	0.9160	4.243	-0.357	127
p-Cresol	0.820	0.870	0.570	0.310	4.312	0.9160	4.130	-0.370	127
2,4-Dimethylphenol	0.843	0.790	0.520	0.400	4.770	1.0569	4.732	0.322	125
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	4.720	0.380	125
3,4-Dimethylphenol	0.830	0.900	0.550	0.380	4.980	1.0569	5.025	0.255	125
3,5-Dimethylphenol	0.830	0.860	0.550	0.370	4.856	1.0569	4.901	0.301	125
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	4.720	0.220	126
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	3.311	-0.569	130
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.153	0.813	130
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	4.748	-0.102	129
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	5.041	-0.119	129
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	5.000	1.350	129
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	4.743	1.033	130
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	4.758	1.398	128

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3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	5.741	-1.319	128
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	5.810	-2.000	128
2,4-Dinitrophenol	1.200	1.490	0.090	0.560	5.981	1.1235	5.904	0.324	133
1-Naphthol	1.520	1.100	0.660	0.340	6.284	1.1441	6.398	0.528	137
2-Naphthol	1.520	1.080	0.610	0.400	6.200	1.1441	6.325	0.375	137
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	3.547	-0.533	121
1-Naphthylamine	1.670	1.260	0.200	0.570	6.490	1.1852	6.467	1.127	139
2-Naphthylamine	1.670	1.280	0.220	0.550	6.540	1.1852	6.566	1.086	139
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	4.287	-4.063	136
Catechol	0.970	1.100	0.880	0.470	4.450	0.8338	4.428	-2.772	136
Hydroquinone	1.063	1.270	1.060	0.570	4.827	0.8338	4.826	-4.044	136
1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	5.143	-2.287	136
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	9.453	-1.097	143
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	8.121	3.053	111
2-Furaldehyde	0.690	1.130	0.000	0.450	3.318	0.6962	3.130	-0.700	144
5-Methylfurfural	0.744	1.110	0.000	0.520	3.933	0.8339	3.632	-0.398	144
2,4-Dinitro-6-aminophenol	1.750	1.850	0.210	0.800	7.466	1.2233	7.304	-1.046	146
Benzoylacetone	0.766	0.990	0.010	0.580	5.647	1.3114	5.690	2.000	145
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	4.650	0.590	134
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	4.610	0.520	134

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Table 4. Experimental log *P* and log *K* data for solutes dissolved in decane at 298 K.

Solute	**E**	**S**	**A**	**B**	**L**	**V**	Log *K*	Log *P*	Ref
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	-1.524	0.496	85
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.364	0.596	85
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.509	0.961	85
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-0.042	1.168	85
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	0.570	1.540	28
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-1.091	0.629	31
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.564	0.946	85
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-0.796	1.004	85
Nitrous Oxide	0.068	0.350	0.000	0.100	0.164	0.2810	0.360	0.590	60
Carbon monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	-0.682	0.938	30
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.200	0.279	60, 79
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.177	1.283	85
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	0.651	1.991	27
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.248	2.688	27
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.786	3.306	27
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.637	3.337	27
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	2.290	3.990	26
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.790	4.610	26
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540	2.650	4.490	26
2,2-Dimethylbutane	0.000	0.000	0.000	0.000	2.352	0.9540	2.480	4.320	26
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	3.300	5.260	26
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949	2.970	5.050	26
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.780	5.890	26

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2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.2358	3.470	5.490	26
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358	3.530	5.410	26
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	4.350	6.500	26
Decane	0.000	0.000	0.000	0.000	4.686	1.5180	4.840	7.160	Unity
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.7045	2.540	3.420	83
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.8454	2.880	4.050	83
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	2.990	3.890	26
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	3.350	4.560	83
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272	3.860	5.440	26
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	0.421	1.361	27
Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.233	2.203	27
1-Butene	0.100	0.080	0.000	0.070	1.529	0.6292	1.773	2.783	27
2-Methylpropene	0.120	0.080	0.000	0.080	1.579	0.6292	1.729	2.589	27
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.632	1.658	85
Trichloroethene	0.520	0.370	0.080	0.030	2.997	0.7146	2.815	2.495	121
Methyl *tert*-butyl ether	0.024	0.220	0.000	0.590	2.380	0.8718	2.548	0.958	76
Methyl *tert*-pentyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	3.052	1.462	76
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	2.910	-0.800	77, 121
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	1.810	-1.020	121
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	2.400	-0.320	77, 121
Pentan-2-one	0.143	0.680	0.000	0.510	2.755	0.8288	2.880	0.300	121
Hexan-2-one	0.136	0.680	0.000	0.510	3.286	0.9697	3.379	0.969	121
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.1106	3.797	1.547	121
3,3-Dimethylbutan-2-one	0.106	0.620	0.000	0.510	2.928	0.9697	3.042	0.762	121
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	2.050	-0.250	124

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Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	2.403	0.243	84, 124
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	2.900	0.850	124
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	3.484	1.544	124
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	3.938	2.098	124
Isopropyl acetate	0.055	0.570	0.000	0.470	2.546	0.8875	2.781	0.841	84
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	2.556	0.406	124
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	3.484	1.504	124
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.1693	4.019	2.189	124
Ethylamine	0.236	0.350	0.160	0.610	1.677	0.4902	1.414	-1.886	140
Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	2.174	-1.046	140
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	2.490	-0.620	140
Dimethylamine	0.189	0.300	0.080	0.660	1.600	0.4902	1.690	-1.460	121
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	1.920	-1.030	77, 121
Water	0.000	0.450	0.820	0.350	0.260	0.1673	0.350	-4.290	57
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	1.030	-2.710	78
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	1.580	-2.090	77, 78
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.023	-1.537	121
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	2.763	-0.697	121
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	3.049	-0.301	120
2-Methyl-2-butanol	0.194	0.300	0.310	0.630	2.721	0.8718	2.922	-0.328	120
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	3.661	0.431	120
2-Methyl-1-pentanol	0.211	0.390	0.310	0.560	3.471	1.0127	3.532	0.362	120
3-Methyl-1-pentanol	0.211	0.390	0.310	0.560	3.493	1.0127	3.509	0.279	120
2-Methyl-2-pentanol	0.169	0.300	0.310	0.640	3.240	1.0127	3.329	0.079	120
3-Methyl-2-pentanol	0.170	0.390	0.330	0.560	3.476	1.0127	3.529	0.279	120

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4-Methyl-1-pentanol	0.196	0.390	0.330	0.530	3.439	1.0127	3.501	0.431	120
2-Methyl-3-pentanol	0.207	0.330	0.330	0.630	3.315	1.0127	3.421	0.041	120
4-Methyl-2-pentanol	0.167	0.330	0.330	0.550	3.263	1.0127	3.340	0.380	120
2,3-Dimethyl-2-butanol	0.208	0.270	0.310	0.650	3.223	1.0127	3.339	0.079	120
3,3-Dimethyl-1-butanol	0.188	0.360	0.310	0.610	3.332	1.0127	3.459	0.079	120
3-Methyl-3-hexanol	0.198	0.300	0.310	0.640	3.805	1.1536	3.912	0.732	120
2-Methyl-3-hexanol	0.200	0.330	0.330	0.620	3.839	1.1536	4.003	0.763	120
3-Methyl-2-hexanol	0.160	0.330	0.330	0.550	3.832	1.1536	3.861	0.991	120
2-Methyl-2-hexanol	0.163	0.300	0.310	0.630	3.686	1.1536	3.823	0.763	120
5-Methyl-2-hexanol	0.160	0.330	0.330	0.570	3.819	1.1536	3.827	0.857	120
3-Ethyl-3-pentanol	0.234	0.300	0.310	0.640	3.838	1.1536	3.912	0.732	120
4,4-Dimethyl-2-pentanol	0.190	0.330	0.330	0.570	3.858	1.1536	3.909	0.919	120
2,3-Dimethyl-3-pentanol	0.190	0.300	0.310	0.630	3.817	1.1536	3.912	0.792	120
2,2-Dimethyl-3-pentanol	0.227	0.300	0.300	0.550	3.856	1.1536	3.553	1.143	120
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	0.041	2.261	25
Mercury	0.850	0.430	0.000	0.040	1.721	0.3400	1.820	1.360	59
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	2.920	2.290	46
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.420	2.770	77, 121
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	3.835	3.255	141
n-Propylbenene	0.604	0.500	0.000	0.150	4.230	1.1391	3.837	3.447	141
trans-Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	7.460	4.680	24
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.220	4.270	103
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.513	4.153	104, 117
Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5850	8.559	5.109	106, 107
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.538	4.508	99

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Phenanthrene	2.055	1.290	0.000	0.290	7.632	1.4544	7.426	4.626	105, 99
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	8.646	5.146	106, 117
Fluorene	1.588	1.060	0.000	0.240	6.922	1.3565	6.832	4.382	110
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	2.551	1.961	121
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	3.613	2.793	121
Hexachlorobenzene	1.490	0.990	0.000	0.000	7.390	1.4508	7.551	6.051	102, 99
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	3.980	2.910	121
9-Fluorenone	1.600	1.490	0.000	0.350	7.474	1.3722	7.255	3.055	96
Thianthrene	2.240	1.390	0.000	0.360	8.541	1.5426	8.256	4.356	96
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.086	4.586	96
1-Nitronaphthalene	1.600	1.590	0.000	0.290	7.056	1.2600	6.885	2.689	95
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	9.106	3.072	92
1,2,4,5-Tetramethylbenzene	0.739	0.600	0.000	0.190	5.029	1.2800	5.192	4.666	94
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	8.235	2.832	93
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	7.560	2.690	97
p-Chloro-1-phenyl-3,3-dimethylurea	1.140	1.500	0.470	0.780	7.180	1.4768	7.185	-0.450	100
2,4-Dichloro-1-phenyl-3,3-dimethylurea	1.280	1.600	0.570	0.700	8.060	1.5992	8.070	0.070	100
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	5.593	3.673	98
2-Ethylanthraquinone	1.410	1.545	0.000	0.557	8.781	1.8106	8.823	4.009	118
4-Nitropyridine N-oxide	0.934	1.920	0.210	0.760	5.271	0.9082	5.250	-2.870	108
Diphenyl sulfone	1.570	2.100	0.000	0.720	8.577	1.6051	8.651	1.261	101
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	4.026	-0.824	133
p-Cresol	0.820	0.870	0.570	0.310	4.312	0.9160	4.398	-0.102	121
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	3.357	-0.523	130
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.128	0.788	129

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3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	4.753	-0.097	129
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	5.052	-0.108	129
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	4.976	1.326	129
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	4.723	1.013	130
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	4.740	1.380	128
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	5.673	-1.387	128
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	5.810	-2.000	128
1-Naphthol	1.520	1.100	0.660	0.340	6.284	1.1441	6.424	0.554	137
2-Naphthol	1.520	1.080	0.610	0.400	6.200	1.1441	6.315	0.365	137
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	9.395	-1.155	143
2-Furaldehyde	0.690	1.130	0.000	0.450	3.318	0.6962	3.307	-0.523	144
5-Methylfurfural	0.744	1.110	0.000	0.520	3.933	0.8339	3.875	-0.155	144
2,4-Dinitro-6-aminophenol	1.750	1.850	0.210	0.800	7.466	1.2233	7.360	-1.000	146
Benzoylacetone	0.766	0.990	0.010	0.580	5.647	1.3114	5.690	2.000	145
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	4.870	0.810	134
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	4.750	0.660	134

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