CORRELATION AND PREDICTION OF PARTITION COEFFICIENT BETWEEN THE GAS PHASE AND WATER, AND THE SOLVENTS DRY METHYL ACETATE, DRY AND WET ETHYL ACETATE, AND DRY AND WET BUTYL ACETATE

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Abstract

Experimental partition coefficient data have been compiled from the published literature for the water/methyl acetate, water/ethyl acetate and water/butyl acetate partition systems, log P data, and for the gas/methyl acetate, gas/ethyl acetate and gas/butyl acetate partition systems, log K data. Application of the Abraham solvation parameter model to the sets of partition coefficients leads to equations that correlate the log P data and log K data to 0.18 log units for the three dry alkyl acetate solvents. Slightly larger deviations were noted for solute partition into both wet ethyl acetate and wet butyl acetate. The derived correlations were validated using training set and test set analyses.

Key Words and Phrases: Partition coefficient, butyl acetate, methyl acetate, ethyl acetate, linear free energy relationship

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Introduction

Knowledge of vapor-liquid equilibria in systems involving organic compounds is important in many commercial manufacturing processes. Practical applications include the design of distillation processes for separating synthesized compounds from reaction solvent mixtures, and the removal of trace impurities from organic solvents using gas stripping methods. Distillation and gas stripping processes are governed by the partitioning of solute and solvent molecules between the vapor and liquid phases. This partitioning is related to the thermodynamic properties of the mixtures, and is described by gas-to-liquid partition coefficients.

In recent years numerous thermodynamic models have been developed for estimating vapor-liquid equilibria and activity coefficients of compounds in binary, ternary and higher-order multi-component liquid mixtures. Predictive methods include equation-of-state models, group contribution approaches, semi-theoretical and strictly empirical activity coefficient models and linear free energy relationship (lfer) correlations. Of the published lfer methods the general solvation parameter model of Abraham [1, 2] is one of the most 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

$$SP = c + e \cdot \mathbf{E} + s \cdot \mathbf{S} + a \cdot \mathbf{A} + b \cdot \mathbf{B} + v \cdot \mathbf{V} \tag{1}$$

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

$$SP = c + e \cdot \mathbf{E} + s \cdot \mathbf{S} + a \cdot \mathbf{A} + b \cdot \mathbf{B} + l \cdot \mathbf{L} \tag{2}$$

The dependent variable, SP, is some property of a series of solutes in a fixed phase. 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 water-to-condensed phase partition coefficients, P, 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. 1 and 2 to correlate solute properties having chemical, environmental and pharmaceutical importance.

At present we are developing/updating correlations for additional/existing systems [3-10] and are developing new computation methodologies for calculating solute descriptors from available experimental data and/or structural information [2, 11-15]. To date we have published Abraham model correlations for describing the gas-to-solvent, K,

$$\log K = \frac{solute\ concentration\ in\ solution}{solute\ concentration\ in\ the\ gas\ phase} \qquad (3)$$

where K is the dimensionless gas-to-solvent partition coefficient (with concentrations in each phase defined in terms of mol dm^{-3}), and water-to-solvent partition coefficients, P, for more than 50 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.

In the present study we report Abraham model correlations for the partitioning of solutes into anhydrous methyl acetate and into both anhydrous and wet ethyl acetate and butyl acetate both from the gas phase (log K data) and from water (log P data). As part of the present study we have updated the log P and log K correlations that we had previously reported for ethyl acetate. The updated correlations are based on much larger databases that include recently published experimental solubility data for several polycyclic aromatic hydrocarbons and substituted benzoic acid derivatives, plus other crystalline organic solutes.

Data Sets and Computation Methodology

Most of the experimental data that we were able to retrieve from the published literature [17-79] pertained either to the infinite dilution activity coefficient, γ_{solute}^{∞}, or Henry’s law constants, K_{Henry}, for solutes dissolved in anhydrous methyl acetate and butyl acetate. In order to apply the Abraham model the infinite dilution activity coefficients needed to be converted to log K values for gas-to-organic solvent partition through Eqns. 4 and 5

$$\log K = \log\left(\frac{RT}{\gamma_{solute}^{\infty} P_{solute}^{o} V_{solvent}}\right) \qquad (4)$$

$$\log K = \log \left(\frac{RT}{K_{Henry} V_{solvent}}\right) \tag{5}$$

or for partition from water to the anhydrous organic solvent through Eqn. 6

$$\text{Log P} = \log K - \log K_w \tag{6}$$

Here 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. The experimental log K and log P values at 298.15 K for anhydrous methyl acetate and anhydrous butyl acetate are listed in Tables 1 and 2, respectively.

Our experimental databases also contain measured solubility data [80-109] for several crystalline solutes dissolved in both neat methyl acetate and neat butyl acetate. 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 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

$$P = C_S / C_W \tag{7}$$

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 values, provided that the solid saturated vapor pressure, P_{solute}^{o}, at 298 K is also available. P_{solute}^{o} can be transformed into the gas phase concentration, C_G, and the gas-to-water and gas-to-solvent partitions, K_w and K, can be obtained through

$$K_w = C_W / C_G \qquad \text{or} \qquad K_S = C_S / C_G \tag{8}$$

Eqn.8. The vapor pressure and aqueous solubility data needed for these calculations are reported in our previous publications.

Molecular descriptors for all of the compounds considered in the present study are also tabulated in Tables 1 and 2. The tabulated values came from our solute descriptor database, which now contains values for more than 3,500 different organic and organometallic compounds. The descriptors 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, 110]. Solute descriptors used in the present study are all based on experimental data. There is also commercial software [111] and several published estimation schemes [18, 112-115] available for calculating the numerical values of solute descriptors from molecular structural information if one is unable to find the necessary partition, solubility and/or chromatographic data.

Results and Discussion

We have assembled in Table 1 log K and log P values for the partitioning of 77 solutes between the gas phase and dry methyl acetate (log K_{MA} data – the subscript MA denotes that the solvent is methyl acetate), and between water and dry methyl acetate (log P_{MA} data). The latter values represent a hypothetical partition process, and the numerical values were computed in the manner described above using measured gas-to-water partition coefficient data reported elsewhere [5, 116-118]. The solutes considered cover a reasonably wide range of compound type and descriptor values. Analysis of the experimental data in accordance with the Abraham model (Eqns. 1 and 2) yielded the following correlation equations:

$$\log P_{MA} = 0.351(0.040) + 0.223(0.072)\,\mathbf{E} - 0.150(0.094)\,\mathbf{S} - 1.035(0.107)\,\mathbf{A} - 4.527(0.132)\,\mathbf{B} + 3.972(0.036)\,\mathbf{V} \quad (9)$$

(with N = 77, SD = 0.184, R^2 = 0.996, R^2_{adj} = 0.995, F = 3175.7)

$$\log K_{MA} = 0.129(0.033) - 0.447(0.072)\,\mathbf{E} + 1.675(0.088)\,\mathbf{S} + 2.625(0.101)\,\mathbf{A} + 0.213(0.125)\,\mathbf{B} + 0.874(0.009)\,\mathbf{L} \quad (10)$$

(with $N = 77$, $SD = 0.175$, $R^2 = 0.998$, $R^2_{adj} = 0.998$, $F = 7734.0$)

Here and elsewhere, N corresponds to the number of solutes, R denotes the correlation coefficient, SD is the standard deviation and F denotes the Fisher F-statistic. All regression analyses were performed using SPSS statistical software. Equations 9 and 10 are statistically very good with standard deviations of 0.194 and 0.175 log units. Both equations can be used to predict the solubility of solutes in dry methyl acetate. Equation 9 might be more useful in some predictive applications, particularly in instances where the L-descriptor and/or C_G (see Eqn. 7) are not known. Equation 10 uses the McGowan volume, V-descriptor, which is easily calculable from the individual atomic sizes and numbers of bonds in the solute molecule [114]. Also for nonvolatile, crystalline solutes one is more likely to know the aqueous solubility than C_G. See Figure 1 for a plot of $\log P_{MA}$ values based on Eqn. 9 against experimental values that cover a range of approximately 14.75 log units, from $\log P_{MA} = -0.98$ for methanol to $\log P_{MA} = 13.76$ for tricosane.

The equation coefficients in the Abraham model are not just fitting constants, but they reflect particular solute-solvent interactions that correspond to chemical properties of the solvent phase. The excess molar refraction, **E**, is derived from the solute refractive index, and hence the e-coefficient gives a measure of general solute-solvent dispersion interactions. The **V** and **L** descriptors were set up as measures of the endoergic effect of disrupting solvent-solvent bonds. However, solute volume is always well correlated with polarizability and so the v- and l-constants will include not only an endoergic cavity effect but also exoergic solute-solvent effects that arise through solute polarizability. The **S** descriptor is a measure of dipolarity and polarizaiblity, and hence the s-coefficient will reflect the ability of a solvent to undergo dipole-dipole and dipole-induced dipole interactions with a solute. The **A** descriptor is a measure of solute hydrogen bond acidity, and hence the a-coefficient will reflect the complimentary solvent hydrogen bond basicity. Similarly the b-coefficient will be a measure of the solvent hydrogen bond acidity. All of this is straightforward for gas-to-solvent partitions because there are no interactions to consider in the gas phase. For water-to-solvent partitions (log P correlations), the coefficients refer to differences between the properties of the organic solvent and water. The numerical equation coefficients calculated above are quite reasonable given molecular structure of methyl acetate and the types of interactions that are expected to be present. The small b-coefficient in Eqn. 10 indicates that methyl acetate should have very little (if any) acidic hydrogen bond character. Dry methyl acetate does not have an acidic hydrogen, and based on structural considerations, the b-coefficient should be zero. We removed the b · **B** term from the log K correlation, and re-performed the regression analysis to give

$$\log K_{MA} = 0.134(0.033) - 0.477(0.070)\,\mathbf{E} + 1.749(0.078)\,\mathbf{S} + 2.678(0.097)\,\mathbf{A} + 0.876(0.009)\,\mathbf{L} \qquad (11)$$

$$(\text{with } N = 77,\ SD = 0.177,\ R^2 = 0.998,\ R^2_{adj} = 0.998,\ F = 9408.6)$$

There was no loss in descriptive ability resulting from setting the b-coefficient equal to zero. The standard deviations of Eqn. 10 (SD = 0.175) and Eqn. 11 (SD = 0.177) are identical. Figure 2 depicts a plot of the calculated log K_{MA} based on Eqn. 11 versus the experimental data.

The log P_{MA} and log K_{MA} databases for methyl acetate contain only 77 solutes. It would be difficult to obtain a good training set correlation by using only half of the experimental values. To assess the predictive ability of Eqns. 10 and 11 the parent data points were divided into three subsets (A, B, C) as follows: the 1^{st}, 4^{th}, 7^{th}, etc. data points comprise the first subset (A); the 2^{nd}, 5^{th}, 8^{th}, etc. data points comprise the second subset (B); and the 3^{rd}, 6^{th}, 9^{th}, etc. data points comprise the third subset (C). Three training sets were prepared as combinations of two subsets (A and B), (A and C), and (B and C).

Each validation computation gave a training set correlation equation having coefficients not too different from that obtained from the parent 74 compound data base. The training set equations were then used to predict log P and log K values for the compounds in the respective test sets (A, B and C). The statistical information for the three test set predictions are summarized in Table 3. For the three test sets the average values of SD = 0.194, AAE = 0.148, and AE = -0.001 were obtained for the water-to-methyl acetate log P correlation, and average values of SD = 0.174, AAE = 0.131, and AE = -0.003 were obtained for the gas-to-methyl acetate log K correlation. We conclude that there is very little bias in the predictions based on the derived Abraham model correlations, and that Eqns. 10 and 11 can be used to predict further values with an SD of about 0.19 log units.

During our search of the published chemical and engineering literature we also found experimental infinite dilution activity coefficient and solubility data for solutes dissolved in neat butyl acetate. The published experimental values have been converted to log P and log K values using Eqns. 3-8. The calculated log P_{BA} and log K_{BA} partition coefficients are tabulated in Table 2. Analysis of the experimental values in accordance with the Abraham model yielded the following two linear free energy relationship correlations

$$\log P_{BA} = 0.248(0.047) + 0.356(0.065)\,\mathbf{E} - 0.501(0.082)\,\mathbf{S} - 0.867(0.096)\,\mathbf{A} - 4.973(0.100)\,\mathbf{B} + 4.281(0.027)\,\mathbf{V} \quad (12)$$

(with N = 73, SD = 0.160, R^2 = 0.998, R^2_{adj} = 0.998, F = 7380)

$$\log K_{BA} = 0.147(0.040) - 0.414(0.064)\,\mathbf{E} + 1.212(0.077)\,\mathbf{S} + 2.623(0.086)\,\mathbf{A} + 0.954(0.007)\,\mathbf{L} \quad (13)$$

(with N = 73, SD = 0.157, R^2 = 0.998, R^2_{adj} = 0.998, F = 6174.7)

Preliminary analysis showed the b · **B** term to be negligible in the log K_{BA} equation, as would be expected for a solvent not possessing an acidic hydrogen. Based on the preliminary analysis the b · **B** term was eliminated from the final regression which is given above (see Eqn. 10). Both derived correlations provide a very good mathematical description of the experimental log P_{BA} and log K_{BA} data.

To assess the predictive ability of Eqns. 12 and 13, the 73 data points were into three subsets (A, B, C) as before: the 1st, 4th, 7th, etc. data points comprise the first subset (A); the 2nd, 5th, 8th, etc. data points comprise the second subset (B); and the 3rd, 6th, 9th, etc. data points comprise the third subset (C). Three training sets were prepared as combinations of two subsets (A and B), (A and C), and (B and C). Each validation computation gave a training set correlation equation having coefficients not too different from that obtained from the parent 74 compound data base. The training set equations were then used to predict log P and log K values for the compounds in the respective test sets (A, B and C). The statistical information for the three test set predictions are summarized in Table 3. For the three test sets the average values of SD = 0.175, AAE = 0.146, and AE = 0.00 were obtained for the water-to-butyl acetate log P correlation, and average values of SD = 0.174, AAE = 0.136, and AE = 0.001 were obtained for the gas-to-butyl acetate log K correlation. We conclude that there is very little bias in the predictions based on the derived Abraham model correlations, and that Eqns. 12 and 13 can be used to predict further values with an SD of about 0.17 log units.

. The linear free energy relationship models that have been derived thus far pertain to solute partitions into neat, anhydrous methyl acetate and butyl acetate. Alkyl acetates are used as solvents in practical extraction systems, and there are sufficient experimental values in the published literature to develop meaningful correlations for partition into "wet" butyl acetate. El Tayar *et al*. [119] compiled published partition coefficient for 121 solutes for the water-to-octanol, water-to-heptane, water-to-chloroform, water-to-diethyl ether and water-to-butyl acetate partition systems. Experimental partition coefficient data were not available for every solute in the five partition systems. For some partition systems there were relatively few experimental log P values. As part of the study the authors reported a log P_{BA} correlation based on an earlier version of the Abraham model

$$\text{Log } P_{BA} = 6.34(0.80)\ (V_I/100) + 0.91(0.60)\ \pi^* - 3.87(1.82)\ \beta + 0.30(0.53)\ \alpha - 1.52 \qquad (14)$$

$$(N = 26,\ SD = 0.259,\ R^2 = 0.966,\ F = 121.6)$$

where V_I is the intrinsic molecular volume of the solute, π^* measures the solute's dipolarity/-polarizability, and α and β denote the solute's hydrogen-bond donor acidity and hydrogen-bond acceptor basicity, respectively. While Eqn. 14 did provide a reasonable mathematical description of the 26 log P_{BA} values that were available to the authors, the correlation needs to be updated using the current version of the Abraham model.

Our search of the published literature [119-128] found practical water-to-butyl acetate partition coefficient data for 81 solutes. The log P_{BA} (wet) values are tabulated in Table 5, along with the corresponding log K_{BA} (wet) values calculated from Eqn. 5. For the most part the experimental log P_{BA} values were taken from the compilation of El Tayar *et al*. [119] and the Pomona MedChem database [120]. The data set contains considerably more compounds than were used in the El Tayar *et al*.study. Analysis of the experimental log P_{BA} and log K_{BA} gave

$$\log P_{BA}(\text{wet}) = -0.475(0.109) + 0.428(0.115)\ \mathbf{E} - 0.094(0.133)\ \mathbf{S} - 0.241(0.102)\ \mathbf{A} - 4.151(0.128)\ \mathbf{B^o} + 4.046(0.128)\ \mathbf{V} \qquad (15)$$

$$(\text{with } N = 81,\ SD = 0.201,\ R^2 = 0.967,\ R^2_{adj} = 0.965,\ F = 442.8)$$

$$\log K_{BA}(\text{wet}) = -0.664(0.100) + 0.061(0.142)\ \mathbf{E} + 1.671(0.145)\ \mathbf{S} + 3.373(0.108)\ \mathbf{A} + 0.824(0.134)\ \mathbf{B}$$

$$+ 0.832(0.036)\ \mathbf{L} \qquad (16)$$

(with $N = 81$, $SD = 0.215$, $R^2 = 0.990$, $R^2_{adj} = 0.989$, $F = 1426$)

$$\log K_{BA}(\text{wet}) = -0.664(0.100) + 0.062(0.144)\ \mathbf{E} + 1.679(0.147)\ \mathbf{S} + 3.380(0.109)\ \mathbf{A} + 0.819(0.136)\ \mathbf{B^o}$$

$$+ 0.829(0.037)\ \mathbf{L} \qquad (17)$$

(with $N = 81$, $SD = 0.216$, $R^2 = 0.989$, $R^2_{adj} = 0.989$, $F = 1404$)

for partition of solutes from water-to-wet butyl acetate and from gas-to-wet butyl acetate. The alternative basicity solute descriptor, $\mathbf{B^o}$, was used in Eqn. 15 because the organic phase contains an appreciable amount of water. Our past practice has been to use the B descriptor for gas-to-organic solvent partitions, even for those organic solvents that contain an appreciable amount of water. We thus report two wet log K_{BA} correlations, one first correlation using **B** (Eqn. 16) and the second using $\mathbf{B^o}$ (Eqn. 17). For most solutes the two Abraham basicity solute descriptors, **B** and $\mathbf{B^o}$, are numerically equivalent. The values differ for only a few solutes, most notably for sulfoxides, anilines and alkylpyridines. Of the 81 solutes listed in Table 5, only five (aniline, 4-methylaniline, 4-pentylaniline, 4-hexylaniline and pyridine) have variable basicity. We did derive the corresponding Abraham model log P_{BA} and log K_{BA} correlations using the **B** solute descriptor. For the five solutes with variable basicity, the log P_{BA} results are AE = 0.039 (obs-calc) for $\mathbf{B^o}$ and AE = -0.111 (obs-calc) for **B**. The systematic error is very slightly larger for **B** solute descriptor.

As noted in the Introduction log P and log K correlations already exist for ethyl acetate

$$\log P_{EA} = 0.358 + 0.362\ \mathbf{E} - 0.449\ \mathbf{S} - 0.668\ \mathbf{A} - 5.016\ \mathbf{B} + 4.155\ \mathbf{V} \qquad (18)$$

$$\log K_{EA} = 0.203 - 0.335\ \mathbf{E} + 1.251\ \mathbf{S} + 2.949\ \mathbf{A} + 0.917\ \mathbf{L} \qquad (19)$$

$$\log P_{EA}(\text{wet}) = 0.253 + 1.157\,\mathbf{E} - 1.397\,\mathbf{S} - 0.054\,\mathbf{A} - 3.755\,\mathbf{B^o} + 3.726\,\mathbf{V} \qquad (20)$$

The correlations have been used in computations illustrating the determination of solute descriptors of crystalline solutes from measured solubility data [80-88] and in principal component analyses comparing the chemical similarity of biological processes and organic solvent/water partition systems [129-132]. The databases employed in deriving the correlations were never published, and no statistical information was ever reported.

For completeness, we have reanalyzed the available log P_{EA} and log K_{EA} partition coefficient data for solutes into both dry [16-20, 42, 44, 80-109, 133-194 and wet ethyl acetate [120] using the Abraham model. The experimental log P_{EA} and log K_{EA} databases for ethyl acetate are given in Tables 6 and 7 for both dry and wet ethyl acetate, respectively. The assembled databases contain log P_{EA} and log K_{EA} values for more than 60 different organic solutes covering a reasonably wide range of compound type and descriptor values. Analyses of the experimental data yielded the following four correlation equations

Dry ethyl acetate:

$$\log P_{EA} = 0.328(0.034) + 0.369(0.057)\,\mathbf{E} - 0.446(0.080)\,\mathbf{S} - 0.700(0.069)\,\mathbf{A} - 4.904(0.113)\,\mathbf{B} + 4.150(0.033)\,\mathbf{V} \qquad (21)$$

(with N = 106, SD = 0.165, R^2 = 0.996, R^2_{adj} = 0.995, F = 4475.1)

$$\log K_{EA} = 0.182(0.026) - 0.352(0.048)\,\mathbf{E} + 1.316(0.050)\,\mathbf{S} + 2.891(0.061)\,\mathbf{A} + 0.916(0.008)\,\mathbf{L} \qquad (22)$$

(with N = 106, SD = 0.148, R^2 = 0.998, R^2_{adj} = 0.998, F = 15635.1)

Wet ethyl acetate:

$$\log P_{EA}(\text{wet}) = 0.441(0.099) + 0.591)0.121)\,\mathbf{E} - 0.669(0.106)\,\mathbf{S} - 0.325(0.125)\,\mathbf{A} - 4.261(0.139)\,\mathbf{B^o}$$

$$+ 3.666(0.122)\ \mathbf{V} \qquad (23)$$

(with N = 62, SD = 0.260, R^2 = 0.963, R^2_{adj} = 0.960, F = 300.7)

$$\log K_{EA}(\text{wet}) = 0.130(0.104) + 0.031(0.160)\ \mathbf{E} + 1.202(0.127)\ \mathbf{S} + 3.199(0.141)\ \mathbf{A} + 0.463(0.168)\ \mathbf{B} + 0.828(0.039)\ \mathbf{L} \qquad (24)$$

(with N = 62, SD = 0.295, R^2 = 0.993, R^2_{adj} = 0.992, F = 1627.3)

$$\log K_{EA}(\text{wet}) = 0.124(0.104) + 0.045(0.160)\ \mathbf{E} + 1.203(0.126)\ \mathbf{S} + 3.203(0.141)\ \mathbf{A} + 0.491(0.160)\ \mathbf{B^o} + 0.823(0.039)\ \mathbf{L} \qquad (25)$$

(with N = 62, SD = 0.293, R^2 = 0.993, R^2_{adj} = 0.993, F = 1647.1)

The statistics of the derived correlations are quite good given the range of values covered by the log P_{EA} and log K_{EA} data. Slightly larger deviations were noted for the two “wet” ethyl acetate correlations. We suspect that the log P_{EA} data for wet ethyl acetate may have a greater uncertainty associated with the reported numerical values due to inherent experimental difficulties associated with partition systems where the organic solvent contains a high proportion of water.

There are 106 experimental data points in both the log P_{EA} and log K_{EA} databases for dry ethyl acetate. To validate the derived correlations we divided the experimental values into a test and training set by allowing the SPSS software to randomly select half of the experimental values. The 53 selected data points became the training set, and the compounds that were left served as the test set. Analyses of the experimental data in the two training sets give

$$\log P_{EA} = 0.424(0.077) + 0.372(0.070)\ \mathbf{E} - 0.402(0.101)\ \mathbf{S} - 0.684(0.099)\ \mathbf{A} - 4.972(0.153)\ \mathbf{B} + 4.030(0.092)\ \mathbf{V} \qquad (26)$$

(with N = 53, SD = 0.149, R^2 = 0.994, R^2_{adj} = 0.993, F = 1527.4)

$$\log K_{EA} = 0.166(0.033) - 0.293(0.075)\,\mathbf{E} + 1.183(0.070)\,\mathbf{S} + 3.058(0.086)\,\mathbf{A} + 0.922(0.014)\,\mathbf{L} \quad (27)$$

$$(\text{with } N = 53,\ SD = 0.142,\ R^2 = 0.999,\ R^2_{adj} = 0.998,\ F = 8615.3)$$

There is very little difference in the equation coefficients for the full data set and training data set correlations. The training set correlations were then used to predict the log P_{EA} and log K_{EA} values for the 53 compounds in the respective test sets. Comparison of the predicted and observed values gave SD = 0.202 and SD = 0.166 log units, AAE = 0.152 and AAE = 0.130 log units, and AE = 0.012 and AE = 0.037 log units for Eqns. 26 and 27. There is therefore very little bias in the predictions using Eqn. 26 (with AE equal to 0.012 log units) and Eqn. 27 (with AE equal to 0.037 log units). This level of predictive error will be sufficient for most practical chemical and engineering applications.

The present study shows that 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 dry methyl acetate, dry ethyl acetate and dry butyl acetate, as well as into wet ethyl acetate and wet butyl acetate. At present we have log P and log correlations for slightly more than 50 organic solvents. The Abraham model has been used successfully to correlate measured solute properties in mixed solvent systems. For example, Baltazar et al. [195] recently correlated the gas chromatographic retention factors of 40 organic solutes on binary mixtures of two room temperature ionic liquids (mixtures of 1-butyl-3-methylimidazolium chloride and 1-butyl-3-methylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide) with Eqn. 2. Qian and Poole [196] described the Folch partition coefficients, log P data, of 86 organic solutes with Eqn. 2. The Folch partition system is a biphasic chloroform-methanol-water mixture (8:4:3 by volume). The approximate compositions of the two layers are 5:48:47 chloroform-methanol-water (volume/volume composition) and 86:14:1 chloroform-methanol-water (volume/volume composition).

The derived correlations presented here do pertain to 298.15 K. Many commercial manufacturing and separation processes take place at higher temperatures, and there is a growing need to estimate 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 both water [197] and dry ethyl acetate [198]. The ΔH_{solv} correlations will allow one to extrapolate the predicted values of log P_{EA} and log K_{EA} based on Eqns. 22 – 25 to other temperatures not too far removed from 298.15 K.

The recommended equation coefficients for partition from the gas phase and for partition from water are summarized in Table 8. There are a large number of comparisons that can be made. For example, the a-coefficient and the b-coefficient always indicate that the wet acetates are stronger hydrogen bond bases (more positive b-coefficient) and stronger hydrogen bond acids (more positive a-coefficient) than the corresponding dry acetates. Going from the methyl to ethyl to butyl acetates, both the v-coefficient and the l-coefficient increase, showing that the larger the acetate the more lipophilic it is. All this is as expected, and demonstrates that the coefficients in Eqns. 1 and 2 are not just fitting coefficients, but encode information about the chemical nature of the systems under study.

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TABLE 1. Solute Descriptors and Experimental Water-to-Methyl Acetate (dry) and Gas-to-Methyl Acetate (Dry) Partition Coefficient Data at 298.15 K

Solute	**E**	**S**	**A**	**B**	**V**	**L**	Log Kw	Log Kobs	Log Pobs
Hydrogen	0.000	0.000	0.000	0.000	0.1086	-1.200	-1.72	-1.04	0.68
Oxygen	0.000	0.000	0.000	0.000	0.1830	-0.723	-1.51	-0.56	0.95
Ozone	0.000	0.100	0.090	0.000	0.2417	0.039	-0.60	0.21	0.81
Nitrogen	0.000	0.000	0.000	0.000	0.2222	-0.978	-1.80	-0.67	1.13
Nitrous oxide	0.068	0.350	0.000	0.100	0.2810	0.164	-0.23	0.80	1.03
Carbon monoxide	0.000	0.000	0.000	0.040	0.2220	-0.836	-1.62	-0.58	1.04
Carbon dioxide	0.000	0.280	0.050	0.100	0.2809	0.058	-0.08	0.83	0.91
Sulfur dioxide	0.370	0.660	0.280	0.100	0.3465	0.778	1.53	2.26	0.73
Methane	0.000	0.000	0.000	0.000	0.2495	-0.323	-1.46	-0.22	1.24
Ethane	0.000	0.000	0.000	0.000	0.3904	0.492	-1.34	0.51	1.85
Pentane	0.000	0.000	0.000	0.000	0.8131	2.162	-1.70	1.97	3.67
Hexane	0.000	0.000	0.000	0.000	0.9540	2.668	-1.82	2.42	4.24
Heptane	0.000	0.000	0.000	0.000	1.0949	3.173	-1.96	2.85	4.81
Octane	0.000	0.000	0.000	0.000	1.2358	3.677	-2.11	3.29	5.40
Nonane	0.000	0.000	0.000	0.000	1.3767	4.182	-2.15	3.72	5.87
2-Methylpentane	0.000	0.000	0.000	0.000	0.9540	2.503	-1.84	2.30	4.14
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	1.0949	2.809	-2.08	2.57	4.65
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	1.2358	3.308	-2.02	3.01	5.03
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	1.2358	3.481	-1.88	3.10	4.98
Cyclohexane	0.305	0.100	0.000	0.000	0.8454	2.964	-0.90	2.64	3.54
Ethylcyclohexane	0.263	0.100	0.000	0.000	1.1272	3.877	-1.58	3.39	4.97
Ethene	0.107	0.100	0.000	0.070	0.3474	0.289	-0.94	0.55	1.49
1-Pentene	0.093	0.080	0.000	0.070	0.7701	2.047	-1.23	2.11	3.34
1-Hexene	0.078	0.080	0.000	0.070	0.9110	2.572	-1.16	2.57	3.73
Acetylene	0.190	0.470	0.120	0.050	0.3044	0.070	0.00	1.29	1.29
Propyne	0.183	0.250	0.120	0.140	0.4453	1.025	0.35	1.84	1.49
1-Butyne	0.178	0.250	0.120	0.100	0.5862	1.520	0.12	2.22	2.10
But-1-en-3-yne	0.327	0.260	0.180	0.010	0.5432	1.467	-0.03	2.34	2.37
Dimethyl ether	0.000	0.270	0.000	0.410	0.4491	1.285	1.40	1.71	0.31
Chloromethane	0.249	0.430	0.000	0.080	0.3719	1.163	0.40	1.81	1.41
Dichloromethane	0.387	0.570	0.100	0.050	0.4943	2.019	0.96	2.95	1.99
Chloroform	0.425	0.490	0.150	0.020	0.6167	2.480	0.79	3.42	2.63
trans 1,2-Dichloroethene	0.425	0.410	0.090	0.050	0.5922	2.278	0.36	2.92	2.56
1,1,2-Trichlorotrifluoroethane	0.010	0.130	0.000	0.000	0.8107	2.210	-1.30	2.48	3.78
2-Bromo-2-chloro-1,1,1-	0.102	0.390	0.130	0.050	0.7409	1.982	0.12	3.38	3.26

trifluoroethane									
Methanol	0.278	0.440	0.430	0.470	0.3082	0.970	3.74	2.76	-0.98
Ethanol	0.246	0.420	0.370	0.480	0.4491	1.485	3.67	3.01	-0.66
1-Propanol	0.236	0.420	0.370	0.480	0.5900	2.031	3.56	3.58	0.02
2-Propanol	0.212	0.360	0.330	0.560	0.5900	1.764	3.48	3.27	-0.21
2-Methoxyethanol	0.269	0.500	0.300	0.840	0.6487	2.490	5.08	4.01	1.07
2-Ethoxyethanol	0.237	0.550	0.290	0.820	0.7896	2.719	4.92	4.32	0.60
Methyl acetate	0.142	0.640	0.000	0.450	0.6057	1.911	2.30	3.03	0.73
Acetonitrile	0.237	0.900	0.070	0.320	0.4042	1.739	2.85	3.32	0.47
Nitromethane	0.313	0.950	0.060	0.310	0.4237	1.892	2.95	3.76	0.81
Nitroethane	0.270	0.950	0.020	0.330	0.5646	2.414	2.72	4.00	1.28
Acetone	0.179	0.700	0.040	0.490	0.5470	1.696	2.79	2.95	0.16
Ethyl oxirane	0.222	0.820	0.040	0.270	0.6223	2.344	2.15	3.04	0.89
Benzene	0.610	0.520	0.000	0.140	0.7164	2.786	0.63	3.21	2.58
Docosane	0.000	0.000	0.000	0.000	3.2084	10.740	-3.57	9.54	13.11
Tricosane	0.000	0.000	0.000	0.000	3.3493	11.252	-3.72	10.04	13.76
Anthracene	2.290	1.340	0.000	0.280	1.4544	7.568	3.03	8.12	5.09
Phenanthrene	2.055	1.290	0.000	0.290	1.4544	7.632	2.80	8.14	5.34
Hexachlorobenzene	1.490	0.990	0.000	0.000	1.4508	7.390	1.50	7.45	5.95
Pyrene	2.808	1.710	0.000	0.280	1.5846	8.833	3.50	9.25	5.75
Acenaphthene	1.604	1.050	0.000	0.220	1.2586	6.469	2.36	6.83	4.47
trans-Stilbene	1.450	1.040	0.000	0.340	1.5630	7.525	2.78	8.21	5.43
Diphenyl sulfone	1.570	2.150	0.000	0.700	1.6051	8.902	7.39	10.80	3.41
Diuron	1.280	1.600	0.570	0.700	1.5992	8.060	8.00	10.69	2.69
Monuron	1.140	1.440	0.510	0.850	1.4768	7.239	7.63	9.61	1.98
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	0.9904	4.732	5.39	7.47	2.08
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	1.0541	4.947	4.80	7.41	2.61
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	1.0726	4.677	4.30	6.54	2.24
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	1.0726	4.819	4.98	7.32	2.34
3-Nitrobenzoic acid	0.990	1.180	0.730	0.520	1.1059	5.601	6.93	8.85	1.92
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	1.1059	5.770	6.90	9.13	2.23
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	1.1313	5.636	6.80	8.30	1.50
Naproxen	1.510	2.020	0.600	0.670	1.7821	9.207	8.80	12.48	3.68
Acetylsalicylic acid	0.781	1.690	0.710	0.670	1.2879	6.279	8.50	9.98	1.48
4-Hydroxyacetanilide	1.060	1.630	1.040	0.860	1.1724	6.430	10.90	10.83	-0.07
Ferrocene	1.350	0.850	0.000	0.200	1.1209	5.622	1.92	5.99	4.07
Benzil	1.445	1.590	0.000	0.620	1.6374	7.611	4.87	9.12	4.25
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	1.6512	9.171	6.03	10.50	4.47
4-Nitroaniline	1.220	1.920	0.460	0.350	0.9904	6.042	7.19	9.66	2.47
Salicylamide	1.160	1.650	0.630	0.480	1.0315	5.910	7.60	9.35	1.75
1*H*-1,2,4-Triazole	0.662	1.500	0.970	0.430	0.4952	3.310	8.52	7.57	-0.95

Betulin	1.790	2.120	0.700	1.140	3.8670	17.466	10.39	20.09	9.70
3-Nitrophthalic acid	1.360	2.010	1.200	0.890	1.3212	7.780	12.67	13.34	0.67

TABLE 2. Solute Descriptors and Experimental Water-to-Butyl Acetate (dry) and Gas-to-Butyl Acetate (Dry) Partition Coefficient Data at 298.15 K

Solute	**E**	**S**	**A**	**B**	**V**	**L**	Log K_w	Log K_{obs}	Log P_{obs}
Hydrogen	0.000	0.000	0.000	0.000	0.1086	-1.200	-1.72	-1.10	0.62
Nitrogen	0.000	0.000	0.000	0.000	0.2222	-0.978	-1.80	-0.80	1.00
Nitrous oxide	0.068	0.350	0.000	0.100	0.2810	0.164	-0.23	0.72	0.95
Carbon monoxide	0.000	0.000	0.000	0.040	0.2220	-0.836	-1.62	-0.64	0.98
Pentane	0.000	0.000	0.000	0.000	0.8131	2.162	-1.70	2.15	3.85
Hexane	0.000	0.000	0.000	0.000	0.9540	2.668	-1.82	2.63	4.45
Heptane	0.000	0.000	0.000	0.000	1.0949	3.173	-1.96	3.10	5.06
Octane	0.000	0.000	0.000	0.000	1.2358	3.677	-2.11	3.56	5.67
Nonane	0.000	0.000	0.000	0.000	1.3767	4.182	-2.15	4.02	6.17
2-Methylpentane	0.000	0.000	0.000	0.000	0.9540	2.503	-1.84	2.49	4.33
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	1.0949	2.809	-2.08	2.79	4.87
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	1.2358	3.308	-2.02	3.27	5.29
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	1.2358	3.481	-1.88	3.34	5.22
Cyclohexane	0.305	0.100	0.000	0.000	0.8454	2.964	-0.90	2.87	3.77
Ethylcyclohexane	0.263	0.100	0.000	0.000	1.1272	3.877	-1.58	3.66	5.24
1-Heptene	0.092	0.080	0.000	0.070	1.0519	3.063	-1.22	3.14	4.36
1,6-Heptadiene	0.189	0.200	0.000	0.100	1.0089	3.028	-0.85	3.24	4.09
Carbon tetrachloride	0.458	0.380	0.000	0.000	0.7391	2.823	-0.19	3.12	3.31
Butyl acetate	0.071	0.600	0.000	0.450	1.0284	3.353	1.94	4.09	2.15
2-Butanol	0.217	0.360	0.330	0.560	0.7309	2.338	3.39	3.59	0.20
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	0.7309	2.413	3.30	3.55	0.25
1-Propanol	0.236	0.420	0.370	0.480	0.5900	2.031	3.56	3.41	0.15
1-Pentanol	0.219	0.420	0.370	0.480	0.8718	3.106	3.35	4.60	1.25
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	0.8718	3.011	3.24	4.24	1.00
1-Hexanol	0.210	0.420	0.370	0.480	1.0127	3.610	3.23	5.01	1.78
Cyclohexanol	0.460	0.540	0.320	0.570	0.9040	3.758	4.01	5.18	1.17
1,3-Dichloro-2-propanol	0.546	0.930	0.420	0.540	0.8348	3.650	5.18	5.56	0.38
Benzene	0.610	0.520	0.000	0.140	0.7164	2.786	0.63	2.84	2.21
Toluene	0.601	0.520	0.000	0.140	0.8573	3.325	0.65	4.03	3.38
o-Xylene	0.663	0.560	0.000	0.160	0.9982	3.939	0.74	4.56	3.82
m-Xylene	0.623	0.520	0.000	0.160	0.9982	3.839	0.61	4.44	3.83
p-Xylene	0.613	0.520	0.000	0.160	0.9982	3.839	0.59	4.47	3.88
n-Octadecane	0.000	0.000	0.000	0.000	2.6448	8.722	-3.04	8.75	11.79
n-Nonadecane	0.000	0.000	0.000	0.000	2.7857	9.226	-3.21	9.28	12.49
n-Eicosane	0.000	0.000	0.000	0.000	2.9266	9.731	-3.31	9.47	12.78

n-Docosane	0.000	0.000	0.000	0.000	3.2084	10.740	-3.57	10.36	13.93
n-Tricosane	0.000	0.000	0.000	0.000	3.3493	11.252	-3.72	10.93	14.65
n-Tetracosane	0.000	0.000	0.000	0.000	3.4902	11.758	-3.84	11.26	15.10
n-Octacosane	0.000	0.000	0.000	0.000	4.0538	13.780	-4.34	13.09	17.43
Anthracene	2.290	1.340	0.000	0.280	1.4544	7.568	3.03	8.16	5.13
Pyrene	2.808	1.710	0.000	0.280	1.5846	8.833	3.50	9.29	5.79
Fluoranthene	2.377	1.550	0.000	0.240	1.5846	8.827	3.44	9.27	5.83
Acenaphthene	1.604	1.050	0.000	0.220	1.2586	6.469	2.36	6.91	4.55
Phenanthrene	2.055	1.290	0.000	0.290	1.4544	7.632	2.80	8.09	5.29
Methyl 4-hydroxybenzoate	0.900	1.370	0.690	0.450	1.1313	5.665	6.84	8.68	1.84
Benzoic acid	0.730	0.900	0.590	0.400	0.9317	4.657	5.10	6.81	1.71
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	0.9904	4.732	5.39	7.34	1.95
4-Hydroxybenzoic acid	0.930	0.900	0.810	0.560	0.9904	4.867	6.78	7.89	1.11
trans-Stilbene	1.450	1.040	0.000	0.340	1.5630	7.525	2.78	8.20	5.42
Diuron	1.280	1.600	0.570	0.700	1.5992	8.060	8.00	10.61	2.61
Monouron	1.140	1.440	0.510	0.850	1.4768	7.239	7.63	9.39	1.76
Hexachlorobenzene	1.490	0.990	0.000	0.000	1.4508	7.390	1.50	7.62	6.12
Diphenyl sulfone	1.570	2.150	0.000	0.700	1.6051	8.902	7.39	10.44	3.05
4-Nitrobenzyl chloride	1.080	1.350	0.000	0.350	1.1539	5.806	3.77	7.09	3.32
Paracetamol	1.060	1.630	1.040	0.860	1.1724	6.430	10.90	10.38	-0.52
Ferrocene	1.350	0.850	0.000	0.200	1.1209	5.622	1.92	6.01	4.09
3-Chlorobenzoic acid	0.840	0.950	0.630	0.320	1.0541	5.197	5.15	7.50	2.35
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	1.0541	4.947	4.80	7.21	2.41
3-Nitrobenzoic acid	0.990	1.180	0.730	0.520	1.1059	5.601	6.93	8.53	1.60
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	1.1059	5.770	6.90	8.76	1.86
3,5-Dinitrobenzoic acid	1.250	1.630	0.700	0.590	1.2801	6.984	8.30	10.18	1.88
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	1.0726	4.677	4.30	6.42	2.12
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	1.0726	4.819	4.98	7.10	2.12
Naproxen	1.510	2.020	0.600	0.670	1.7821	9.207	8.80	12.20	3.40
Acetylsalicylic acid	0.781	1.690	0.710	0.670	1.2879	6.279	8.50	9.58	1.08
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	1.1313	5.636	6.80	7.88	1.08
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	1.1313	5.741	6.70	8.41	1.71
Benzil	1.445	1.590	0.000	0.620	1.6374	7.611	4.87	8.93	4.06
4-Nitroaniline	1.220	1.920	0.460	0.350	0.9904	6.042	7.19	9.29	2.10
Haloperidol	1.900	1.390	0.400	1.760	2.7980	12.819	11.30	14.32	3.02
Hydroquinone	1.063	1.270	1.060	0.570	0.8338	4.827	8.82	8.96	0.14
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	1.6512	9.171	6.03	10.29	4.26
Salicylamide	1.160	1.650	0.630	0.480	1.0315	5.910	7.60	9.01	1.41

TABLE 3. Summary of test set computations for methyl acetate

Training Set	Test Set	Predictions (log units)		
		SD	AAE	AE
Log P Correlation				
A + B	C	0.155	0.116	-0.027
A + C	B	0.231	0.178	0.032
B + C	A	0.195	0.150	-0.009
Log K Correlation				
A + B	C	0.164	0.121	-0.034
A + C	B	0.230	0.167	0.019
B + C	A	0.127	0.104	0.006

TABLE 4. Summary of test set computations for butyl acetate

Training Set	Test Set	Predictions (log units)		
		SD	AAE	AE
Log P Correlation				
A + B	C	0.171	0.143	0.002
A + C	B	0.170	0.148	0.060
B + C	A	0.185	0.148	-0.055
Log K Correlation				
A + B	C	0.185	0.151	-0.024
A + C	B	0.174	0.136	0.041
B + C	A	0.162	0.121	-0.016

TABLE 5. Solute Descriptors and Practical Partition Coefficient Data for Solutes

Between Water and Wet Butyl Acetate at 298.15 K

Solute	**E**	**S**	**A**	**B**	**B^o**	**V**	**L**	Log K_w	Log K_{obs}	Log P_{obs}
Methanol	0.278	0.44	0.43	0.47	0.47	0.3082	0.970	3.74	2.00	-1.74
Ethanol	0.246	0.42	0.37	0.48	0.48	0.4491	1.485	3.67	2.67	-1.00
1-Propanol	0.236	0.42	0.37	0.48	0.48	0.5900	2.031	3.56	3.33	-0.23
1-Butanol	0.224	0.42	0.37	0.48	0.48	0.7309	2.601	3.46	3.78	0.32
1-Pentanol	0.219	0.42	0.37	0.48	0.48	0.8718	3.106	3.35	4.20	0.85
1-Hexanol	0.210	0.42	0.37	0.48	0.48	1.0170	3.610	3.23	4.83	1.60
1-Heptanol	0.211	0.42	0.37	0.48	0.48	1.1536	4.115	3.09	4.99	1.90
Phenol	0.805	0.89	0.60	0.30	0.30	0.7751	3.766	4.85	6.54	1.69
2-Nitrophenol	1.015	1.05	0.05	0.37	0.37	0.9493	4.760	3.36	5.68	2.32
3-Nitrophenol	1.050	1.57	0.79	0.23	0.23	0.9493	5.692	7.06	9.48	2.42
4-Nitrophenol	1.070	1.72	0.82	0.26	0.26	0.9493	5.876	7.81	10.11	2.30
2-Fluorophenol	0.660	0.69	0.61	0.26	0.26	0.7930	3.453	3.88	5.79	1.91
3-Fluorophenol	0.667	0.98	0.68	0.17	0.17	0.7930	3.842	4.62	6.82	2.20
4-Fluorophenol	0.670	0.97	0.63	0.23	0.23	0.7930	3.844	4.54	6.49	1.95
2-Chlorophenol	0.853	0.88	0.32	0.31	0.31	0.8975	4.178	3.34	5.73	2.39
3-Chlorophenol	0.909	1.06	0.69	0.15	0.15	0.8975	4.773	4.80	7.48	2.68
4-Chlorophenol	0.915	1.08	0.67	0.21	0.21	0.8975	4.775	5.16	7.67	2.51
2-Bromophenol	1.037	0.90	0.35	0.31	0.31	0.9501	4.802	3.71	6.17	2.46
3-Bromophenol	1.060	1.16	0.70	0.16	0.16	0.9501	5.144	5.11	8.02	2.91
4-Bromophenol	1.080	1.17	0.67	0.20	0.20	0.9501	5.135	5.23	7.75	2.52
2-Iodophenol	1.360	1.00	0.40	0.35	0.35	1.0333	4.964	4.55	7.33	2.78
3-Iodophenol	1.370	1.20	0.70	0.18	0.18	1.0333	5.528	5.68	8.62	2.94
4-Iodophenol	1.380	1.22	0.68	0.20	0.20	1.0333	5.492	5.58	8.68	3.10
2-Methylphenol	0.840	0.86	0.52	0.30	0.30	0.9160	4.218	4.31	6.55	2.24
3-Methylphenol	0.822	0.88	0.57	0.34	0.34	0.9160	4.310	4.60	6.73	2.13
4-Methylphenol	0.820	0.87	0.57	0.31	0.31	0.9160	4.312	4.50	6.81	2.31
2-Ethylphenol	0.831	0.84	0.52	0.37	0.37	1.0569	4.612	4.42	7.21	2.79
4-Ethylphenol	0.800	0.90	0.55	0.36	0.36	1.0569	4.737	4.50	6.95	2.45
2-Methoxyphenol	0.837	0.91	0.22	0.52	0.52	0.9747	4.449	4.09	5.81	1.72
3-Methoxyphenol	0.879	1.17	0.59	0.38	0.38	0.9747	4.803	5.80	7.63	1.83
4-Methoxyphenol	0.900	1.17	0.57	0.48	0.48	0.9747	4.773	6.15	7.70	1.55
2,4-Dimethylphenol	0.843	0.80	0.53	0.39	0.39	1.0569	4.770	4.41	6.92	2.51
2,5-Dimethylphenol	0.840	0.83	0.50	0.38	0.38	1.0569	4.774	4.34	6.86	2.52
2,6-Dimethylphenol	0.850	0.82	0.51	0.37	0.37	1.0569	4.680	3.86	6.49	2.63

3,4-Dimethylphenol	0.830	0.86	0.56	0.39	0.39	1.0569	4.980	4.77	7.22	2.45
3.5-Dimethylphenol	0.820	0.84	0.57	0.36	0.36	1.0569	4.856	4.60	7.26	2.66
4-Propylphenol	0.793	0.88	0.54	0.35	0.35	1.1978	5.185	4.45	7.30	2.85
1-Naphthol	1.520	1.10	0.66	0.34	0.34	1.1441	6.284	5.87	8.40	2.53
2-Naphthol	1.520	1.08	0.61	0.40	0.40	1.1441	6.200	5.95	9.06	3.11
Acetic acid	0.265	0.64	0.62	0.44	0.44	0.4648	1.816	4.88	4.48	-0.40
Propanoic acid	0.233	0.65	0.61	0.44	0.44	0.6057	2.276	4.73	4.82	0.09
Butanoic acid	0.210	0.64	0.61	0.45	0.45	0.7466	2.750	4.63	5.32	0.69
Pentanoic acid	0.205	0.63	0.62	0.45	0.45	0.8875	3.227	4.45	5.66	1.21
Heptanoic acid	0.149	0.64	0.62	0.44	0.44	1.1693	4.183	4.20	6.41	2.21
2-Hydroxybenzoic acid	0.900	0.85	0.73	0.37	0.37	0.9904	4.732	5.39	7.76	2.37
3-Hydroxybenzoic acid	0.910	0.88	0.86	0.58	0.58	0.9904	4.860	7.00	8.30	1.30
4-Hydroxybenzoic acid	0.930	0.90	0.81	0.56	0.56	0.9904	4.867	6.78	8.14	1.36
2,4-Dihydroxybenzoic acid	1.140	1.16	1.06	0.56	0.56	1.0491	5.573	8.39	10.02	1.63
4-Methoxybenozic acid	0.899	0.91	0.61	0.48	0.48	1.1313	5.305	5.51	7.87	2.36
2-Methyl-1-propanol	0.217	0.39	0.37	0.48	0.48	0.7309	2.413	3.30	3.51	0.21
3-Methyl-1-butanol	0.192	0.39	0.37	0.48	0.48	0.8718	3.011	3.24	4.16	0.92
2-Butanol	0.217	0.36	0.33	0.56	0.56	0.7309	2.338	3.39	3.44	0.05
Pentobarbital	1.030	1.11	0.47	1.23	1.23	1.7966	7.945	8.63	10.63	2.00
Hexobarbital	1.500	1.58	0.17	1.33	1.33	1.7859	8.972	9.45	11.25	1.80
Phenobarbital	1.630	1.72	0.71	1.18	1.18	1.6999	8.952	11.32	13.12	1.80
Aniline	0.955	0.96	0.26	0.41	0.50	0.8162	3.934	4.30	5.63	1.33
4-Methylaniline	0.923	0.95	0.23	0.45	0.52	0.9571	4.452	4.09	5.75	1.66
4-Pentylaniline	0.916	0.88	0.20	0.53	0.60	1.5207	6.448	3.82	7.27	3.45
4-Hexylaniline	0.912	0.88	0.21	0.52	0.60	1.6616	6.969	3.69	7.59	3.90
Pyridine	0.631	0.84	0.00	0.52	0.47	0.6753	3.022	3.44	3.89	0.45
Ephedrine	0.916	0.76	0.24	1.19	1.19	1.4385	6.211	6.92	7.48	0.56
Tetrahydrofuran	0.289	0.52	0.00	0.48	0.48	0.6223	2.636	2.55	2.89	0.34
4-Aminobenzoic acid	1.075	1.65	0.94	0.60	0.60	1.0315	5.916	9.43	10.60	1.17
2,4-Dichlorophenol	0.960	0.82	0.54	0.17	0.17	1.0199	4.896	3.65	6.59	2.94
2,6-Dichlorophenol	0.900	0.86	0.36	0.24	0.24	1.0199	4.777	3.37	5.92	2.55
2,4,6-Trichlorophenol	1.010	0.80	0.60	0.15	0.15	1.1423	5.670	3.63	7.02	3.39
1-Naphthylamine	1.670	1.27	0.19	0.51	0.51	1.1852	6.490	5.35	8.04	2.69
2-Naphthylamine	1.670	1.30	0.18	0.51	0.51	1.1852	6.540	5.39	8.11	2.72
2-Aminophenol	1.110	1.31	0.61	0.60	0.60	0.8749	4.975	7.45	7.87	0.42
2-Hydroxybenzaldehyde	0.962	1.05	0.12	0.33	0.33	0.9317	4.570	3.48	5.82	2.34
Methyl 2-hydroxybenzoate	0.850	0.82	0.01	0.48	0.48	1.1313	4.961	2.97	5.51	2.54
Methyl 4-hydroxybenzoate	0.900	1.37	0.69	0.45	0.45	1.1313	5.665	6.86	9.22	2.36
1-Nitroso-2-naphthol	1.434	1.41	0.06	0.58	0.58	1.2596	6.706	5.36	7.87	2.51

2-Nitroso-1-naphthol	1.434	1.26	0.44	0.58	0.58	1.2596	6.691	6.44	8.70	2.26
4-Nitrosophenol	0.900	0.73	0.55	0.58	0.58	0.8906	4.256	5.51	6.66	1.15
2-Hydroxy-3-methoxybenzaldehyde	1.040	1.26	0.07	0.61	0.61	1.1313	5.608	5.05	6.96	1.91
Catechol	0.970	1.10	0.88	0.47	0.47	0.8338	4.450	7.20	8.34	1.14
Resorcinol	0.980	1.11	1.09	0.52	0.52	0.8338	4.618	8.35	9.35	1.00
Hydroquinone	1.063	1.27	1.06	0.57	0.57	0.8338	4.827	8.87	9.53	0.66
Vanillin	1.028	1.28	0.33	0.68	0.68	1.1313	5.730	6.42	7.87	1.45
Peracetic acid	0.305	0.92	0.58	0.46	0.46	0.5235	2.392	5.49	5.06	-0.43

TABLE 6. Solute descriptors and observed values of log P_{EA}, log K_{EA}, and log K_w for the gas and water to dry ethyl acetate systems at 298.15 K

Solute	**E**	**S**	**A**	**B**	**V**	**L**	Log P_{obs}	Log K_{obs}	Log K_w
Radon	0.000	0.00	0.00	0.00	0.3840	0.877	1.46	0.81	-0.65
Hydrogen	0.000	0.00	0.00	0.00	0.1086	-1.200	0.65	-1.07	-1.72
Oxygen	0.000	0.00	0.00	0.00	0.1830	-0.723	0.85	-0.66	-1.51
Nitrogen	0.000	0.00	0.00	0.00	0.2222	-0.978	1.04	-0.76	-1.80
Carbon monoxide	0.000	0.00	0.00	0.04	0.2220	-0.836	1.02	-0.60	-1.62
Sulfur dioxide	0.370	0.66	0.28	0.10	0.3465	0.778	0.83	2.36	1.53
Ethane	0.000	0.00	0.00	0.00	0.3904	0.492	1.83	0.49	-1.34
2-Methylpropane	0.000	0.00	0.00	0.00	0.6722	1.409	3.28	1.58	-1.70
Pentane	0.000	0.00	0.00	0.00	0.8131	2.162	3.79	2.09	-1.70
Hexane	0.000	0.00	0.00	0.00	0.9540	2.668	4.36	2.54	-1.82
Heptane	0.000	0.00	0.00	0.00	1.0949	3.173	4.94	2.98	-1.96
Octane	0.000	0.00	0.00	0.00	1.2358	3.677	5.56	3.45	-2.11
Nonane	0.000	0.00	0.00	0.00	1.3767	4.182	6.06	3.91	-2.15
2-Methylpentane	0.000	0.00	0.00	0.00	0.9540	2.503	4.25	2.41	-1.84
2,4-Dimethylpentane	0.000	0.00	0.00	0.00	1.0949	2.809	4.78	2.70	-2.08
2,5-Dimethylhexane	0.000	0.00	0.00	0.00	1.2358	3.308	5.18	3.16	-2.02
2,3,4-Trimethylpentane	0.000	0.00	0.00	0.00	1.2358	3.481	5.11	3.23	-1.88
Cyclohexane	0.305	0.10	0.00	0.00	0.8454	2.964	3.66	2.76	-0.90
Ethylcyclohexane	0.263	0.10	0.00	0.00	1.1272	3.877	5.12	3.54	-1.58
Propene	0.103	0.08	0.00	0.07	0.4883	0.946	2.08	1.11	-0.97
trans-But-2-ene	0.126	0.08	0.00	0.05	0.6292	1.664	3.14	2.03	-1.11
Pent-1-ene	0.093	0.08	0.00	0.07	0.7701	2.047	3.40	2.17	-1.23
2-Methylprop-1-ene	0.120	0.08	0.00	0.08	0.6292	1.579	2.73	1.87	-0.86
3-Methylbut-1-ene	0.063	0.06	0.00	0.05	0.7701	1.933	3.35	2.01	-1.34
Hept-1-ene	0.092	0.08	0.00	0.07	1.0519	3.063	4.20	2.98	-1.22
But-1,3-diene	0.320	0.23	0.00	0.10	0.5862	1.543	2.53	2.08	-0.45
2-Methylbuta-1,3-diene	0.313	0.23	0.00	0.10	0.7271	2.101	2.91	2.41	-0.50
Hept-1,6-diene	0.189	0.20	0.00	0.10	1.0089	3.028	4.22	3.37	-0.85
Dichloromethane	0.387	0.57	0.10	0.05	0.4943	2.019	2.00	2.96	0.96
Trichloromethane	0.425	0.49	0.15	0.02	0.6167	2.480	2.59	3.38	0.79
Tetrachloromethane	0.458	0.38	0.00	0.00	0.7391	2.823	3.29	3.10	-0.19
1,2-Dichloroethane	0.416	0.64	0.10	0.11	0.6352	2.573	2.19	3.46	1.27
1-Chloropropane	0.216	0.40	0.00	0.10	0.6537	2.202	2.46	2.70	0.24

1-Chlorobutane	0.210	0.40	0.00	0.10	0.7946	2.722	3.04	3.16	0.12
2-Chloro-2-methylpropane	0.142	0.30	0.00	0.03	0.7946	2.273	3.41	2.61	-0.80
Bromoethane	0.366	0.40	0.00	0.12	0.5654	2.120	2.05	2.59	0.54
2-Bromo-2-methylpropane	0.305	0.29	0.00	0.07	0.8472	2.609	3.57	2.97	-0.60
Iodomethane	0.676	0.43	0.00	0.12	0.5077	2.106	1.89	2.54	0.65
Iodoethane	0.640	0.40	0.00	0.14	0.6486	2.573	2.42	2.96	0.54
1,1,2-Trifluorotrichloroethane	0.010	0.13	0.00	0.00	0.8107	2.210	3.79	2.49	-1.30
1,2-Difluorotetrachloroethane	0.227	0.33	0.00	0.02	0.9154	3.034	4.03	3.39	-0.64
Tetrahydrofuran	0.289	0.52	0.00	0.48	0.6223	2.636	0.46	3.01	2.55
1,4-Dioxane	0.329	0.75	0.00	0.64	0.6810	2.892	-0.04	3.67	3.71
2-Methylproprionaldehyde	0.144	0.62	0.00	0.45	0.6879	2.120	0.87	2.97	2.10
Propanone	0.179	0.70	0.04	0.49	0.5470	1.696	0.03	2.86	2.83
Butanone	0.166	0.70	0.00	0.51	0.6879	2.287	0.54	3.26	2.72
Ethyl acetate	0.106	0.62	0.00	0.45	0.7466	2.314	1.14	3.30	2.16
Acetonitrile	0.237	0.90	0.07	0.32	0.4042	1.739	0.22	3.07	2.85
Proprionitrile	0.162	0.90	0.02	0.36	0.5450	2.082	0.61	3.43	2.82
Diethylamine	0.154	0.30	0.08	0.69	0.7720	2.395	-0.24	2.75	2.99
Triethylamine	0.101	0.15	0.00	0.79	1.0538	3.040	0.77	3.13	2.36
Nitromethane	0.313	0.95	0.06	0.31	0.4237	1.892	0.66	3.61	2.95
N,N-Dimethylformamide	0.367	1.31	0.00	0.74	0.6468	3.173	-1.26	4.47	5.73
Methanol	0.278	0.44	0.43	0.47	0.3082	0.970	-1.04	2.70	3.74
Ethanol	0.246	0.42	0.37	0.48	0.4491	1.485	-0.65	3.02	3.67
Propan-2-ol	0.212	0.36	0.33	0.56	0.5900	1.764	-0.45	3.03	3.48
Dimethylsulfoxide	0.522	1.72	0.00	0.97	0.6126	3.459	-2.97	4.88	7.85
Carbon disulphide	0.876	0.26	0.00	0.03	0.4905	2.370	2.44	2.29	-0.15
Tetramethyltin	0.324	0.11	0.00	0.10	1.0431	2.651	4.17	2.64	-1.53
Benzene	0.610	0.52	0.00	0.14	0.7164	2.786	2.61	3.24	0.63
Toluene	0.601	0.52	0.00	0.14	0.8573	3.325	3.04	3.69	0.65
trans-Stilbene	1.450	1.04	0.00	0.34	1.5630	7.525	5.45	8.23	2.78
Acenaphthene	1.604	1.05	0.00	0.22	1.2586	6.469	4.56	6.92	2.36
Anthracene	2.290	1.34	0.00	0.28	1.4544	7.568	5.12	8.15	3.03
Phenanthrene	2.055	1.29	0.00	0.29	1.4544	7.632	5.32	8.12	2.80
Fluoranthene	2.377	1.55	0.00	0.24	1.5846	8.827	5.84	9.28	3.44
Pyrene	2.808	1.71	0.00	0.28	1.5846	8.833	5.78	9.28	3.50
Chlorobenzene	0.718	0.65	0.00	0.07	0.8388	3.657	3.33	4.15	0.82
Aniline	0.955	0.96	0.26	0.41	0.8162	3.934	1.19	5.49	4.30
Benzoic acid	0.730	0.90	0.59	0.40	0.9317	4.657	1.79	6.91	5.12
2-Hydroxybenzoic acid	0.900	0.85	0.73	0.37	0.9904	4.732	2.02	7.41	5.39
4-Hydroxybenzoic acid	0.930	0.90	0.81	0.56	0.9904	4.867	1.33	8.11	6.78

4-Hydroxybenzoic acid	0.930	0.90	0.81	0.56	0.9904	4.867	1.24	8.02	6.78
Methyl 4-hydroxybenzoate	0.900	1.37	0.69	0.45	1.1313	5.665	1.90	8.75	6.85
2-Methylpyridine	0.598	0.75	0.00	0.58	0.8162	3.422	0.76	4.16	3.40
2,4-Dichloro-1-phenyl-3,3-dimethylurea	1.280	1.60	0.57	0.70	1.5992	8.060	2.70	10.70	8.00
2-Furaldehyde	0.690	1.13	0.00	0.45	0.6929	3.318	0.79	4.62	3.83
Phenylacetic acid	0.730	1.08	0.66	0.57	1.0726	4.962	1.67	8.14	6.47
4-Hydroxyphenylacetic acid	1.030	1.45	0.94	0.74	1.1313	5.902	0.44	9.95	9.51
4-Ethoxyacetanilide	0.940	1.48	0.48	0.86	1.4542	6.893	1.42	9.42	8.00
Betulin	1.790	2.12	0.70	1.14	3.8670	17.470	10.02	20.41	10.39
3-Nitrophthalic acid	1.360	2.01	1.20	0.89	1.3212	7.780	0.01	12.68	12.67
Acetylsalicylic acid	0.781	1.69	0.71	0.67	1.2879	6.279	1.33	9.90	8.57
3-Chlorobenzoic acid	0.840	0.95	0.63	0.32	1.0541	5.197	2.46	7.61	5.15
4-Chlorobenzoic acid	0.840	1.02	0.63	0.27	1.0541	4.947	2.61	7.41	4.80
3-Nitrobenzoic acid	0.990	1.18	0.73	0.52	1.1059	5.601	1.82	8.75	6.93
4-Nitrobenzoic acid	0.990	1.52	0.68	0.40	1.1059	5.770	2.08	8.98	6.90
3,5-Dinitrobenzoic acid	1.250	1.63	0.70	0.59	1.2801	6.984	2.11	10.41	8.30
4-Chloro-3-nitrobenzoic acid	1.250	1.47	0.70	0.44	1.2283	6.685	2.55	9.76	7.21
2-Chloro-5-nitrobenzoic acid	1.250	1.40	0.67	0.46	1.2283	6.513	2.46	9.41	6.95
2-Methoxybenzoic acid	0.899	1.41	0.45	0.62	1.1313	5.636	1.37	8.17	6.80
4-Methoxybenzoic acid	0.899	1.25	0.62	0.52	1.1313	5.741	1.92	8.62	6.70
2-Methylbenzoic acid	0.730	0.84	0.42	0.44	1.0726	4.677	2.23	6.53	4.30
3-Methylbenzoic acid	0.730	0.89	0.60	0.40	1.0726	4.819	2.28	7.26	4.98
Ketoprofen	1.650	2.26	0.55	0.89	1.9779	10.527	3.30	13.76	10.46
Naproxen	1.510	2.02	0.60	0.67	1.7821	9.207	3.70	12.50	8.80
Salicylamide	1.160	1.58	0.61	0.51	1.0315	5.818	1.63	9.23	7.60
Benzil	1.445	1.59	0.00	0.62	1.6374	7.611	4.17	9.04	4.87
1-Chloroanthraquinone	1.900	1.79	0.00	0.57	1.6512	9.171	4.38	10.41	6.03
Monuron	1.140	1.50	0.47	0.78	1.4768	7.180	1.95	9.58	7.63
Diuron	1.280	1.60	0.57	0.70	1.5992	8.060	2.70	10.70	8.00
Ferrocene	1.350	0.85	0.00	0.20	1.1209	5.622	4.10	6.02	1.92
Diphenylsulfone	1.570	2.15	0.00	0.70	1.6051	8.902	3.28	10.67	7.39
Hexachlorobenzene	1.490	0.99	0.00	0.00	1.4508	7.390	6.10	7.51	1.50
Docosane	0.000	0.00	0.00	0.00	3.2084	10.740	13.58	10.01	-3.57
Tricosane	0.000	0.00	0.00	0.00	3.3493	11.252	14.26	10.54	-3.72
Hydroquinone	1.063	1.27	1.06	0.57	0.8338	4.827	0.18	9.05	8.87

TABLE 7. Solute descriptors[a] and observed values of log P_{EA}, log K_{EA}, and log K_w for the gas and water to wet ethyl acetate systems at 298.15 K

Solute	**E**	**S**	**A**	**B**^{o}	**V**	**L**	log P_{obs}	log K_{obs}	log K_w
Radon	0.000	0.00	0.00	0.00	0.3840	0.877	1.41	0.76	-0.65
Hydrogen peroxide	0.451	0.66	0.78	0.41	0.2260	1.226	-0.72	4.97	5.69
Cyanamide	0.450	1.36	0.26	0.32	0.3631	2.265	-0.19	4.74	4.93
Formic acid	0.343	0.75	0.76	0.33	0.3239	1.545	-0.23	5.10	5.33
Acetic acid	0.265	0.64	0.62	0.44	0.4648	1.816	-0.15	4.73	4.88
Propanonic acid	0.233	0.65	0.61	0.44	0.6057	2.276	0.36	5.09	4.73
Butanoic acid	0.210	0.64	0.61	0.45	0.7466	2.750	0.72	5.35	4.63
Pentanoic acid	0.205	0.63	0.62	0.45	0.8875	3.227	1.31	5.76	4.45
Heptanoic acid	0.149	0.64	0.62	0.44	1.1693	4.183	1.95	6.15	4.20
Fumaric acid	0.710	0.94	0.87	0.59	0.7780	3.916	0.23	7.53	7.30
Methanol	0.278	0.44	0.43	0.47	0.3082	0.970	-0.85	2.89	3.74
Ethanol	0.246	0.42	0.37	0.48	0.4491	1.485	-0.40	3.27	3.67
Propan-1-ol	0.236	0.42	0.37	0.48	0.5900	2.031	0.18	3.74	3.56
Butan-1-ol	0.224	0.42	0.37	0.48	0.7309	2.601	0.77	4.23	3.46
Pentan-1-ol	0.219	0.42	0.37	0.48	0.8718	3.106	1.36	4.71	3.35
Hexan-1-ol	0.210	0.42	0.37	0.48	1.0127	3.610	1.80	5.03	3.23
Heptan-1-ol	0.211	0.42	0.37	0.48	1.1536	4.115	2.30	5.39	3.09
Octan-1-ol	0.199	0.42	0.37	0.48	1.2945	4.619	3.16	6.16	3.00
Ethane-1,2-diol	0.404	0.90	0.58	0.78	0.5078	2.661	-1.82	5.28	7.10
Propane-1,3-diol	0.397	0.91	0.77	0.85	0.6487	3.263	-1.55	6.35	7.90
Butane-1,4-diol	0.395	0.93	0.72	0.90	0.7896	3.795	-1.19	6.55	7.74
Pentane-1,5-diol	0.388	0.90	0.72	0.92	0.9305	4.200	-0.68	7.64	8.32
Hexane-1,6-diol	0.385	0.96	0.72	0.96	1.0714	4.600	-0.10	8.11	8.21
Heptane-1,7-diol	0.381	0.96	0.75	0.96	1.2123	5.070	0.48	8.76	8.28
Octane-1,8-diol	0.380	0.96	0.75	0.95	1.3532	5.510	1.07	9.11	8.04
Aniline	0.955	0.96	0.26	0.50	0.8162	3.934	1.25	5.55	4.30
p-Toluidine	0.923	0.95	0.23	0.52	0.9571	4.452	1.53	5.62	4.09
p-Nitroaniline	1.220	1.92	0.46	0.35	0.9904	6.042	1.98	9.16	7.18
Ethyl p-aminobenzoate	1.030	0.95	0.35	0.82	1.3133	6.136	1.19	7.35	6.16
4-Aminobenzoic acid	1.075	1.65	0.94	0.60	1.0315	5.916	1.29	10.72	9.43
4-Aminosalicylic acid	1.250	1.53	0.99	0.65	1.0902	6.228	1.00	10.61	9.61
Phenol	0.805	0.89	0.60	0.30	0.7751	3.766	1.53	6.38	4.85
2,4-Dimethylphenol	0.843	0.79	0.52	0.40	1.0569	4.770	2.59	7.00	4.41

2,5-Dimethylphenol	0.840	0.83	0.50	0.38	1.0569	4.774	2.59	6.93	4.34
3,4-Dimethylphenol	0.830	0.90	0.55	0.38	1.0569	4.980	2.53	7.30	4.77
3,5-Dimethylphenol	0.830	0.86	0.55	0.37	1.0569	4.856	2.59	7.19	4.60
4-Ethylphenol	0.800	0.90	0.55	0.36	1.0569	4.737	2.54	7.04	4.50
2-Fluorophenol	0.660	0.69	0.61	0.26	0.7928	3.453	2.00	5.88	3.88
2-Chlorophenol	0.853	0.88	0.32	0.31	0.8975	4.178	2.30	5.64	3.34
2-Bromophenol	1.037	0.90	0.35	0.31	0.9501	4.802	2.52	6.23	3.71
2-Iodophenol	1.360	1.00	0.40	0.35	1.0333	4.964	2.84	7.39	4.55
Picric acid	1.430	2.66	0.46	0.42	1.2977	8.128	2.75	12.05	9.30
2-Hydroxybenzoic acid	0.900	0.85	0.73	0.37	0.9904	4.732	1.69	7.08	5.39
Catechol	0.970	1.10	0.88	0.47	0.8338	4.450	1.25	8.45	7.20
Resorcinol	0.980	1.11	1.09	0.52	0.8338	4.618	0.96	9.31	8.35
Hydroquinone	1.063	1.27	1.06	0.57	0.8338	4.827	0.79	9.66	8.87
Chlorohydroquinone	1.080	1.13	0.65	0.49	0.9562	5.059	1.92	8.45	6.53
4-Hydroxyacetanilide	1.060	1.63	1.04	0.86	1.1724	6.430	-0.30	10.60	10.90
1-Naphthol	1.520	1.10	0.66	0.34	1.1441	6.284	2.61	8.48	5.87
2-Naphthol	1.520	1.08	0.61	0.40	1.1441	6.200	3.16	9.11	5.95
2-Furaldehyde	0.690	1.13	0.00	0.45	0.6929	3.318	0.58	4.41	3.83
Cocaine	1.355	1.92	0.00	1.50	2.2977	10.530	2.00	12.02	10.02
Antipyrine	1.300	1.83	0.00	1.37	1.4846	7.764	-0.13	9.61	9.74
1,2,4-Triazole	0.662	1.50	0.97	0.43	0.4952	3.271	-1.00	7.52	8.52
Purine	1.320	1.58	0.56	0.78	0.8231	5.343	-0.68	8.29	8.97
Uracil	0.810	0.88	0.44	1.00	0.7516	3.610	-0.85	6.70	7.55
Thymine	0.800	1.67	0.38	0.79	0.8925	4.888	-0.74	7.48	8.22
Theobromine	1.500	1.60	0.50	1.38	1.2223	7.078	-1.15	10.30	11.45
Caffeine	1.500	1.72	0.05	1.28	1.3632	7.833	-0.23	9.56	9.79
Hydrocortisone	2.030	3.49	0.71	1.90	2.7976	14.800	1.09	19.74	18.65
Prednisolone	2.210	3.10	0.71	1.92	2.7546	14.370	1.05	18.96	17.91
Estriol	1.970	1.74	1.06	1.63	2.2575	11.700	1.38	15.93	14.55
Phenytoin	1.713	2.19	0.85	1.00	1.8693	10.137	2.29	14.41	12.12

[a] The numerical values of $\mathbf{B}$ and $\mathbf{B}^{o}$ are identical for all of the tabulated solutes except for aniline ($\mathbf{B}$ = 0.41 and $\mathbf{B}^{o}$ = 0.50); p-toluidine ($\mathbf{B}$ = 0.45 and $\mathbf{B}^{o}$ = 0.52) and purine ($\mathbf{B}$ = 1.00 and $\mathbf{B}^{o}$ = 0.78).

TABLE 8. A summary of the coefficients in equations for log P and log K

System	c	e	s	a	b	v	l
Gas to dry methyl acetate	0.134	-0.477	1.749	2.678	0.000		0.876
Gas to dry ethyl acetate	0.182	-0.352	1.316	2.891	0.000		0.916
Gas to dry butyl acetate	0.147	-0.414	1.212	2.623	0.000		0.954
Water to dry methyl acetate	0.351	0.223	-0.150	-1.035	-4.527	3.972	
Water to dry ethyl acetate	0.328	0.369	-0.446	-0.700	-4.904	4.150	
Water to dry butyl acetate	0.248	0.356	-0.501	-0.867	-4.973	4.281	
Gas to wet ethyl acetate	0.130	0.031	1.202	3.199	0.463		0.828
Gas to wet butyl acetate	-0.664	0.061	1.671	3.373	0.824		0.832
Water to wet ethyl acetate	0.441	0.591	-0.669	-0.325	-4.261[a]	3.666	
Water to wet butyl acetate	-0.475	0.428	-0.094	-0.241	-4.151 [a]	4.046	

[a] Coefficient for the $\mathbf{B}^{o}$ descriptor.

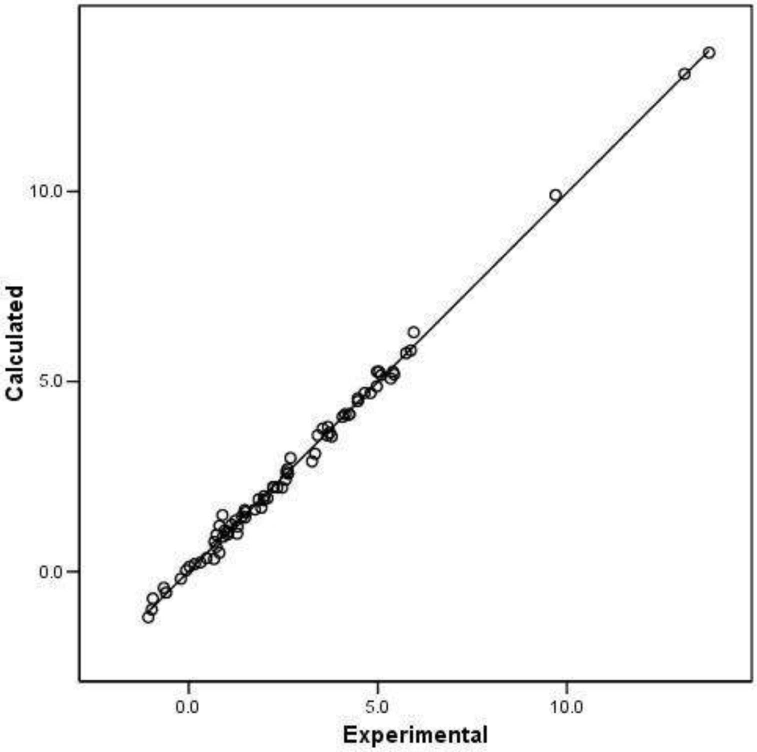

Figure 1. Comparison of calculated water-to-methyl acetate log P based on Eqn. 9 versus experimental data.

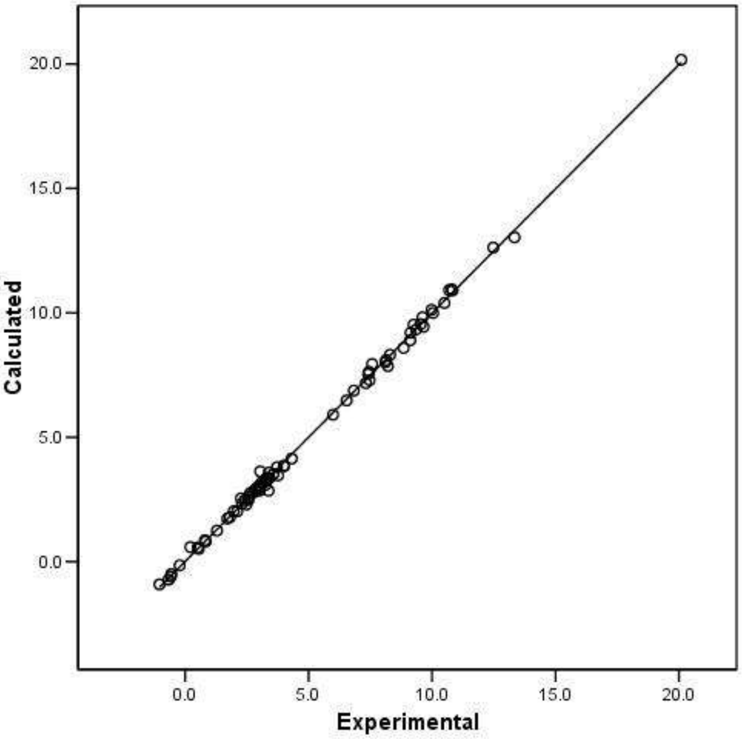

Figure 2. Comparison of calculated gas-to-methyl acetate log K values based on Eqn. 11 versus experimental data.