DEVELOPMENT OF ABRAHAM MODEL CORRELATIONS FOR SOLVATION CHARACTERISTICS OF LINEAR ALCOHOLS

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Abstract

Data have been compiled from the published literature on the partition coefficients of solutes and vapors into the anhydrous linear alcohols (methanol through 1-heptanol, and 1-decanol) from both water and from the gas phase. The logarithms of the water-to-alcohol partition coefficients ($\log P$) and gas-to-alcohol partition coefficients ($\log K$) were correlated with the Abraham solvation parameter model. The derived correlations described the observed $\log P$ and $\log K$ values to within average standard deviations of 0.14 and 0.12 log units, respectively. The predictive abilities of the each correlation were assessed by dividing databases into a separate training set and test set.

KEY WORDS AND PHRASES: Partition Coefficients, Alcohol Solvents, Linear Free Energy
Correlations, Activity Coefficients, Solubilities, Henry's Constants

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1. Introduction

The solubility of crystalline solutes in both neat organic solvents and mixtures has received considerable attention in recent years due to the important role that solubility plays in the manufacture of new chemical materials and pharmaceutical products. For newly synthesized compounds, supply is often very limited and there is not always sufficient material to measure the compound's solubility in every solvent of possible interest. To address this concern, researchers have turned to predictive methods for estimating solubility when experimental data are unavailable. Several methods have been developed for predicting solubility from solely molecular structure considerations, from measured physical properties, or from experimental solubility data for the solute dissolved in a few select organic solvents.

The predictive method that we have been using is based on the Abraham general solvation model [1-6] for solute transfer between two condensed phases

$$\log P = c + e \cdot \mathbf{E} + s \cdot \mathbf{S} + a \cdot \mathbf{A} + b \cdot \mathbf{B} + v \cdot \mathbf{V} \quad (1)$$

and for processes involving solute transfer from the gas phase to a condensed phase

$$\log K = c + e \cdot \mathbf{E} + s \cdot \mathbf{S} + a \cdot \mathbf{A} + b \cdot \mathbf{B} + l \cdot \mathbf{L} \quad (2)$$

The dependent variables in Eqns. 1 and 2 are the logarithm of the solute's water-to-organic solvent partition coefficient, $\log P$, and the logarithm of the solute's gas-to-organic solvent partition coefficient, $\log K$. For solubility predictions, the model assumes that the partition between water and the organic solvent is given by the ratio of molar solubilities of the solute in the organic solvent, C_S^{sat} , and in water, C_W^{sat} (i.e., $P = C_S^{\text{sat}}/C_W^{\text{sat}}$). The gas-to-organic solvent partition is similarly calculated as the molar solubility in the organic solvent divided the solute

gas phase concentration (i.e., $K = C_S^{\text{sat}}/C_G$), the latter value calculable from the solute vapor pressure above the solid at the solution temperature. The computation methodology is described in detail elsewhere. [3-24]

The independent variables in Eqns. 1 and 2 are solute descriptors as follows: **E** and **S** refer to the excess molar refraction and dipolarity/polarity descriptors of the solute, respectively, **A** and **B** are measures of the solute hydrogen-bond acidity and hydrogen-bond 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 regression coefficients and constants (c, e, s, a, b, v and l) are obtained by regression analysis of experimental data for a specific process (*i.e.*, a given partitioning process, a given stationary phase and mobile phase combination, *etc.*). In the case of partition coefficients, where two solvent phases are involved, the c, e, s, a, b, v and l coefficients represent differences in the solvent phase properties. For any fully characterized system/process (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. This is the major advantage of using Eqns. 1 and 2 to correlate solute partitioning properties having environmental, pharmaceutical and chemical importance.

The predictive procedure that we have developed for estimating solute solubility requires knowledge of both the solute descriptors and regression coefficients for the solvent of interest. If the solute descriptors are not available, then the first step is to calculate them from measured solubilities and whatever other appropriate data are available. Of the six descriptors in Eqns. 1 and 2, **V** can always be calculated from the solute molecular formula, known atomic sizes and number of chemical bonds in the molecule [25]. For compounds that are liquid at 293 K, the

excess molar refraction descriptor, **E** (in units of (cm³ mol⁻¹)/10), can be obtained from the experimental refractive index. In the case of crystalline solutes, either the hypothetical refractive index can be calculated, or **E** can be obtained through the addition of values for fragments or sub-structures [2, 26]. This leaves three descriptors in Eqn. 1 to be determined (a fourth descriptor **L** is needed if both Eqns. 1 and 2 are to be used). If three log **P** values are available, either from direct practical partitioning experiments or indirectly through solubility ratios, then the remaining **S**, **A** and **B** descriptors can be calculated by solving the three corresponding Eqn. 1 equations simultaneously. In practice, more than three log **P** values will be used. The number of equations can be increased by converting all of the log **P** values into log **K** values through Eqn. 3

$$\text{Log } K = \log P - \log K_w \quad (3)$$

where K_w is the gas-to-water partition coefficient (unitless if concentrations in the gas phase and the aqueous phase are both in mol/L), or by combining the Abraham model and the Goss Modified Abraham model correlations, as we illustrated recently in determining solute descriptors for benzil [27]. Equation coefficients for the Goss Modified Abraham model have been reported for a few select organic solvents [27, 28]. For the present discussion, we assume that five log **P** values are available from measured solubility ratios and practical partition coefficient data. Five more equations in log **K** can be constructed with Eqn. 3, and two more equations in log K_w are also available. The gas-to-water partition coefficient of crystalline solutes, log K_w , will normally have to be found by trial-and-error as vapor pressure data are not generally available. Starting with five log **P** values, no fewer than twelve equations will be available to calculate the four missing solute descriptors (**S**, **A**, **B** and **L**) and log K_w . Once the

solute descriptors are known, one can estimate the solute's solubility in more than 50 organic solvents using the Abraham model equation coefficients that we have published thus far.

Several of the Abraham model correlations that we are currently using to calculate solute descriptors were derived more than ten years ago. These earlier correlations are based on the limited experimental data that were available at the time. It is important to update periodically earlier correlations as additional experimental data become available to ensure that the predictive equations span as wide a range of descriptor space as possible. In the present study we have reanalyzed the available experimental log P and log K partition coefficient data for solutes dissolved in the anhydrous linear alcohols (methanol through 1-heptanol, and 1-decanol). Abraham model correlations have been previously reported for these alcohol solvents [29-32]. The correlations that are presented here are based on much larger databases, and include a much larger number of the more acidic solutes (such as the crystalline benzoic acid derivatives) and a much larger number of the more nonvolatile solutes. The larger databases allow us to validate the derived correlations through training set and test set analyses. The experimental log P and log K databases are also given, as well as the literature references for where the published data were taken. Our previous publications reported the databases for only methanol [29], ethanol [30] and 1-propanol [31]. Updated correlations for the dry linear, secondary and branched alcohols are needed. Several research groups have begun publishing solubility data for crystalline pesticides and pesticide intermediates (i.e., 2-(4-ethylbenzoyl)benzoic acid [33]) and pharmaceutical drug molecules and intermediates (such as lovastatin [34], isonicotinic acid [35], pimozone [36], 4-aminobenzenesulfonamide [37] and meloxicam [38]) dissolved in alcohol solvents. Updated correlations allow us to utilize better the recently published solubility data in solute descriptor computers.

2. Data Sets and Computation Methodology

Most of the experimental data that we were able to retrieve from the published literature pertained either to the Raoult's law infinite dilution activity coefficient, $\gamma_{\text{solute}}^{\infty}$, Henry's law constants, K_{Henry} , or solubilities for solutes dissolved in the eight 1-alcohol solvents (methanol through 1-heptanol, and 1-decanol). 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. 4 and 5

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

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

or log P values for partition from water to the anhydrous 1-alcohols through Eqn. (2). In equations 4 and 5 R is the universal gas constant, T is the system temperature, $P_{\text{solute}}^{\circ}$ is the vapor pressure of the solute at T, and V_{solvent} is the molar volume of the solvent. The calculation of log P requires knowledge of the solute's gas phase partition coefficient into water, K_w , which is available for most of the solutes being studied. The experimental log K and log P values at 298 K for anhydrous methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol and 1-decanol are listed in Tables S1-S8 (Supporting information). Also included in the Supporting information are the literature references pertaining to the log K and log P data. As an informational note, the calculated log P values for the anhydrous alcohols refer to a hypothetical partition coefficient. Even though hypothetical, these log P correlations are still quite useful in that predicted log P values can be used to estimate the solute's infinite dilution activity

coefficient or molar solubility in the anhydrous alcohol solvent for those solutes for which the solute descriptors are known.

Our experimental databases also contain measured solubility data for several crystalline solutes dissolved in both the anhydrous 1-alcohols and in water. The solubility data were taken largely from our previously published solubility studies. At the time that our solubility studies were performed we included solvents for which we planned to update and to derive correlation equations in the future. In the case of crystalline solutes, the partition coefficient between water and the anhydrous organic solvent is calculated as a solubility ratio

$$P = C_S/C_W \quad (6)$$

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 equilibrium vapor pressure of the solute above crystalline solute, $P_{\text{solute}}^{\circ}$, at 298 K is also available. $P_{\text{solute}}^{\circ}$ can be transformed into the gas phase concentration, C_G , and the gas-to-water and gas-to-organic solvent partitions, K_W and K , can be obtained through the following equations

$$K_W = C_W/C_G \quad \text{or} \quad K = C_S/C_G \quad (7)$$

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

As noted in an earlier publication [3], three conditions must be met to calculate partition coefficients from solubility data. The conditions are as follows: (1) the same solid phase must be in equilibrium with the saturated solutions in the solvent and in water (in practice this means that there should be no solvate or hydrate formation); (ii) the secondary medium activity coefficient

of the solid in the saturated solutions must be unity (or near unity); and (iii) for the solutes that are ionized in aqueous solution, C_w , must refer to the solubility of the neutral form. The second condition would restrict the method to those solutes that are sparingly soluble in water and in the organic solvent. Past applications [3, 10, 21, 27, 39] have shown that the Abraham model does accurately describe the solubility of several fairly soluble solutes. For example, Eqns. 2 and 3 described the molar solubility of benzil in 24 organic solvents to within overall standard deviations of 0.124 and 0.109 log units, respectively. [39] Standard deviations for acetylsalicylic acid dissolved in 13 alcohols, 4 ethers and ethyl acetate were 0.123 and 0.138 log units. [10] Flanagan and coworkers [21] further showed that Eqs. 1 and 2 of the Abraham model predicted the experimental solubilities of 1,2,4,5-tetramethylbenzene in 25 different solvents to within an overall standard deviation of 0.15 log units using numerical values of the solute descriptors that had been previously calculated from infinite dilution partition coefficient and chromatographic retention data. Benzil, acetylsalicylic acid and 1,2,4,5-tetramethylbenzene exhibited solubilities exceeding 1 Molar in many of the organic solvents.

Molecular descriptors for all of the compounds considered in the present study are also tabulated in Tables S1 – S8. 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. [2, 4]

3. Results and Discussion

We have assembled in Table S1 (Supporting Information) 148 log P values and 146 log K values for solutes dissolved in methanol covering a reasonably wide range of compound type and descriptor values. Our previously derived methanol correlations were based on 93 log P and 93 log K values, and did not contain the highly acidic (large **A** values) or basic solutes (large **B** values) or many polycyclic aromatic aromatics. The latter class of compounds typically have the larger **E** values. As noted above in using predictive equations it is important to stay within the chemical space defined by the range of solute descriptors covered. Analysis of the experimental data yielded the following correlation equations

$$\begin{aligned} \text{Log P} = & 0.276(0.027) + 0.334(0.041) \text{ E} - 0.714(0.058) \text{ S} + 0.243(0.057) \text{ A} - 3.320(0.066) \text{ B} \\ & + 3.549(0.033) \text{ V} \end{aligned} \quad (8)$$

$$(N = 148, \text{SD} = 0.162, R^2 = 0.992, F = 3412)$$

and

$$\begin{aligned} \text{Log K} = & -0.039(0.020) - 0.338(0.044) \text{ E} + 1.317(0.059) \text{ S} + 3.826(0.057) \text{ A} + 1.396(0.062) \text{ B} \\ & + 0.773(0.008) \text{ L} \end{aligned} \quad (9)$$

$$(N = 146, \text{SD} = 0.149, R^2 = 0.999, F = 25384)$$

All regression analyses were performed using SPSS statistical software. The standard errors in the calculated coefficients are given in parenthesis. 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 correlation coefficients and by the small

standard deviations of $SD = 0.162$ and $SD = 0.149$ log units. 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 13.6 and 36 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

$$\begin{aligned} \text{Log P} = & 0.269(0.043) + 0.402(0.068) \mathbf{E} - 0.761(0.092) \mathbf{S} + 0.243(0.084) \mathbf{A} - 3.253(0.118) \mathbf{B} \\ & + 3.531(0.054) \mathbf{V} \end{aligned} \quad (10)$$

$$(N = 74, SD = 0.169, R^2 = 0.991, F = 1445)$$

and

$$\begin{aligned} \text{Log K} = & -0.032(0.029) - 0.309(0.063) \mathbf{E} + 1.261(0.089) \mathbf{S} + 3.871(0.096) \mathbf{A} + 1.363(0.101) \mathbf{B} \\ & + 0.776(0.013) \mathbf{L} \end{aligned} \quad (11)$$

$$(N = 73, SD = 0.158, R^2 = 0.999, F = 15631)$$

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 versus experimental values, we found $SD = 0.164$ (Eqn. 10) and $SD = 0.142$ (Eqn. 11),

AAE (average absolute error) = 0.125 (Eqn. 10) and AAE = 0.099 (Eqn. 11), and AE (average error) = -0.017 (Eqn. 10) and AE = 0.014 (Eqn. 11). There is therefore very little bias in using Eqns. 10 and 11 with AE equal to -0.017 and 0.014 log units. The training and test set analyses were performed twice more with similar results.

The experimental log P and log K values for ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol and 1-decanol in Tables S2 – S8 (Supporting Information) were analyzed in similar fashion. To conserve journal space we have tabulated the calculated equation coefficients and the associated statistical information in Tables 1 and 2. Listed below the equation coefficients are the respective standard errors. For convenience we have also included in Tables 1 and 2 the equation coefficients for methanol and ethanol reported above. Examination of the statistical information reveals that the Abraham solvation parameter model does provide very accurate mathematical descriptions for the observed gas-to-alcohol and water-to-alcohol partition coefficient data for solutes dissolved in the eight anhydrous alcohol solvents studied here. (See Figures S1 – S14 of the Supporting Information for additional plots of the observed data versus calculated values based on the Abraham model.) Each derived correlation was validated through training set and test set analyses. Full details of the validation results are given in Tables S9 – S11 (Supporting information).

The coefficients in Eqns. 1 and 2 are not just fitting coefficients, but encode important information on the chemical nature of the phases in question. The coefficients in Eqn. 1 refer to the difference in chemical properties of water and the phase, whereas the coefficients in Eqn. 2 refer directly to the chemical properties of the phase and are rather easier to interpret. In Figure 3 are plotted the coefficients in Eqn. 2 against the number of carbon atoms in the alcohol, using the

coefficients in Table 2, together with those for dry 1-octanol [34] and for water [41]. The coefficients for the alcohols fall on quite smooth curves, thus showing that the coefficients are consistent between one alcohol and another. The e-coefficient becomes slightly more positive along the alcohol series. The s-coefficient becomes less positive, indicating that the higher alcohols behave as being less dipolar than the lower alcohols. The a-coefficient relates to the hydrogen bond basicity of the phase, which decreases only slightly along the series. On the other hand, the b-coefficient, corresponding to the hydrogen bond acidity, decreases significantly. The l-coefficient, which may be taken as a measure of the phase hydrophobicity, increases as the alcohol becomes larger, as expected.

It is very interesting to compare the alcohol coefficients with those for solubility in water, because there are very large differences in several of the coefficients. Water is significantly more dipolar than the alcohols (with a large s-coefficient of 2.74), and is a very much stronger hydrogen bond acid (with a b-coefficient no less than 4.81). However, water is only slightly stronger as a hydrogen bond base (the a-coefficient is 3.90). These hydrogen bond properties of bulk water and bulk alcohols relative to each other would be difficult to deduce by other methods. Finally, again as expected, the l-coefficient for water (-0.213) is quite different from those for the alcohols. Indeed, we have found no dry organic solvent with an l-coefficient less than 0.44, for formamide [42].

The present study shows that the correlations derived from the Abraham solvation parameter model provide reasonably accurate mathematical descriptions of solute transfer from both water and from the gas phase into the linear 1-alcohols. The derived correlations presented here do pertain to 298 K. Many manufacturing and separation processes take place at higher

temperatures, and there is a growing need to determine partition properties into organic solvents at other temperatures. In this regard, we have recently published enthalpy of solvation correlations, ΔH_{solv} , for organic gases and gaseous solutes into water [43], methanol [44], ethanol [44] and 1-butanol [44]. The ΔH_{solv} correlations will allow one to extrapolate the predicted log P and log K based on Eqns. 1 and 2 to other temperatures not too far removed from 298 K.

Acknowledgements

Racheal Pointer thanks the National Science Foundation for support received under NSF-REU grant (CHE-0648843). Sai Achi thanks the University of North Texas's Texas Academy of Math and Science (TAMS) program for a summer research award.

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Table 1. Abraham model correlation equation coefficients for the transfer of solutes from water to the anhydrous (dry) alcohol solvents (log P correlation).

Solvent	c	e	s	a	b	v	N	SD	R	F
Methanol	0.276	0.334	-0.714	0.243	-3.320	3.549	148	0.162	0.992	3412
	(0.027)	(0.041)	(0.058)	(0.057)	(0.066)	(0.033)				
Ethanol	0.222	0.471	-1.035	0.326	-3.596	3.857	130	0.158	0.995	4607
	(0.026)	(0.040)	(0.058)	(0.049)	(0.065)	(0.030)				
1-Propanol	0.139	0.405	-1.029	0.247	-3.767	3.986	145	0.151	0.996	6363
	(0.024)	(0.038)	(0.052)	(0.048)	(0.060)	(0.025)				
1-Butanol	0.165	0.401	-1.011	0.056	-3.958	4.044	151	0.159	0.995	5594
	(0.025)	(0.040)	(0.053)	(0.058)	(0.062)	(0.027)				
1-Pentanol	0.150	0.536	-1.229	0.141	-3.864	4.077	120	0.121	0.997	8874
	(0.022)	(0.039)	(0.055)	(0.048)	(0.071)	(0.022)				
1-Hexanol	0.115	0.492	-1.164	0.054	-3.978	4.131	90	0.136	0.997	5308
	(0.032)	(0.049)	(0.069)	(0.054)	(0.094)	(0.027)				
1-Heptanol	0.035	0.398	-1.063	0.002	-4.342	4.317	69	0.109	0.994	2075
	(0.041)	(0.058)	(0.052)	(0.052)	(0.126)	(0.067)				
1-Decanol	-0.058	0.616	-1.319	0.026	-4.153	4.279	85	0.120	0.998	6901
	(0.029)	(0.051)	(0.064)	(0.058)	(0.082)	(0.025)				

Table 2. Abraham model correlation equation coefficients for the transfer of solutes from gas to the anhydrous (dry) alcohol solvents
(log K correlation).

Solvent	c	e	s	a	b	l	N	SD	R	F
Methanol	-0.039	-0.338	1.317	3.826	1.396	0.773	146	0.149	0.999	25384
	(0.020)	(0.044)	(0.059)	(0.057)	(0.062)	(0.008)				
Ethanol	0.017	-0.232	0.867	3.894	1.192	0.846	128	0.142	0.999	31122
	(0.020)	(0.040)	(0.057)	(0.049)	(0.061)	(0.006)				
1-Propanol	-0.042	-0.246	0.749	3.888	1.076	0.874	140	0.136	0.999	33108
	(0.019)	(0.039)	(0.052)	(0.049)	(0.056)	(0.006)				
1-Butanol	-0.004	-0.285	0.768	3.705	0.879	0.890	151	0.149	0.999	27583
	(0.019)	(0.042)	(0.054)	(0.055)	(0.059)	(0.007)				
1-Pentanol	-0.002	-0.161	0.535	3.778	0.960	0.900	112	0.106	0.999	30919
	(0.017)	(0.038)	(0.052)	(0.052)	(0.070)	(0.005)				
1-Hexanol	-0.014	-0.205	0.583	3.621	0.891	0.913	83	0.116	0.999	20739
	(0.024)	(0.047)	(0.062)	(0.056)	(0.089)	(0.006)				
1-Heptanol	-0.056	-0.216	0.554	3.596	0.803	0.933	65	0.082	1.000	28612
	(0.020)	(0.048)	(0.057)	(0.055)	(0.115)	(0.012)				
1-Decanol	-0.139	-0.090	0.356	3.547	0.727	0.958	79	0.097	0.999	22372
	(0.022)	(0.047)	(0.056)	(0.060)	(0.078)	(0.005)

Figure 1. Comparison of the experimental log P data for solutes dissolved in methanol against calculated values based on Eqn. 8.

Figure 2. Comparison of the experimental log K data for solutes dissolved in methanol against calculated values based on Eqn. 9.

Figure 3. Plots of the coefficients in Eqn. 2 against the number of carbon atoms in the alcohol ($N = 0$ denotes water): ● e-coefficient, ■ s-coefficient, Δ a-coefficient, ○ b-coefficient, ▲ l-coefficient.