

ABRAHAM MODEL CORRELATIONS FOR DESCRIBING SOLUTE TRANSFER INTO 2-BUTOXYETHANOL FROM BOTH WATER AND THE GAS PHASE AT 298 K

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Abstract

Infinite dilution activity coefficients (γ_∞) were measured at 298 K for 12 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 11 different aromatic compounds (benzene, alkylbenzenes, halobenzenes, naphthalene), and 2-chloro-2-methylpropane dissolved in 2-butoxyethanol at 298 K using a headspace gas chromatographic method. As part of the experimental study solubilities of 19 crystalline nonelectrolyte solutes (2-hydroxybenzoic acid, acetylsalicylic acid, 3,5-dinitro-2-methylbenzoic acid, acenaphthene, *trans*-stilbene, xanthene, phenothiazine, 3,5-dinitrobenzoic acid, 3-chlorobenzoic acid, 2-methylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-chloro-5-nitrobenzoic acid, benzoic acid, 4-aminobenzoic acid, benzil, thioxanthen-9-one, 3-nitrobenzoic acid, fluoranthene, and diphenyl sulfone) were determined in 2-butoxyethanol at 298 K using a static, spectrophotometric method. The experimental values

were converted to gas-to-2-butoxyethanol, water-to-2-butoxyethanol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. Abraham model correlations for solute transfer into 2-butoxyethanol were derived from the calculated partition coefficients and solubility ratios. The derived Abraham model describes the observed partition coefficient and solubility data to within 0.14 log units (or less).

KEYWORDS: Infinite dilution activity coefficients; Solubilities of crystalline nonelectrolyte solutes; Partition coefficients; Solubility ratios; Solute transfer between immiscible phases

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1. Introduction

Organic solvents and ionic liquids are used extensively in analytical chemistry for two-phase extractions and chemical separations based on both gas-liquid chromatography (glc) and high-performance liquid chromatography (hplc). Solvent selection is determined largely by the solvent's physical and chemical properties, and by the molecular interactions between the solvent and analyte molecule(s) present in the sample being analyzed. Differences in solvent-analyte interactions govern analyte transfer between the various phases present, and play an important role in determining solubilities, chemical selectivities, and recovery factors. For liquid-liquid extractions the organic solvent and/or ionic liquid must be partly miscible with the sample solvent media in order to establish a two-phase partitioning system. Trial-and-error methods were once used to select the most appropriate solvent for a given analytical application. Mathematical approaches based on empirical solution models, linear free energy relationships (LFERs), and quantitative structure-property relationships (QSPRs), however, have facilitated solvent selection in the modern chemical separation methods.

Lesellier [1] recently compared several commonly used approaches for selecting solvents for chemical separations based on the Snyder solvent selectivity triangle, the Kamlet-Taft solvatochromic solvent selectivity method, the Hansen solubility parameter model, the COSMO-RS model, and the Abraham solvation parameter model. For several of the comparisons the author likely utilized solute parameters/properties rather than solvent parameters/properties because the required information was not readily available. This was particularly true in the case of the Abraham model as solvent parameters (called process or solvent equation coefficients) had been determined for about 300 water/organic solvent, air/organic solvent, and totally organic solvents biphasic partitioning systems [2-20]. Abraham model solvent equation coefficients were not

available for solvents such as acetic acid, pyridine, propionitrile, diethyl phthalate, limonene, α -pinene, α -terpineol, glycerol and 1,3-propanediol. Even when solvent parameters were available the author still elected to use solute descriptors. We also note that one of the listed solvents in the author's discussion was paracetamol, which is a drug molecule having a melting point temperature of about 442 K.

Our contributions in the area of solvent selection has been to characterize numerous organic solvents and ionic liquids in terms of their solubilizing abilities using both measured partition coefficient and solubility data. The model that we have been using in our studies has been the Abraham solvation parameter model [2,21-26], which allows one to describe solute transfer between two condensed phases (a biphasic aqueous-organic or organic-organic system) or solute transfer to a condensed phase from the vapor phase. During the past five years we have published Abraham model correlations for 11 additional organic solvents (e.g., diisopropyl ether [27], tributyl phosphate [28], 2-hexadecene [29,30], 1,9-decadiene [29,30], sulfolane [31], benzonitrile [32], ethylbenzene [33], *o*-xylene [34], *m*-xylene [34], *p*-xylene [34], 2-ethoxyethanol [35], and propylene glycol [36]) and several ionic liquids [37-47], as well as updating our existing correlations for hexane [48], heptane [48], octane [48], decane [48], isooctane [49], toluene [33], tetrahydrofuran [50], and 1,4-dioxane [50].

In the present communication we are extending our considerations to include 2-butoxyethanol, which contains both an ether (R-O-R) and hydroxyl (R-OH) functional group. This is the third alkoxyalcohol that we have studied. 2-Methoxyethanol [51] and 2-ethoxyethanol [35] were studied previously. 2-Butoxyethanol is a technical solvent widely used to dissolve cleaning products, enamels, paints and surface coatings. It has weak surfactant properties, moderate polarity and the ability to be a hydrogen bond donor and/or acceptor. Both polar and apolar organic

substances are well-soluble in it. Prediction of the solubility for various substances in this solvent may be interesting from the practical point of view.

Infinite dilution activity coefficients (γ_∞) were measured at 298 K for 12 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 11 different aromatic compounds (benzene, alkylbenzenes, halobenzenes, naphthalene), and 2-chloro-2-methylpropane dissolved in 2-butoxyethanol using a gas chromatographic headspace analysis method, and gas-to-liquid partition coefficients (K) were calculated using these results and saturated vapor pressures of solutes taken from literature. As part of this study solubilities were also measured for 2-hydroxybenzoic acid, acetylsalicylic acid, 3,5-dinitro-2-methylbenzoic acid, acenaphthene, fluoranthene, *trans*-stilbene, xanthene, phenothiazine, 3,5-dinitrobenzoic acid, 3-chlorobenzoic acid, 2-methylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-chloro-5-nitrobenzoic acid, benzoic acid, 4-aminobenzoic acid, benzil, thioxanthen-9-one, 3-nitrobenzoic acid, and diphenyl sulfone dissolved in 2-butoxyethanol at 298.15 K. The measured partition coefficients and solubilities, combined with published gas solubility data for carbon dioxide [52] and hydrogen gas [53], and our previously reported solubility data for anthracene [54], pyrene [55], benzoin [56], 3,4-dichlorobenzoic acid [57], 3,4-dimethoxybenzoic acid [58], 3-methylbenzoic acid [59], salicylamide [59], 4-nitrobenzoic acid [59], 2-methoxybenzoic acid [59], 4-methoxybenzoic acid [59], 4-chlorobenzoic acid [59], biphenyl [59] and 4-hydroxyacetanilide [59] dissolved in 2-butoxyethanol, were used to derive Abraham model correlations for both water-to-2-butoxyethanol partition coefficients (as $\log P$) and gas-to-2-butoxyethanol partition coefficients (as $\log K$).

2. Experimental Methods

2.1 Gas Chromatographic Headspace Measurements

Measurements of activity coefficients at infinite dilution for a set of low polar volatile organic substances were made using headspace analysis technique. In a typical experiment, 5 ml of dilute solution of the studied compound in 2-butoxyethanol is placed into 22 ml glass vial, sealed and thermostated at 298 K. An autosampler takes samples of equilibrium vapor phase from the vials. These samples are transferred through a heated quartz glass line into the injector of a gas chromatograph. The area of a peak S corresponding to a solute is calculated. Such measurements are repeated at 3–4 different concentrations of a solute in the range 0.1–1.5 vol %. After that, 5 ml of pure solute is put into a vial, and the peak area S_{solute} for the sample of its saturated vapor is determined. The whole experiment is repeated 2 times. The ratio of the areas of the peaks corresponding to a solution and a pure solute is equal to the ratio of the solute vapor pressure over this solution p to saturated vapor pressure:

$$p_{solute}^o : S / S_{solute} = p / p_{solute}^o \quad (1)$$

In turn, the activity coefficient of a solute γ is given by:

$$\gamma = p / (p_{solute}^o \cdot x) \quad (2)$$

where x is the equilibrium molar fraction of this solute in the liquid phase. The values of p_{solute}^o were taken from literature [60]. To obtain the value of x taking into account partial evaporation of a solute, we subtracted the quantity of evaporated solute from the initial quantity of a solute in a vial x_0 using a formula:

$$x = x_0 - \frac{p_{solute}^o V_{free} S}{RT S_{solute} V_{solvent}} \quad (3)$$

where $v_{solvent}$ is the number of moles of solvent in a vial and $V_{free} = 17$ ml is a volume of the head space [61]. Since the considered solutes form no dimers or other associates and γ is found to be

virtually independent of x , it is concluded that at such concentrations $\gamma = \gamma_{\infty}$, where γ_{∞} is the limiting activity coefficient. Dimensionless gas-to-liquid partition coefficients K are calculated by the following equation:

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

where $V_{solvent}$ is the molar volume of 2-butoxyethanol. The Gibbs free energy of solvation is given by:

$$\Delta_{solv} G = RT \ln \left(\gamma_{\infty} P_{solute}^o / bar \right) \quad (5)$$

if the standard state is a hypothetical ideal solution at unit mole fraction and a gas at 1 bar fugacity.

2.2 Solubility Measurements

Acenaphthene (Aldrich, 98%), acetylsalicylic acid (Aldrich, 99%), 4-aminobenzoic acid (Aldrich, 99%), benzil (Aldrich, 97%), benzoic acid (Aldrich, 99+%), 3-chlorobenzoic acid (Aldrich, 99%), 4-chloro-3-nitrobenzoic acid (Acros Organics, 99.5%), 2-chloro-5-nitrobenzoic acid (Acros Organics, 99+%), 3,5-dinitrobenzoic acid (Aldrich, 99+%), 3,5-dinitro-2-methylbenzoic acid (Aldrich, 99+%), diphenyl sulfone (Aldrich, 97%), fluoranthene (Aldrich, 98+%), 2-hydroxybenzoic acid (Aldrich, 99+%), 2-methylbenzoic acid (Aldrich, 99 %), 3-nitrobenzoic acid (Aldrich, 99%), phenothiazine (Acros Organics, 99%), *trans*-stilbene (Aldrich, 96 %), thioxanthen-9-one (Aldrich, 98%), and xanthene (Aldrich, 98%) were all purchased from commercial sources. Acenaphthene, benzil, fluoranthene, thioxanthen-9-one, xanthene and *trans*-stilbene were recrystallized several times from anhydrous methanol prior to use. The remaining 13 solutes were used as received. 2-Butoxyethanol (Acros Organics, 99%) was stored

over molecular sieves and distilled shortly before use. Gas chromatographic analysis showed that the purity of 2-butoxyethanol was 99.8 mass percent.

Solubilities were determined using a static, spectrophotometric method. Aliquots of the saturated solutions were transferred into weighed volumetric flasks after the samples had equilibrated in a constant temperature water bath at 298.15 ± 0.05 for at least three days with periodic agitation. The transferred aliquot was weighed and diluted quantitatively with 2-propanol. Absorbances of the diluted solutions were recorded on a Milton Roy Spectronic 1000 Plus spectrophotometer. The concentration of each diluted solution was calculated from a Beer-Lambert law absorbance versus concentration curve generated from the measured absorbances of nine carefully prepared standard solutions of known solute concentration. The analysis wavelengths and concentration ranges used for each solute have been reported in our earlier publications [62-79]. Molar concentrations were converted into mole fraction solubilities using the mass of the sample analyzed, molar mass of 2-butoxyethanol and the respective solutes, volume of the volumetric flasks, and any dilutions needed to get the measured absorbances on the Beer-Lambert law curve. To insure that there was no solvate formation we determined the melting point temperature of the equilibrated solid phases after the solubility measurements were performed. The equilibrated solid phases were removed, dried, and their melting point temperatures determined. For each crystalline solute studied, the melting point temperature of the equilibrated solid phase was within ± 0.5 K of the melting point temperature of the commercial sample or recrystallized solute prior to contact with 2-butoxyethanol.

2.3. Calculation Procedure

The Abraham model equation coefficients for all derived correlations were determined by regression analysis using the IBM SPSS Statistics Package, Version 22. The statistical

information for each derived correlation equation was also provided by the statistical software package.

3. Theoretical background

The Abraham solvation parameter model is a linear free energy relationship that has been shown to provide a very good mathematical description of solute transfer between two condensed phases:

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \quad (6)$$

or solute transfer to a condensed phase from the vapor phase:

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L} \quad (7)$$

where P and K denote the respective partition coefficients. Equations 6 and 7 have also been used to describe the logarithm of molar solubility ratios, $\log (C_{S,\text{organic}}/C_{S,\text{water}})$ and $\log (C_{S,\text{organic}}/C_{S,\text{gas}})$, with the subscripts indicating the phase to which the solute molar concentrations pertain. The numerical values of the equation coefficients (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) are determined by regression analysis by fitting measured partition coefficient data and solubility ratios in accordance with Eqns. 6 and 7, and have been reported in several of our earlier publications for more than 80 different common organic solvents. For approximately one fifth of the organic solvents that have been studied we have also reported Abraham model correlations that describe the transfer of ions and ionic species from water to the organic solvent:

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} + j_p^+ \cdot \mathbf{J}^+ + j_p^- \cdot \mathbf{J}^- \quad (8)$$

by including two additional terms, $j_p^+ \cdot J^+ + j_p^- \cdot J^-$, to describe interactions involving cations and anions, respectively. For nonionic solutes the $j_p^+ \cdot J^+ + j_p^- \cdot J^-$ terms are zero, and the coefficients c_p , e_p , s_p , a_p , b_p and v_p in Eq. 8 are the same as those in Eq. 6 for nonionic solutes in the same partitioning system. Numerical values of the j_p^+ and j_p^- equation coefficients are reported elsewhere [3, 17, 80] for 18 organic solvents, as well as the values of solute descriptors for inorganic ions and ionic species such as alkanoate anions, substituted benzoate anions, phenoxide anions, tetraalkylammonium cations, and pyridinium cations.

The Abraham model contains both solute and solvent parameters that when multiplied together describe a type of molecular interaction. The solute parameters (called solute descriptors) are defined as follows: **E** refers to the solute excess molar refractivity in units of $(\text{cm}^3 \text{ mol}^{-1})/10$, **S** measures the solute dipolarity/polarizability, **A** and **B** quantify the overall or total hydrogen-bond acidity and basicity, **V** is the McGowan volume in units of $(\text{cm}^3 \text{ mol}^{-1})/100$, and **L** is defined as the logarithm of the gas-to-hexadecane partition coefficient at 298 K. Equation coefficients provide the complimentary information regarding the solubilizing media's ability to interact with the dissolved solute. It is the solvent coefficients that Lesellier [1] should have used in his discussion regarding solvent selection, however, the lack of equation coefficients for several of the organic solvents likely led the author to use solute descriptors instead. Solute descriptors are available for more than 5,000 different organic, inorganic and organometallic compounds, while process/solvent equation coefficients are available for approximately 300 partitioning systems.

4. Results and Discussion

The measured infinite dilution activity coefficients, average values of $\log K$ and $\Delta_{sol}G$, are presented in Table 1 for 12 different aliphatic hydrocarbons, 11 different aromatic compounds, and 2-chloro-2-methylpropane, along with the standard uncertainty in the measured infinite

dilution activity coefficient, $u(\gamma_\infty)$. Reported in Table 2 are the mole fraction solubilities of the 19 crystalline nonelectrolyte solutes dissolved in 2-butoxyethanol that were measured as part of the present study. The numerical values tabulated in Table 2 represent the average of between four and eight independent experimental measurements. The reproducibility of the measured values was ± 1.5 % (relative error). To our knowledge, this is the first time that the solubilities of these solutes have been measured in 2-butoxyethanol.

Table 1. Experimental values of limiting activity coefficients, gas-to-liquid partition coefficients, and the Gibbs free energies of solvation in 2-butoxyethanol at $T = 298.15$ K^a

Solute	γ_∞	$u(\gamma_\infty)$	Log K	$\Delta_{solv} G / (\text{kJ} \cdot \text{mol}^{-1})$
n-Hexane	4.41	0.20	2.327	−0.3
n-Heptane	4.55	0.12	2.830	−3.2
n-Octane	5.34	0.15	3.274	−5.7
n-Nonane	6.14	1.00	3.714	−8.2
n-Decane	7.78	0.30	4.105	−10.4
n-Undecane	10.41	1.40	4.518	−12.8
Cyclohexane	2.95	0.13	2.695	−2.4
Methylcyclopentane	2.95	0.12	2.541	−1.5
Methylcyclohexane	3.54	0.09	2.939	−3.8
Cyclooctane	4.24	0.40	3.782	−8.6
Cyclohexene	2.32	0.08	2.836	−3.2
1,7-Octadiene	2.30	0.10	3.437	−6.6
Benzene	1.50	0.05	2.998	−4.1
Toluene	1.81	0.05	3.440	−6.6

Fluorobenzene	1.29	0.05	3.153	−5.0
Chlorobenzene	1.46	0.10	3.907	−9.3
Bromobenzene	1.89	0.20	4.253	−11.3
o-Dichlorobenzene	1.90	0.20	4.739	−14.0
m-Xylene	2.20	0.10	3.890	−9.2
p-Xylene	3.37	0.20	3.677	−8.0
Ethylbenzene	2.17	0.20	3.832	−8.9
p-Cymene	2.24	0.15	4.638	−13.5
Naphthalene	6.49	0.70	5.409	−17.9
<i>tert</i> -Butyl chloride	1.76	0.05	2.418	−0.8

^a Standard uncertainty for temperature $u(T) = 0.2$ K.

Table 2. Experimental mole fraction solubilities, X_S^{exp} , of crystalline nonelectrolyte solutes dissolved in 2-butoxyethanol at 298.15 K

Solute	X_S^{exp}
Xanthene	0.05288
Acenaphthene	0.06484
Fluoranthene	0.04991
<i>trans</i> -Stilbene	0.01862
Thioxanthen-9-one	0.004036
Phenothiazine	0.05625
Diphenyl sulfone	0.03016
3,5-Dinitrobenzoic acid	0.08966
4-Chloro-3-nitrobenzoic acid	0.06793
2-Chloro-5-nitrobenzoic acid	0.1562
2-Methylbenzoic acid	0.1959
3-Chlorobenzoic acid	0.1411
3,5-Dinitro-2-methylbenzoic acid	0.07014
Benzil	0.06671
2-Hydroxybenzoic acid	0.2430
Acetylsalicylic acid	0.09255
3-Nitrobenzoic acid	0.2081

4-Aminobenzoic acid	0.04336
Benzoic acid	0.2582

The organic compounds considered in the present study cover a wide range of chemical diversity and include ten alkanes (hexane, heptane, octane, nonane, decane, undecane, methylcyclopentane, cyclohexane, methylcyclohexane, and cyclooctane), benzene and four alkylbenzenes (toluene, ethylbenzene, m-xylene, p-xylene and 4-isopropyltoluene), six polycyclic aromatic hydrocarbons (naphthalene, anthracene, fluoranthene, biphenyl, acenaphthene, and pyrene) and eighteen benzoic acid derivatives (2-hydroxybenzoic acid, acetylsalicylic acid, 3,5-dinitro-2-methylbenzoic acid, 3,5-dinitrobenzoic acid, 3-chlorobenzoic acid, 4-chlorobenzoic acid, 3,4-dichlorobenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 2-methoxybenzoic acid, 4-methoxybenzoic acid, 3,4-dimethoxybenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-chloro-5-nitrobenzoic acid, benzoic acid, 4-aminobenzoic acid, 3-nitrobenzoic acid, and 4-nitrobenzoic acid). The benzoic acid derivatives possess both electron donating ($-\text{CH}_3$, $-\text{OCH}_3$, $-\text{OH}$) and electron withdrawing ($-\text{Cl}$, $-\text{OC}(=\text{O})\text{CH}_3$, $-\text{NO}_2$) substituents. The chemical diversity of the solutes included in the present should be sufficient to enable development of Abraham model correlations capable of predicting partition coefficients and solubilities of solutes dissolved in 2-butoxyethanol.

The dependent solute properties in Abraham model eqns. 6 and 7 are the logarithm of the water-to-organic solvent partition coefficient ($\log P$), the logarithm of the gas-to-organic solvent partition coefficient ($\log K$), and the two logarithms of the molar solubility ratios ($\log (C_{\text{S,organic}}/C_{\text{S,water}})$ and $\log (C_{\text{S,organic}}/C_{\text{S,gas}})$). The published mole fraction solubility data [57-59]

and mole fraction solubility data in Table 2 are converted to molar solubilities by converted to molar solubilities by dividing $X_{S,organic}^{exp}$ by the ideal molar volume of the saturated solution:

$$C_{S,organic}^{exp} \approx X_{S,organic}^{exp} / [X_{S,organic}^{exp} V_{Solute} + (1 - X_{S,organic}^{exp}) V_{Solvent}] \quad (9)$$

The numerical values used for the molar volumes of the hypothetical subcooled liquid solutes were obtained by summing group values for the functional groups contained in the solute molecules. The molar solubility ratios of $(C_{S,organic}/C_{S,water})$ and $(C_{S,organic}/C_{S,gas})$ are obtained by dividing the solute's molar solubility in 2-butoxyethanol by the solute's molar solubility in water, $C_{S,water}$, and by the solute's gas phase molar concentration, $C_{S,gas}$. Numerical values of $C_{S,water}$ and $C_{S,gas}$ are available in our earlier publications [56-58, 68-75, 79, 81-85] for all of the crystalline solutes considered in the current study. The measured $\log K$ data given in Table 1 are converted $\log P$ values using $\log P = \log K - \log K_w$. The calculation of $\log P$ requires knowledge of the solute's gas phase partition coefficient into water, K_w , which is available for all of the liquid organic compounds considered in the present communication. After performing the indicated conversions, we have 59 experimental $\log (P \text{ or } C_{S,organic}/C_{S,water})$ and 59 experimental $\log (K \text{ or } C_{S,organic}/C_{S,gas})$ values to use in developing Abraham model correlations for describing solute transfer into 2-butoxyethanol. The 59 experimental $\log (K \text{ or } C_{S,organic}/C_{S,gas})$ and $\log (P \text{ or } C_{S,organic}/C_{S,water})$ values are tabulated in the eighth and ninth columns of Table 3, respectively. Also given in Table 3 are the molecular solute descriptors for the 59 solutes that will be used in deriving the Abraham model correlations. The descriptors are of experimental origin and were obtained from measured water-to-organic solvent partitions, gas-to-organic solvent partitions, molar solubility ratios and chromatographic retention factor data as described in several earlier publications [2, 22, 25, 68-75].

Table 3. Experimental log (K or $C_{S,organic}/C_{S,gas}$) and log (P or $C_{S,organic}/C_{S,water}$) Data for Solutes Dissolved in 2-Butoxyethanol at 298.15 K.

Solute	E	S	A	B	L	V	log K^a	log P^a	Ref.
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-1.227	0.493	53
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.191	0.271	52
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.330	4.150	This work
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	2.830	4.790	This work
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.270	5.380	This work
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	3.710	5.860	This work
Decane	0.000	0.000	0.000	0.000	4.686	1.5180	4.100	6.420	This work
Undecane	0.000	0.000	0.000	0.000	5.191	1.6590	4.520	6.900	This work
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	2.690	3.590	This work
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.8454	2.540	3.710	This work
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	2.940	4.150	This work
Cyclooctane	0.413	0.100	0.000	0.000	4.329	1.1272	3.740	4.370	This work
Cyclohexene	0.395	0.200	0.000	0.070	3.021	0.8024	2.840	3.110	This work
1,7-Octadiene	0.191	0.200	0.000	0.100	3.415	1.1498	3.440	4.400	This work
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	2.420	3.220	This work
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.000	2.370	This work
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.440	2.790	This work
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	3.830	3.250	This work
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.9982	3.890	3.280	This work
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	3.680	3.090	This work
4-Isopropyltoluene	0.607	0.490	0.000	0.190	4.590	1.2800	4.640	4.140	This work
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.410	3.680	This work
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.918	4.888	54
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.104	5.604	55
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.590	4.230	This work
Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5850	8.943	5.493	This work
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.341	4.391	59
<i>trans</i> -Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	7.727	4.947	This work
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	3.150	2.560	This work
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	3.910	3.090	This work
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	4.740	3.840	This work
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	4.250	3.180	This work
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.310	4.810	This work
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	10.128	4.725	This work
Benzoic acid	0.730	0.900	0.590	0.400	4.657	0.9317	7.006	1.866	This work
3-Nitrobenzoic acid	0.990	1.180	0.730	0.520	5.601	1.1059	8.818	1.888	This work

4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.1059	9.160	2.260	59
3,5-Dinitrobenzoic acid	1.250	1.630	0.700	0.590	6.984	1.2801	10.550	2.250	This work
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.1313	8.351	1.551	59
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313	8.965	2.265	59
3,4-Dimethoxybenzoic acid	0.950	1.646	0.570	0.755	6.746	1.3309	9.993	1.546	58
4-Aminobenzoic acid	1.075	1.650	0.940	0.600	5.916	1.0315	10.320	0.890	This work
4-Hydroxyacetanilide	1.060	1.630	1.040	0.860	6.430	1.1724	11.603	0.703	59
3-Chlorobenzoic acid	0.840	0.950	0.630	0.320	5.197	1.0541	7.836	2.686	This work
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	4.947	1.0541	7.717	2.917	59
3,5-Dinitro-2-methylbenzoic acid	1.310	2.120	0.750	0.650	8.040	1.4210	12.278	2.322	This work
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726	6.538	2.238	This work
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	4.819	1.0726	7.342	2.362	59
4-Chloro-3-nitrobenzoic acid	1.250	1.470	0.700	0.440	6.685	1.2283	9.922	2.712	This work
2-Chloro-5-nitrobenzoic acid	1.250	1.400	0.670	0.460	6.513	1.2283	9.612	2.662	This work
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	4.732	0.9904	7.556	2.206	This work
Acetylsalicylic acid	0.781	1.690	0.710	0.670	6.279	1.2879	10.023	1.523	This work
3,4-Dichlorobenzoic acid	0.950	0.920	0.670	0.260	5.623	1.1766	8.201	3.461	57
Diphenylsulfone	1.570	2.150	0.000	0.700	8.902	1.6051	10.386	2.996	This work
Benzoin	1.585	2.115	0.196	0.841	9.159	1.6804	11.310	2.579	56
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	8.613	3.743	This work
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.093	4.025	This work
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.0315	9.266	1.581	59
2-Butoxyethanol	0.201	0.530	0.260	0.830	3.656	1.0714	5.215	0.625	Unity

^a For solid solutes the tabulated values represent molar solubility ratios, except for naphthalene.

The experimental log (K or $C_{S,organic}/C_{S,gas}$) values in the eighth column of Table 3 give a set of 59 Abraham model equations containing six process coefficients (c_k , e_k , s_k , a_k , b_k and l_k), and the experimental log (P or $C_{S,organic}/C_{S,water}$) values in the ninth column of Table 4 give a second set of 59 Abraham model equations containing six process coefficients (c_p , e_p , s_p , a_p , b_p , v_p). Each set of 59 equations was solved simultaneously for the optimal set of processes coefficients that best describes the respective experimental log (K or $C_{S,organic}/C_{S,gas}$) and log (P or $C_{S,organic}/C_{S,water}$) data. Regression analysis of the experimental data in Table 3 yielded the following two mathematical expressions:

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = -0.055(0.075) + 0.377(0.069) \mathbf{E} - 0.607(0.104) \mathbf{S} - 0.080(0.087) \mathbf{A} \\ -4.371(0.166) \mathbf{B} + 4.234(0.077) \mathbf{V} \quad (10)$$

(with N = 59, SD = 0.134, R² = 0.992, F = 1278)

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.109(0.043) - 0.304(0.057) \mathbf{E} + 1.126(0.081) \mathbf{S} + 3.407(0.065) \mathbf{A} \\ + 0.660(0.126) \mathbf{B} + 0.914(0.015) \mathbf{L} \quad (11)$$

(with N = 59, SD = 0.103, R² = 0.999, F = 9908)

where the standard error in each calculated equation coefficients is given in parenthesis immediately following the respective coefficient. The statistical information pertaining to each derived correlation is given below the respective equation, and includes the number of experimental data points used in the regression analysis (N), the standard deviation (SD), the squared correlation coefficient (R²) and the Fisher F-statistic (F).

The Abraham model eqns. 10 and 11 provide a reasonably accurate mathematical description of the solubility and partitioning behavior of organic solutes into 2-butoxyethanol as documented by the relatively small standard deviations of 0.134 and 0.103 log units, respectively. Figures 1 and 2 graphically compare the experimental data to the back-calculated values based on eqns. 11 and 10. In the case of the $\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$ comparison the experimental values span a range of approximately 13.51 log units, from $\log K = -1.23$ for hydrogen gas to $\log (C_{S,\text{organic}}/C_{S,\text{gas}}) = 12.28$ for 3,5-dinitro-2-methylbenzoic acid. The $\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$ comparison spans a much smaller range, from $\log P = 0.28$ for carbon dioxide gas to $\log P = 6.90$ for undecane. There is unfortunately insufficient experimental data to perform training set and test set analyses to assess the predictive ability of the derived expressions. Based upon our past experience with Abraham model, and having performed many training set and test analyses on derived Abraham model correlations when there were a sufficient number of experimental data

points [31, 33-35], we expect that eqns. 10 and 11 should be capable of predicting molar solubility ratios and partition coefficients of additional solutes dissolved in 2-butoxyethanol to within 0.14 log units. The standard deviations of the training set correlations and test set calculations performed in the past have always been very similar to the standard deviations of the derived correlations for the full data set.

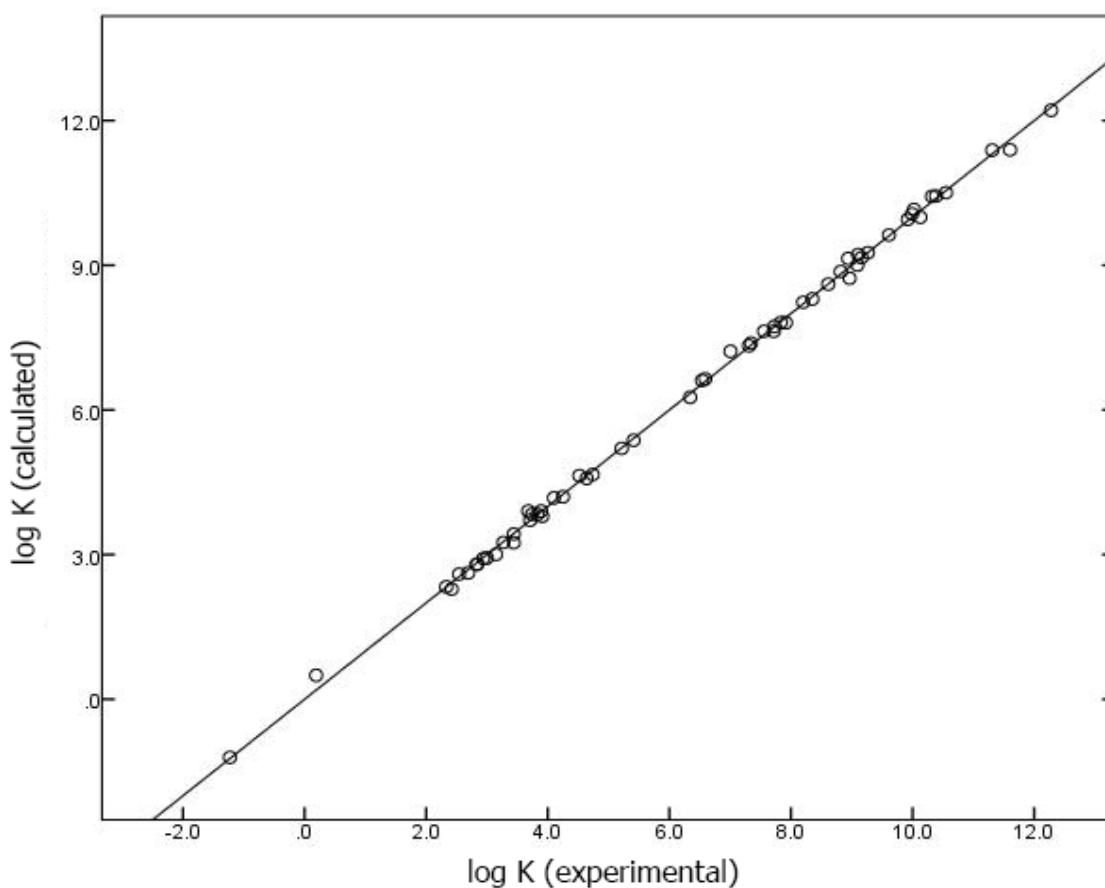


Figure 1. Comparison between experimental log K data and back-calculated values based on eqn. 11.

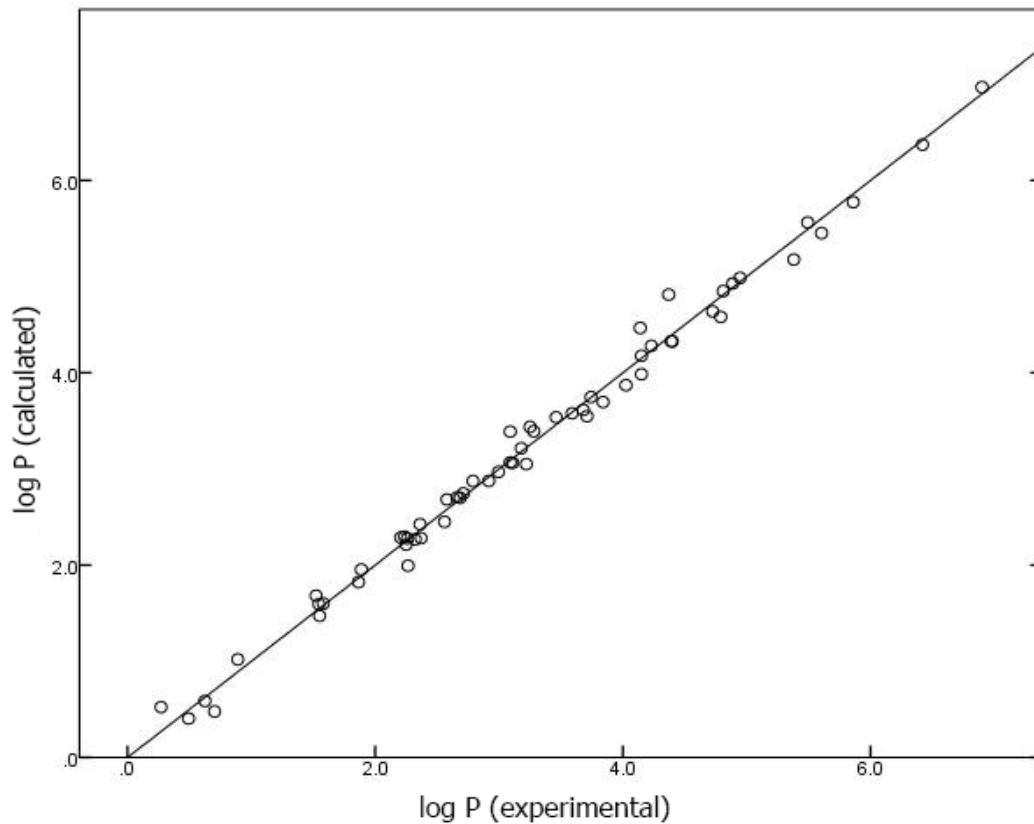


Figure 2. Comparison between experimental $\log P$ data and back-calculated values based on eqn. 10.

As mentioned in the introduction 2-butoxyethanol represents the third alkoxyalcohol solvent that we have studied. A comparison of the obtained experimental gas-to-liquid partition coefficient data with the previously reported values for the same solutes in 2-ethoxyethanol [35] and 2-methoxyethanol [51] shows a good intercorrelation between the three 2-alkoxyalcohol solvents. The intercorrelations can be expressed by the equations:

$$\log K \text{ (2-butoxyethanol)} = 0.927(0.010) \log K \text{ (2-methoxyethanol)} + 0.432(0.065) \quad (12)$$

$$(n = 48, \sigma = 0.223, R^2 = 0.9949)$$

$$\log K \text{ (2-butoxyethanol)} = 0.959(0.005) \log K \text{ (2-ethoxyethanol)} + 0.218(0.037) \quad (13)$$

$$(n = 49, \sigma = 0.121, R^2 = 0.9985)$$

The solutes include both liquid and crystalline nonelectrolyte compounds, both hydrogen-bonding and nonhydrogen-bonding compounds, and both polar and nonpolar organic compounds. High correlation coefficients speak about similar solvation properties of the three solvents and the absence of large experimental errors in the data sets.

Similar solubilizing properties of the three alkoxyalcohol solvents can also be seen in the equation coefficients for the log K correlations, which for 2-methoxyethanol and 2-ethoxyethanol are given by eqns. 14 and 15, respectively.

For 2-methoxyethanol: [51]

$$\begin{aligned} \log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = & -0.141(0.052) - 0.265(0.076) \mathbf{E} + 1.810(0.096) \mathbf{S} + 3.641(0.085) \mathbf{A} \\ & + 0.590(0.141) \mathbf{B} + 0.790(0.018) \mathbf{L} \end{aligned} \quad (14)$$

(with $N = 62$, $SD = 0.139$, $R^2 = 0.998$, $F = 6044$)

For 2-ethoxyethanol: [35]

$$\begin{aligned} \log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = & -0.064(0.032) - 0.257(0.049) \mathbf{E} + 1.452(0.047) \mathbf{S} + 3.672(0.055) \mathbf{A} \\ & + 0.662(0.141) \mathbf{B} + 0.842(0.012) \mathbf{L} \end{aligned} \quad (15)$$

(with $N = 76$, $SD = 0.126$, $R^2 = 0.999$, $F = 17838$)

Careful examination of eqns. 11, 14 and 15 reveals that 5 of the 6 equation coefficients are very similar. To within the standard uncertainty in the calculated equation coefficients the H-bond donor (as reflected in the b_k coefficient) and H-bond acceptor (as reflected in the a_k coefficient) properties are nearly the same. It is only the s_k coefficient in the three correlations that differs significantly between the three correlations. The s_k coefficient decreases with increasing length of the alkoxy-chain, from $s_k = 1.810$ for 2-methoxyethanol to $s_k = 1.452$ for 2-ethoxyethanol to $s_k = 1.126$ for 2-butoxyethanol. This tendency is similar to that observed for the log K correlations for

normal aliphatic alcohols. For these solvents, s_k is also the coefficient changing (decreases) most rapidly with the growing alkyl chain length [86]. While we do not yet have a $\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$ correlation for 2-propoxyethanol, we suspect that one could obtain a reasonable estimate of the solubility and partitioning behavior of solutes dissolved in 2-propoxyethanol simply by using an Abraham model correlation based on

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.087 - 0.281 \mathbf{E} + 1.289 \mathbf{S} + 3.540 \mathbf{A} + 0.661 \mathbf{B} + 0.878 \mathbf{L} \quad (16)$$

the arithmetic average of the $\log K$ equation coefficients for 2-ethoxyethanol and 2-butoxyethanol. Similarly, the average of the $\log P$ equation coefficients for water to 2-ethoxyethanol (35) and water to 2-butoxyethanol leads to an estimate of the equation coefficients for water to 2-propoxyethanol,

$$\text{Log } (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.039 + 0.385 \mathbf{E} - 0.513 \mathbf{S} + 0.022 \mathbf{A} - 4.285 \mathbf{B} + 4.061 \mathbf{V} \quad (17)$$

An arithmetic average of the equation coefficients for ethyl acetate and butyl acetate provided a fairly reasonable estimate of the solubility behavior of 3,4-dichlorobenzoic acid in propyl acetate [57].

4. Conclusion

Mathematical expressions have been derived for predicting the solubility and partitioning behavior of neutral, nonelectrolyte solutions into 2-butoxyethanol based on the Abraham solvation parameter model. The derived mathematical expressions are expected to predict the solute transfer properties to 2-butoxyethanol ($\log P$, $\log K$, $\log (C_{S,\text{organic}}/C_{S,\text{water}})$, and $\log (C_{S,\text{organic}}/C_{S,\text{gas}})$) for additional solutes to within 0.14 log units, provided that the numerical values of the solute descriptors fall within the range of values used in obtaining the predictive expressions. Comparison of the derived $\log K$ correlations for 2-butoxyethanol to correlations derived

previously for 2-methoxyethanol and 2-ethoxyethanol indicates that the solubilizing properties of the three 2-alkoxyethanol solvents are very similar. To within the standard uncertainty in the calculated equation coefficients the H-bond donor (b_k coefficient) and H-bond acceptor (a_k coefficient) properties are nearly the same. It is only the s_k coefficient in the three correlations that differs significantly between the three correlations.

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References

- [1] E. Lesellier, J. Chromatogr. A 1389 (2015) 49-64.
- [2] M.H. Abraham, R.E. Smith, R. Luchtefeld, A.J. Boorem, R. Luo, W.E. Acree, Jr., J. Pharm. Sci. 99 (2010) 1500-1515.
- [3] M.H. Abraham, W.E. Acree, Jr., New J. Chem. 34 (2010) 2298-2305.
- [4] T.C. Ariyasena, C.F. Poole, Chromatographia 76 (2013) 1031-1039.
- [5] T.C. Ariyasena, C.F. Poole, Chromatographia 76 (2013) 157-164.
- [6] T. Karunasekara, C.F. Poole, J. Chromatogr. A 1218 (2011) 4525-4536.
- [7] T. Karunasekara, C.F. Poole, Chromatographia 73 (2011) 941-951.
- [8] T. Karunasekara, C.F. Poole, J. Chromatogr. A 1218 (2011) 809-816.
- [9] T. Karunasekara, C.F. Poole, Talanta 83 (2011) 1118-1125.
- [10] T. Karunasekara, C.F. Poole, J. Sep. Sci. 33 (2010) 1167-1173.
- [11] C.F. Poole, S.N. Atapattu, S.K. Poole, A.K. Bell, Anal. Chim. Acta 652 (2009) 32-53.
- [12] S.N. Atapattu, K. Eggers, C.F. Poole, W. Kiridena, W.W. Koziol, J. Chromatogr. A 1216 (2009) 1640-1649.
- [13] C.F. Poole, S.K. Poole, J. Chromatogr. A 1184 (2008) 254-280.
- [14] J. Qian, C.F. Poole, J. Sep. Sci. 30 (2007) 2326-2331.
- [15] J. Qian, C.F. Poole, J. Chromatogr. A 1143 (2007) 276-283.
- [16] H. Ahmed, C.F. Poole, J. Sep. Sci. 29 (2006) 2158-2165.
- [17] M.H. Abraham, W.E. Acree, Jr., J. Org. Chem. 75 (2010) 1006-1015.
- [18] L.M. Sprunger, W.E. Acree, Jr., M.H. Abraham, QSAR Comb. Sci. 27 (2008) 890-900.
- [19] M.H. Abraham, A. Nasezadeh, W.E. Acree, Jr., Ind. Eng. Chem. Res. 47 (2008) 3990-3995.

- [20] M.H. Abraham, J.R.M. Gola, J. Gil-Lostes, W.E. Acree, Jr., J.E. Cometto-Muniz, J. Chromatogr. A 1293 (2013) 133-141.
- [21] M.H. Abraham, Chem. Soc. Rev. 22 (1993) 73-83.
- [22] M.H. Abraham, A. Ibrahim, A.M. Zissimos, J. Chromatogr. A 1037 (2004) 29-47.
- [23] L.M. Sprunger, J. Gibbs, W.E. Acree, Jr., M.H. Abraham, QSAR Comb. Sci. 28 (2009) 72-88.
- [24] L. Sprunger, W.E. Acree, Jr., M.H. Abraham, J. Chem. Inf. Model. 47 (2007) 1808-1817.
- [25] A.M. Zissimos, M.H. Abraham, M.C. Barker, K.J. Box, K.Y. Tam, J. Chem. Soc., Perkin Trans. 2 (2002) 470-477.
- [26] L.M. Sprunger, J. Gibbs, W.E. Acree, Jr., M.H. Abraham, QSAR & Comb. Sci. 27 (2008) 1130-1139.
- [27] M. Brumfield, W.E. Acree, Jr., M.H. Abraham, Phys. Chem. Liq. 53 (2015) 25-37.
- [28] M. Brumfield, A. Wadawadigi, N. Kuprasertkul, S. Mehta, W.E. Acree, Jr., M.H. Abraham, Phys. Chem. Liq. 53 (2015) 10-24
- [29] M.H. Abraham, W.E. Acree, Jr., New J. Chem. 36 (2012) 1798-1806.
- [30] M.H. Abraham, W.E. Acree, Jr., New J. Chem. 37 (2013) 882-885.
- [31] T.W. Stephens, N.E. De La Rosa, M. Saifullah, S. Ye, V. Chou, A.N. Quay, W.E. Acree, Jr., M.H. Abraham, Fluid Phase Equilibr. 309 (2011) 30-35.
- [32] M.H. Abraham, W.E. Acree, Jr., Thermochim. Acta 526 (2011) 22-28.
- [33] T.W. Stephens, M. Loera, A.N. Quay, V. Chou, C. Shen, A. Wilson, W.E. Acree, Jr., M.H. Abraham, Open Thermodyn. J. 5 (2011) 104-121.
- [34] T.W. Stephens, N.E. De La Rosa, M. Saifullah, S. Ye, V. Chou, A.N. Quay, W.E. Acree, Jr., M.H. Abraham, Fluid Phase Equilibr. 308 (2011) 64-71.

- [35] I.A. Sedov, M.A. Stolov, E. Hart, D. Grover, H. Zettl, V. Koshevarova, W.E. Acree, Jr., M.H. Abraham, *J. Mol. Liq.* 208 (2015) 63-70.
- [36] D.M. Stovall, C. Dai, S. Zhang, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.*, (2015) submitted for publication.
- [37] T.W. Stephens, E. Hart, N. Kuprasertkul, S. Mehta, A. Wadawadigi, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 52 (2014) 777-791.
- [38] P. Twu, J.L. Anderson, T.W. Stephens, H. Lu, K. Satish, D. Shan, W.E. Acree, Jr., M.H. Abraham, *Eur. Chem. Bull.* 2 (2013) 954-964.
- [39] R. Jiang, J.L. Anderson, T.W. Stephens, W.E. Acree, Jr., M.H. Abraham, *Eur. Chem. Bull.* 2 (2013) 741-751.
- [40] P. Twu, J.L. Anderson, T.W. Stephens, A. Wilson, W.E. Acree, Jr., M.H. Abraham, *J. Solut. Chem.* 42 (2013) 772-799.
- [41] T.W. Stephens, W.E. Acree, Jr., P. Twu, J.L. Anderson, G.A. Baker, M.H. Abraham, *J. Solut. Chem.* 41 (2012) 1165-1184.
- [42] L.M. Grubbs, S. Ye, M. Saifullah, W.E. Acree, Jr., P. Twu, J.L. Anderson, G.A. Baker, M.H. Abraham, *J. Solut. Chem.* 40 (2011) 2000-2022
- [43] L.M. Sprunger, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 48 (2010) 385-393.
- [44] F. Mutelet, E.-S.R.E Hassan, T.W. Stephens, W.E. Acree, Jr., G.A. Baker, *Chem. Eng. Data* 58 (2013) 2210-2218.
- [45] W.E. Acree, Jr., G.A. Baker, A.-L. Revelli, J.-C. Moise, F. Mutelet, *J. Chem. Eng. Data* 57 (2012) 3510-3518.
- [46] W.E. Acree, Jr., G.A. Baker, F. Mutelet, J.-C. Moise, *J. Chem. Eng. Data* 56 (2011) 3688-3697.

- [47] F. Mutelet, A.-L. Revelli, J.-N. Jaubert, L.M. Sprunger, W.E. Acree, Jr., G.A. Baker, J. Chem. Eng. Data 55 (2010) 234-242.
- [48] T.W. Stephens, A.N. Quay, V. Chou, M. Loera, C. Shen, A. Wilson, W.E. Acree, Jr., M.H. Abraham, Glob. J. Phys. Chem. 3 (2012) 1/1-1/42.
- [49] T.W. Stephens, A. Wilson, N. Dabadge, A. Tian, H.H. Hensley, M. Zimmerman, W.E. Acree, Jr., M.H. Abraham, Glob. J. Phys. Chem. 3 (2012) 9/1-9/16.
- [50] M. Saifullah, S. Ye, L.M. Grubbs, N.E. La Rosa, W.E. Acree, Jr., M.H. Abraham, J. Solut. Chem. 40 (2011) 2082-2094.
- [51] E. Hart, D. Grover, H. Zettl, V. Koshevarova, S. Zhang, C. Dai, W.E. Acree, Jr., I.A. Sedov, M.A. Stolov, M.H. Abraham, J. Mol. Liq., (2015) accepted for publication.
- [52] A. Henni, P. Tontiwachwuthikul, A. Chakma, Can. J. Chem. Eng. 83 (2005) 358-361.
- [53] E. Brunner, Ber. Bunsen-Gesell. 83 (1979) 715-721.
- [54] M.E.R. McHale, A.-S.M. Kauppila, J.R. Powell, W.E. Acree, Jr., J. Chem. Thermodyn. 28 (1996) 209-214.
- [55] M.E.R. McHale, K.S. Coym, K.A. Fletcher, W.E. Acree, Jr., J. Chem. Eng. Data 42 (1997) 511-513.
- [56] T.W. Stephens, M. Loera, M. Calderas, R. Diaz, N. Montney, W.E. Acree, Jr., M.H. Abraham, Phys. Chem. Liq. 50 (2012) 254-265.
- [57] A. Wilson, A. Tian, V. Chou, A.N. Quay, W.E. Acree, Jr., M.H. Abraham, Phys. Chem. Liq. 50 (2012) 324-335.
- [58] K.R. Bowen, T.W. Stephens, H. Lu, K. Satish, D. Shan, W.E. Acree, Jr., M.H. Abraham, Eur. Chem. Bull. 2 (2013) 577-583.

- [59] L.M. Grubbs, M. Saifullah, N.E. De La Rosa, S. Ye, S.S. Achi, W.E. Acree, Jr., M.H. Abraham, *Fluid Phase Equilib.* 298 (2010) 48-53.
- [60] US EPA. 2011. Estimation Programs Interface Suite™ for Microsoft® Windows. United States Environmental Protection Agency, Washington, DC, USA.
- [61] I.A. Sedov, M.A. Stolov, B.N. Solomonov, *Fluid Phase Equilib.* 354 (2013) 95-101.
- [62] K.A. Fletcher, M.E.R. McHale, K.S. Coym, W.E. Acree, Jr., *Can. J. Chem.* 75 (1997) 258-261.
- [63] K.M. De Fina, T.L. Sharp, W.E. Acree, Jr., *Can. J. Chem.* 77 (1999) 1537-1541.
- [64] K.M. De Fina, T.L. Sharp, W.E. Acree, Jr., *Can. J. Chem.* 77 (1999) 1589-1593.
- [65] C. Monarrez, D.M. Stovall, J.H. Woo, P. Taylor, W.E. Acree, Jr., *Phys. Chem. Liq.* 40 (2002) 703-714.
- [66] D.M. Stovall, W.E. Acree, Jr., M.H. Abraham, *Fluid Phase Equilib.* 232 (2005) 113-121.
- [67] K.M. De Fina, T.L. Sharp, L.E. Roy, W.E. Acree, Jr., *J. Chem. Eng. Data* 44 (1999) 1262-1264.
- [68] S. Ye, M. Saifullah, L.M. Grubbs, M.C. McMillan-Wiggins, P. Acosta, D. Mejorado, I. Flores, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 49 (2011) 821-829.
- [69] D.M. Stovall, C. Givens, S. Keown, K.R. Hoover, R. Barnes, C. Harris, J. Lozano, M. Nguyen, E. Rodriguez, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 43 (2005) 351-360.
- [70] C.R. Daniels, A.K. Charlton, R.M. Wold, R.J. Moreno, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 42 (2004) 633-641.
- [71] K.R. Hoover, R. Coaxum, E. Pustejovsky, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 42 (2004) 457-466.

- [72] A.K. Charlton, C.R. Daniels, R.M. Wold, E. Pustejovsky, W.E. Acree, Jr., M.H. Abraham, *J. Mol. Liq.* 116 (2004) 19-28.
- [73] R. Coaxum, K.R. Hoover, E. Pustejovsky, D.M. Stovall, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 42 (2004) 313-322.
- [74] A.K. Charlton, C.R. Daniels, W.E. Acree, Jr., M.H. Abraham, *J Solut. Chem.* 32 (2003) 1087-1102.
- [75] W.E. Acree, Jr., M.H. Abraham, *J Solut. Chem.* 31 (2002) 293-303.
- [76] K.A. Fletcher, C.E. Hernandez, L.E. Roy, K.S. Coym, W.E. Acree, Jr., *Can. J. Chem.* 77 (1999) 1214-1217.
- [77] C.E. Hernandez, W.E. Acree, Jr., *Can. J. Chem.* 76 (1998) 1312-1316.
- [78] K.A. Fletcher, K.S. Coym, L.E. Roy, C.E. Hernandez, M.E.R. McHale, W.E. Acree, Jr., *Phys. Chem. Liq.* 35 (1998) 243-252.
- [79] K.R. Hoover, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 44 (2006) 367-376.
- [80] M.H. Abraham, W.E. Acree, Jr., *J. Org. Chem.* 75 (2010) 3021-3026.
- [81] B.H. Blake-Taylor, V.H. Deleon, W.E. Acree, Jr., M.H. Abraham. *Phys. Chem. Liq.* 45 (2007) 389-398.
- [82] K.R. Hoover, D.M. Stovall, E. Pustejovsky, R. Coaxum, K. Pop, W.E. Acree, Jr., M.H. Abraham, *Can. J. Chem.* 82 (2004) 1353-1360.
- [83] K.R. Hoover, R. Coaxum, E. Pustejovsky, D.M. Stovall, W.E. Acree, Jr., M.H. Abraham, *Phys. Chem. Liq.* 42 (2004) 339-347.
- [84] W.E. Acree, Jr., M.H. Abraham, *Fluid Phase Equilib.* 201 (2002) 245-258.
- [85] M.H. Abraham, A.M. Zissimos, W.E. Acree, Jr., *Phys. Chem. Chem. Phys.* 3 (2001) 3732-3736.

- [85] L. M. Sprunger, S. S. Achi, R. Pointer, B. H. Blake-Taylor, W. E. Acree, Jr., M. H. Abraham, *Fluid Phase Equilibr.* 286 (2009) 170-174.

HIGHLIGHTS FOR
ABRAHAM MODEL CORRELATIONS FOR DESCRIBING SOLUTE TRANSFER INTO 2-
BUTOXYETHANOL FROM BOTH WATER AND THE GAS PHASE AT 298 K

- Activity coefficients measured for 24 organic solutes in 2-butoxyethanol
- Solubilities measured for 19 crystalline organic solutes in 2-butoxyethanol
- Expressions derived for predicting molar solubilities in 2-butoxyethanol
- Expressions derived for predicting gas-to-liquid partition coefficients of solutes in 2-butoxyethanol

The diagram illustrates the Abraham Model Correlations, showing the relationship between properties in the gas phase and water phase for a solute. It is structured as follows:

- Top Level (Gas Phase):** Labeled "SOLUTE IN GAS PHASE" in green. It contains five red text elements: "BtoxyEtOH", "BtoxyEtOH", "Solute", "BtoxyEtOH", and "BtoxyEtOH".
- Middle Level (Water Phase):** Labeled "Solute" in black. It contains five red text elements: "BtoxyEtOH", "BtoxyEtOH", "Solute", "BtoxyEtOH", and "BtoxyEtOH".
- Bottom Level (Water Phase):** Labeled "Water" in orange. It contains five orange text elements: "Water", "Water", "Solute", "Water", and "Water".

Arrows indicate the relationships between these levels:

- A blue arrow labeled "Log K" points from the "Solute" in the Gas Phase to the "Solute" in the Water Phase.
- A blue arrow labeled "Log P" points from the "Solute" in the Water Phase to the "Solute" in the Water Phase.