DEVELOPMENT OF ABRAHAM MODEL CORRELATIONS FOR SOLUTE TRANSFER
INTO BOTH 2-PROPOXYETHANOL AND 2-ISOPROPOXYETHANOL AT 298.15 K

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Abstract

Infinite dilution activity coefficients (γ_∞) were measured at 298 K for 9 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 7 different aromatic compounds (benzene, alkylbenzenes, halobenzenes), and for 1,2-dichloropropane, dichloromethane, acetone, acetonitrile, tetrahydrofuran, 1,4-dioxane and 2-propanol dissolved in both 2-propoxyethanol and 2-isopropoxyethanol at 298 K using a headspace gas chromatographic method. As part of the experimental study solubilities of 18 and 20 crystalline organic nonelectrolyte solutes were determined in 2-propoxyethanol and 2-isopropoxyethanol, respectively, at 298 K using a uv/visible spectrophotometric method. The experimental values were converted to gas-to-alkoxyethanol, water-to-alkoxyethanol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. Abraham model correlations for solute transfer into both alkoxyethanols were derived from the calculated solubility ratios and partition coefficients. The

derived Abraham model describes the observed solubility ratios and partition coefficients to within 0.12 log units (or less).

Keywords and Phrases: Activity coefficients; partition coefficients; solubilities; headspace chromatographic measurements; 2-propoxyethanol; 2-isopropoxyethanol

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1. Introduction

Organic solvents represent a significant quantity of the chemicals used in industrial manufacturing processes. Increased chemical and disposal costs, coupled with environmental concerns and governmental regulations controlling the release of hazardous materials into the environment, have prompted the manufacturing sector to find ways reduce organic solvent consumption. Implementation of solvent-free processes provide one solution to the problem; however, from a practical standpoint it is not feasible to completely eliminate organic solvents from all synthetic methods and chemical separations. Organic solvents provide a critical role in dissolving organic starting materials, in facilitating heat and mass transfer, and serve as mobile phases for chemical separations involving high-performance liquid chromatography. A more viable and more practical solution to the problem is to replace expensive solvents derived from petroleum with solvents made from renewable resources, and to replace hazardous solvents with ones that exhibit better environmental, health and safety properties.

Solvent selection includes economical, toxicological and chemical considerations. Our contributions in the area of solvent selection has focused on chemical considerations and specifically on the solubilizing properties of potential solvent candidates. For organic synthesis the solvent must be able to dissolve the starting material(s) and provide for the convenient isolation of the synthesized product from the reaction solvent media. This can either be accomplished by selecting a solvent in which the product is not soluble or by evaporation of the solvent once the reaction is complete. In the case of purification by extraction one needs to find a two-phase partitioning system (usually water and an organic solvent) where the compounds to be separated have vastly different relative solubilities in the respective immiscible liquid phases. Purification by recrystallization is also based on solubility differences of the compound in the hot

versus cold solvent, or in the dissolving solvent versus precipitating anti-solvent. The solubility of a dissolved solute in different solvents is controlled by molecular interactions between the solute and surrounding solvent molecules, as well as by solvent-solvent and solute-solute interactions.

In past several years we have reported mathematical correlations for describing measured partition coefficient and solubility data for solutes dissolved in both traditional organic solvents and in ionic liquid solvents based on the Abraham solvation parameter model [1-7]. Solute partitioning can be between two condensed phases (a biphasic aqueous-organic or organic-organic system):

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \quad (1)$$

or involve partitioning between a condensed phase and the gas phase:

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L} \quad (2)$$

where P and K denote the respective partition coefficients. Equations 1 and 2 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 “organic”, “water” and “gas” indicating the phase to which the solute molar concentrations pertain. The independent variables in Eqns. (1) and (2), or descriptors, are solute properties as follows: $\mathbf{E}$ and $\mathbf{S}$ correspond to the excess molar refraction and dipolarity/polarizability descriptors of the solute, respectively, $\mathbf{A}$ and $\mathbf{B}$ are measures of the solute hydrogen-bond acidity and basicity, $\mathbf{V}$ refers to the McGowan volume of the solute and $\mathbf{L}$ is the logarithm of the solute gas phase dimensionless gas to hexadecane partition coefficient at 298 K. The complementary solvent (or process) properties are indicated by the lower case letters in Eqns. (1) and (2). The numerical values of the solvent 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 of partition coefficients and solubility ratios for a series of solutes dissolved in the given solvent or two-phase partitioning system.

Specific solvents studied in the past five years include diisopropyl ether [8], 2-hexadecene [9,10], 1,9-decadiene [9,10], benzonitrile [2], 2-methoxyethanol [11], 2-ethoxyethanol [12], 2-butoxyethanol [13], 1,2-propylene glycol [14], acetophenone [15], aniline [15] and acetic acid [16]. All of the solvents listed above contain a single type of functional group attached to either an alkyl chain or aromatic benzene ring, except for the three 2-alkoxyalcohols. We are particularly interested in developing Abraham model correlations for organic solvents possessing multiple functional groups as our goal is to one day be able to predict the five equation coefficients in Eqns. (1) and (2) from only structural considerations. This will require an extensive database of equation coefficients for a chemically diverse set of solvents possessing different types of functional groups and hydrogen-bonding capabilities. In the present study we extend our earlier considerations to include two additional 2-alkoxyethanol solvents, namely 2-propoxyethanol and 2-isopropoxyethanol. Alkoxyalcohols contain both an ether functional group (-O-) and a hydroxyl functional group (-OH). This will allow us to search for possible synergistic effects between adjacent ether and hydroxyl groups once we begin our search for methods to predict the solvent/process coefficients.

Infinite dilution activity coefficients (γ_∞) were measured at 298 K for a series of organic solutes containing up to 9 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), up to 9 different aromatic compounds (benzene, alkylbenzenes, halobenzenes), two cyclic ethers (tetrahydrofuran, 1,4-dioxane), chloroalkanes (dichloromethane, 1,2-dichloropropane), acetone, acetonitrile, 2-propanol, and butyl acetate (in 2-isopropoxyethanol only) dissolved in both 2-propoxyethanol and 2-isopropoxyethanol using a gas chromatographic headspace analysis

method. Gas-to-liquid partition coefficients (K) were calculated using these results and saturated vapor pressures of solutes taken from the published literature. As part of this study solubilities were measured at 298 K for acetylsalicylic acid, acenaphthene, benzil, benzoic acid, 1-chloroanthraquinone, 4-chloro-3-nitrobenzoic acid, 3,5-dinitrobenzoic acid, 3,5-dinitro-2-methylbenzoic acid, diphenyl sulfone, fluorene, 2-hydroxybenzoic acid, 3-hydroxybenzoic acid, 2-methylbenzoic acid, phenothiazine, *trans*-stilbene, thioxanthen-9-one, and xanthene dissolved in the two 2-alkoxyethanol solvents as well. Solubilities were also determined for 3-chlorobenzoic acid, 2-ethylanthraquinone and pyrene dissolved in 2-isopropoxyethanol and for 3,4-dimethoxybenzoic acid dissolved in 2-propoxyethanol. The measured gas-to-liquid partition coefficient and solubility data, combined with published solubility data for anthracene [17,18], benzoin [19], pyrene [20], 4-nitrobenzoic acid [21], 2-methoxybenzoic acid [21], 4-methoxybenzoic acid [21], 4-hydroxyacetanilide [21], 4-chlorobenzoic acid [21], 3-methylbenzoic acid [21], 3,4-dimethoxybenzoic acid [22], 3,4-dichlorobenzoic acid [23], biphenyl [21], and salicylamide [21], were used to derive Abraham model $\log(P$ or $C_{S,organic}/C_{S,water})$ and $\log(K$ or $C_{S,organic}/C_{S,gas})$ correlations for describing solute transfer into 2-propoxyethanol and 2-isopropoxyethanol both from water and from the gas phase.

2. Experimental Methodology

2.1 Gas Chromatographic Headspace Measurements

2-Propoxyethanol (Acros Organics, 98%), 2-isopropoxyethanol (Aldrich, 99%), n-hexane (Sigma-Aldrich, 99%), n-heptane (Acros Organics, 99%), n-octane (Sigma-Aldrich, 99%), n-nonane (Acros Organics, 99%), cyclohexane (Acros Organics, 99.5%), methylcyclohexane (Aldrich, 99%), 1,7-octadiene (Acros Organics, 99%), 1-heptyne (Acros Organics, 99%), 1-octyne (Alfa Aesar, 98%), benzene (Sigma-Aldrich, 99%), fluorobenzene (Acros Organics,

99%), chlorobenzene (Acros Organics, 99.6%), bromobenzene (Acros Organics, 99%), toluene (Sigma-Aldrich, 99.8%), ethylbenzene (Fluka, 99%), *o*-xylene (Sigma-Aldrich, 99%), *m*-xylene (Sigma-Aldrich, 99%), *p*-xylene (Sigma-Aldrich, 99%), dichloromethane (Kupavnareaktiv, 99.9%), 1,2-dichloropropane (Fluka, 98.5%), acetone (Ecos-1, 99.8%), acetonitrile (J.T.Baker, 99.9%), butyl acetate (Ecos-1, 99.5%), 1,4-dioxane (Komponent-Reaktiv, 99.5%), 2-propanol (Ecos-1, 99.8%), tetrahydrofuran (Ecos-1, 99.5%) were purchased. Most of the compounds were used in the experiments without further purification except tetrahydrofuran and 1,4-dioxane which were distilled over sodium, and 2-propanol which was dried with calcium hydride and distilled. Gas chromatograms of all the substances show no peaks with the area exceeding 0.5% of that of the peak corresponding to the main substance.

In a typical experiment, for each solute-solvent pair we prepared 6 solutions containing different concentrations of a solute in the range 0.1–0.8 volume percents. At such concentrations, solutions are thought to behave as infinitely diluted ones, which was confirmed by the absence of dependence of the results from concentration. The activity coefficient of a solute at infinite dilution γ_∞ is given by $\gamma_\infty = p / (p_{solute}^o \cdot x)$, where x is the equilibrium molar fraction of a solute in the liquid phase, p is the saturated vapor pressure of a solute over the solution, and p_{solute}^o is the saturated vapor pressure of the same solute over its pure liquid phase. The ratio p / p_{solute}^o was determined by means of gas chromatographic headspace technique using PerkinElmer Clarus 580 chromatograph with a headspace autosampler.

The samples (5 ml) of solutions and pure solutes are placed into sealed 22 ml vials and thermostated at 298.15 K. Portions of equilibrium vapor phase are taken from these vials by autosampler and transferred into the chromatographic column, and the areas of chromatographic

peaks that are proportional to the vapor pressure of each compound inside the vial are calculated. We also take into account that the actual value of x due to partial evaporation of a solute into the headspace can be different from the initial molar fraction of a solute by introducing a correction.

Gas-to-liquid partition coefficients K can be calculated using a formula

$$\log K = \log \left(\frac{RT}{\gamma_{\infty} P_{solute}^o V_{solvent}} \right), \text{ where } V_{solvent} \text{ is the molar volume of a solvent. The values of}$$

P_{solute}^o were taken from literature [24]. The Gibbs energy of solvation with the standard states defined as a hypothetical ideal solution at unit mole fraction and a gas at 1 bar fugacity is given by $\Delta_{solv} G = RT \ln(\gamma_{\infty} P_{solute}^o)$. Results are presented in Tables 1 and 2.

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

Solute	γ_{∞}	$u(\gamma_{\infty})$	Log K	$\Delta_{solv} G / (\text{kJ} \cdot \text{mol}^{-1})$
n-Hexane	5.11	0.14	2.323	0.1
n-Heptane	6.12	0.22	2.761	-2.4
n-Nonane	8.63	0.25	3.626	-7.4
Cyclohexane	3.85	0.10	2.639	-1.7
Methylcyclohexane	4.55	0.10	2.890	-3.2
1,7-Octadiene	3.48	0.11	3.316	-5.6
1-Heptyne	2.25	0.06	3.138	-4.6
Benzene	1.62	0.04	3.024	-3.9
Fluorobenzene	1.41	0.04	3.173	-4.8
Chlorobenzene	1.61	0.07	3.924	-9.1
Bromobenzene	1.79	0.05	4.336	-11.4

Toluene	2.03	0.10	3.449	−6.4
Ethylbenzene	2.56	0.08	3.820	−8.5
<i>o</i> -Xylene	2.52	0.09	3.989	−9.4
<i>m</i> -Xylene	2.71	0.10	3.859	−8.7
<i>p</i> -Xylene	2.58	0.07	3.852	−8.7
Dichloromethane	0.70	0.02	2.727	−2.2
1,2-Dichloropropane	1.46	0.06	3.319	−5.6
Acetone	1.53	0.02	2.660	−1.9
Acetonitrile	2.18	0.03	2.923	−3.4
1,4-Dioxane	1.52	0.04	3.447	−6.3
2-Propanol	1.47	0.03	3.386	−6.0
Tetrahydrofuran	1.03	0.03	2.988	−3.7

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

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

Solute	γ_{∞}	$u(\gamma_{\infty})$	Log K	$\Delta_{solv} G / (\text{kJ} \cdot \text{mol}^{-1})$
n-Hexane	5.08	0.11	2.322	0.1
n-Heptane	6.00	0.32	2.766	−2.5
n-Octane	6.77	0.20	3.227	−5.1
n-Nonane	8.72	0.17	3.618	−7.3
Cyclohexane	3.95	0.09	2.624	−1.7
1-Heptyne	2.23	0.07	3.139	−4.6
1-Octyne	2.99	0.08	3.598	−7.2
Benzene	1.60	0.05	3.026	−4.0

Fluorobenzene	1.33	0.05	3.196	−4.9
Chlorobenzene	1.62	0.05	3.919	−9.0
Bromobenzene	1.76	0.10	4.341	−11.5
Ethylbenzene	2.68	0.13	3.797	−8.4
<i>o</i> -Xylene	2.67	0.06	3.960	−9.3
<i>m</i> -Xylene	2.46	0.08	3.898	−8.9
<i>p</i> -Xylene	2.60	0.08	3.846	−8.6
Dichloromethane	0.63	0.02	2.769	−2.5
1,2-Dichloropropane	1.52	0.07	3.299	−5.5
Acetone	1.48	0.03	2.672	−1.9
Acetonitrile	2.04	0.05	2.949	−3.5
Butyl acetate	2.70	0.12	3.715	−7.9
1,4-Dioxane	1.26	0.04	3.526	−6.8
2-Propanol	1.19	0.04	3.475	−6.5
Tetrahydrofuran	1.01	0.04	2.993	−3.8

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

2.2 Solubility Measurements

Acenaphthene (Aldrich, 98 %), acetylsalicylic acid (Aldrich, 99 %), benzil (Aldrich, 97 %), benzoic acid (Aldrich, 99+ %), 1-chloroanthraquinone (Aldrich, 99 %), 3-chlorobenzoic acid (Aldrich, 99 %), 4-chloro-3-nitrobenzoic acid (Acros Organics, 99.5 %), 3,4-dimethoxybenzoic acid (Acros Organics, 99+ %), 3,5-dinitrobenzoic acid (Aldrich, 99+ %), 3,5-dinitro-2-methylbenzoic acid (Aldrich, 99+ %), diphenyl sulfone (Aldrich, 97 %), 2-ethylanthraquinone (Aldrich, 99+ %), fluorene (Aldrich, 98 %), 2-hydroxybenzoic acid (Aldrich, 99+ %), 3-hydroxybenzoic acid (Acros Organics, 99 %), 2-methylbenzoic acid (Aldrich, 99 %),

phenothiazine (Acros Organics, 99 %), pyrene (Aldrich, 98 %), *trans*-stilbene (Aldrich, 96 %), thioxanthen-9-one (Aldrich, 98 %), and xanthene (Aldrich, 98 %) were all purchased from commercial sources. Acenaphthene, benzil, 1-chloroanthraquinone, 2-ethylanthraquinone, fluorene, pyrene, *trans*-stilbene, thioxanthen-9-one, and xanthene were recrystallized several times from anhydrous methanol before use. The remaining 12 solutes were used as received. 2-Propoxyethanol (Sigma-Aldrich, 99.4 %) and 2-isopropoxyethanol (Aldrich, 99 %) were stored over molecular sieves and distilled shortly before use. Gas chromatographic analysis showed that the purity of both 2-propoxyethanol and 2-isopropoxyethanol 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 [20, 22, 25-41]. Molar concentrations were converted into mole fraction solubilities using the mass of the sample analyzed, molar masses of the solvent and the respective solutes, volume of the volumetric flasks, and any dilutions that may have been needed in order to put 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 recovered from the saturated solutions after the solubility measurements were performed. For

each crystalline solute -solvent combination 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-propoxyethanol and 2-isopropoxyethanol.

The experimental mole fraction solubilities of the crystalline organic solutes dissolved in 2-propoxyethanol and 2-isopropoxyethanol are reported in Tables 3 and 4, respectively. The numerical values represent the average of 4 to 8 independent experimental measurements. The reproducibilities of the replicate measurements were ± 1.5 % (relative error).

Table 3. Experimental mole fraction solubilities, X_S^{exp} , of crystalline nonelectrolyte solutes dissolved in 2-propoxyethanol at 298.15 K^a

Solute	X_S^{exp}
Xanthene	0.05649
Acenaphthene	0.06082
Fluorene	0.05161
<i>trans</i> -Stilbene	0.02164
Thioxanthen-9-one	0.003447
Phenothiazine	0.07241
Diphenyl sulfone	0.02622
1-Chloroanthraquinone	0.003717
3,5-Dinitrobenzoic acid	0.1058
4-Chloro-3-nitrobenzoic acid	0.07763
2-Methylbenzoic acid	0.1975
3,5-Dinitro-2-methylbenzoic acid	0.08413
3,4-Dimethoxybenzoic acid	0.02158
Benzil	0.06887
2-Hydroxybenzoic acid	0.2734
3-Hydroxybenzoic acid	0.1621
Acetylsalicylic acid	0.1127
Benzoic acid	0.2673

^a Standard uncertainty for temperature $u(T) = 0.05$ K.

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

Solute	X_S^{exp}
Xanthene	0.05285
Acenaphthene	0.05996
Pyrene	0.02919
Fluorene	0.04574
<i>trans</i> -Stilbene	0.01884
Thioxanthen-9-one	0.002827
Phenothiazine	0.07122
Diphenyl sulfone	0.02538
1-Chloroanthraquinone	0.003156
2-Ethylanthraquinone	0.01829
3,5-Dinitrobenzoic acid	0.1226
4-Chloro-3-nitrobenzoic acid	0.09291
2-Methylbenzoic acid	0.1798
3-Chlorobenzoic acid	0.1795
3,5-Dinitro-2-methylbenzoic acid	0.0997
Benzil	0.06612
2-Hydroxybenzoic acid	0.2864
3-Hydroxybenzoic acid	0.1600
Acetylsalicylic acid	0.1182
Benzoic acid	0.2765

^a Standard uncertainty for temperature $u(T) = 0.05$ K.

3. Development of Abraham Model Correlations

The dependent variables in Eqns. (1) and (2) are the logarithms of the water-to-liquid partition coefficients, $\log P$, the logarithms of the gas-to-liquid partition coefficients, $\log K$, and the logarithms of the two molar solubility ratios, $\log (C_{S,\text{organic}}/C_{S,\text{water}})$ and $\log (C_{S,\text{organic}}/C_{S,\text{gas}})$. The $\log K$ values for the organic liquid solutes were determined from the gas chromatographic headspace measurements and are given in Tables 1 and 2, along with the respective infinite

dilution activity coefficients and Gibbs energies of solvation. Water-to-liquid and gas-to-liquid partition coefficients are inter-related through the following thermodynamic relationship:

$$\log P = \log K - \log K_w \quad (3)$$

The gas-to-water partition coefficients, $\log K_w$, required for the calculation of $\log P$ are available for all of the liquid solutes considered in the present study.

Headspace chromatographic measurements provide a convenient experimental method for determining $\log K$ values for volatile organic liquid solutes having quantifiable partial pressures at low solute concentrations. Headspace measurements are more difficult in the case of crystalline organic solutes as the vapor pressure is often extremely small. For crystalline solutes one can use the logarithm of the molar solubility ratios as the measured solute property. The mole fraction solubility data in Tables 3 and 4 were converted to molar solubilities by dividing $X_{S,organic}^{exp}$ by the ideal molar volume of the saturated solution:

$$C_{S,organic}^{exp} \approx X_{S,organic}^{exp} / [X_{S,organic}^{exp} V_{Solute} + (1 - X_{S,organic}^{exp}) V_{Solvent}] \quad (4)$$

Numerical values of the molar volumes of the crystalline solutes were computed by a group contribution method that involved summing group values for the functional groups found in the solute molecules. The molar solubility ratios of $(C_{S,organic}/C_{S,water})$ and $(C_{S,organic}/C_{S,gas})$ were determined by dividing the solute's molar solubility in 2-propoxyethanol and/or 2-isopropoxyethanol by the solute's molar solubility in water, $C_{S,water}$, and by the solute's gas phase molar concentration, $C_{S,gas}$. The experimental mole fraction solubility data in Tables 3 and 4 gave $\log (C_{S,organic}/C_{S,water})$ and $\log (C_{S,organic}/C_{S,gas})$ values for 18 and 20 solutes dissolved in 2-propoxyethanol and 2-isopropoxyethanol, respectively. The number of experimental data points was increased by including published solubility data from several of our earlier solubility studies

[17-23]. Numerical values of $C_{S,\text{water}}$ and $C_{S,\text{gas}}$ were taken from published papers [19, 22, 23, 27, 29-39, 41-46] for all of the crystalline solutes considered in the current study.

Our experimental measurements and search of the chemical literature yielded nearly 55 data points for each solvent. This is sufficient chemical diversity and more than enough experimental values in each of the solvent data sets to develop meaningful Abraham model $\log P$ and $\log K$ correlations. Each data set contains several nonpolar alkane solutes, several polycyclic aromatic hydrocarbons (anthracene, $E = 2.290$; pyrene, $E = 2.808$; acenaphthene, $E = 1.604$) and polycyclic aromatic hetero-atom compounds (xanthene, $E = 1.502$; phenothiazine, $E = 1.890$) having large E solute descriptors, several carboxylic acid solutes possessing strong H-bond donor capability (3,5-dinitrobenzoic acid, $A = 0.700$; acetylsalicylic acid, $A = 0.710$; 2-hydroxybenzoic acid, $A = 0.730$; 3-hydroxybenzoic acid, $A = 0.860$; 3,5-dinitro-2-methylbenzoic acid, $A = 0.750$), and several organic solutes possessing fairly strong H-bond acceptor character (benzoin, $B = 0.841$; 4-hydroxyacetanilide, $B = 0.860$; diphenyl sulfone, $B = 0.700$). As documented in Tables 5 and 6 the organic solutes considered in the present study cover a fairly large range in the numerical values of their solute descriptors.

Preliminary regression analysis of the experimental $\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$ and $\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$ values in Tables 5 and 6 revealed that the $a_p \cdot A$ term in the $\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$ made a negligible contribution in the case of 2-propoxyethanol. The calculated numerical of a_p coefficient was small and the standard error in the coefficient was larger than the coefficient itself. The $a_p \cdot A$ term was removed from the $\log P$ correlation for 2-propoxyethanol, and reanalysis of the experimental data gave the following Abraham model expressions for 2-propoxyethanol:

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.053(0.059) + 0.419(0.049) E - 0.569(0.062) S - 4.327(0.098) B$$

$$+ 4.095(0.070) \mathbf{V} \quad (5)$$

(with $N = 54$, $SD = 0.100$, $R^2 = 0.996$, $F = 2810$)

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.091(0.042) - 0.288(0.057) \mathbf{E} + 1.265(0.066) \mathbf{S} + 3.566(0.055) \mathbf{A} \\ + 0.390(0.094) \mathbf{B} + 0.902(0.017) \mathbf{L} \quad (6)$$

(with $N = 54$, $SD = 0.094$, $R^2 = 0.999$, $F = 10096$)

and for 2-isopropoxyethanol:

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.107(0.065) + 0.391(0.056) \mathbf{E} - 0.525(0.082) \mathbf{S} + 0.071(0.063) \mathbf{A} \\ - 4.439(0.131) \mathbf{B} + 4.051(0.073) \mathbf{V} \quad (7)$$

(with $N = 55$, $SD = 0.113$, $R^2 = 0.994$, $F = 1676$)

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.045(0.043) - 0.264(0.057) \mathbf{E} + 1.296(0.075) \mathbf{S} + 3.046(0.054) \mathbf{A} \\ + 0.352(0.115) \mathbf{B} + 0.880(0.017) \mathbf{L} \quad (8)$$

(with $N = 55$, $SD = 0.099$, $R^2 = 0.999$, $F = 9143$)

where N represents the number of experimental data points used in the regression analysis, SD refers to the standard deviation of the correlation, R^2 corresponds to the squared correlation coefficient, and F denotes the Fisher F-statistic. The standard error in the calculated equation coefficients is given in parentheses after the respective coefficient.

The derived Abraham model correlations provide a reasonably accurate mathematical description of the observed solubility ratios and partition coefficient data. The standard deviations were $SD = 0.094$ log units and $SD = 0.099$ log units for the log K correlations for 2-propoxyethanol and 2-isopropoxyethanol, respectively. Slightly larger standard deviations of $SD = 0.100$ log units (2-propoxyethanol) and $SD = 0.113$ log units (2-isopropoxyethanol) were calculated for the two log P correlations. Figures 1 - 4 depict a graphical comparison of the observed experimental solubility ratios and partition coefficients and back-calculated values

based on Eqns. (5) - (8). There is not sufficient experimental values to perform training set and test set analyses. We have performed many such analyses in the past on other organic solvents that had larger $\log P$ and $\log K$ datasets. Our past experience has been that the analyses when they could be performed gave very similar standard deviations to the parent data sets.

Table 5. Experimental $\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$ and $\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$ data for solutes dissolved in 2-propoxyethanol at 298.15 K.

Solute	E	S	A	B	L	V	$\log K^a$	$\log P^a$	Ref
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.323	4.143	This work
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	2.761	4.721	This work
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	3.626	5.776	This work
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	2.639	3.539	This work
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	2.890	4.140	This work
1,7-Octadiene	0.191	0.200	0.000	0.100	3.415	1.1498	3.316	4.276	This work
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.0089	3.138	3.578	This work
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943	2.727	1.767	This work
1,2-Dichloropropane	0.370	0.630	0.000	0.170	2.836	0.7761	3.319	2.349	This work
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.024	2.394	This work
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.449	2.799	This work
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	3.820	3.240	This work
<i>o</i> -Xylene	0.663	0.560	0.000	0.160	3.939	0.9982	3.989	3.329	This work
<i>m</i> -Xylene	0.623	0.520	0.000	0.160	3.839	0.9982	3.859	3.249	This work
<i>p</i> -Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	3.852	3.262	This work
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	2.988	0.438	This work
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	3.447	-0.263	This work
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	2.660	-0.170	This work
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	2.923	0.073	This work
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	3.386	-0.094	This work
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.924	4.894	17
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.114	5.614	20
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.618	4.258	This work
Fluorene	1.588	1.060	0.000	0.250	6.922	1.3565	7.096	4.646	This work
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.424	4.474	21
<i>trans</i> -Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	7.850	5.070	This work
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	3.173	2.583	This work
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	3.924	3.104	This work

Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	4.336	3.266	This work
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.394	4.894	This work
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	10.291	4.888	This work
Benzoic acid	0.730	0.900	0.590	0.400	4.657	0.9317	7.067	1.927	This work
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.1059	9.213	2.313	21
3,5-Dinitrobenzoic acid	1.250	1.630	0.700	0.590	6.984	1.2801	10.675	2.375	This work
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.1313	8.304	1.504	21
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313	8.961	2.261	21
3,4-Dimethoxybenzoic acid	0.950	1.646	0.570	0.755	6.746	1.3309	10.213	1.766	This work
4-Hydroxyacetanilide	1.060	1.630	1.040	0.860	6.430	1.1724	11.778	0.878	21
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	4.947	1.0541	7.790	2.990	21
3,5-Dinitro-2-methylbenzoic acid	1.310	2.120	0.750	0.650	8.040	1.4210	12.410	2.454	This work
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726	6.590	2.290	This work
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	4.819	1.0726	7.378	2.398	21
4-Chloro-3-nitrobenzoic acid	1.250	1.470	0.700	0.440	6.685	1.2283	10.035	2.826	This work
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	4.732	0.9904	7.668	2.308	This work
3-Hydroxybenzoic acid	0.910	0.880	0.860	0.580	4.860	0.9904	8.423	1.423	This work
Acetylsalicylic acid	0.781	1.690	0.710	0.670	6.279	1.2879	10.160	1.630	This work
3,4-Dichlorobenzoic acid	0.950	0.920	0.670	0.260	5.623	1.1766	8.327	3.587	23
Diphenyl sulfone	1.570	2.150	0.000	0.700	8.902	1.6051	10.384	2.994	This work
Benzoin	1.585	2.115	0.196	0.841	9.159	1.6804	11.382	2.651	19
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	8.680	3.810	This work
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.084	4.016	This work
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.0315	9.409	1.724	21
2-Propoxyethanol	0.212	0.500	0.300	0.830	3.310	0.9305	4.815	0.115	Unity ^b
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	10.083	4.049	This work

^a For solid solutes the tabulated values represent molar solubility ratios.

^b Activity coefficient is unity.

Table 6. Experimental $\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$ and $\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$ data for solutes dissolved in 2-isopropoxyethanol at 298.15 K.

Solute	E	S	A	B	L	V	Log K^a	log P^a	
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.322	4.142	This work
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	2.766	4.726	This work
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.227	5.337	This work
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	3.618	5.768	This work
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	2.624	3.524	This work
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.0089	3.139	3.579	This work

1-Octyne	0.155	0.220	0.090	0.100	3.521	1.1498	3.598	4.118	This work
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943	2.769	1.809	This work
1,2-Dichloropropane	0.370	0.630	0.000	0.170	2.836	0.7761	3.299	2.329	This work
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.026	2.396	This work
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	3.797	3.217	This work
<i>o</i> -Xylene	0.663	0.560	0.000	0.160	3.939	0.9982	3.960	3.300	This work
<i>m</i> -Xylene	0.623	0.520	0.000	0.160	3.839	0.9982	3.898	3.288	This work
<i>p</i> -Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	3.846	3.256	This work
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	2.993	0.443	This work
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	3.526	-0.184	This work
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470	2.672	-0.158	This work
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	2.949	0.099	This work
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	3.715	1.775	This work
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	3.475	-0.005	This work
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.885	4.855	18
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.045	5.545	This work
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.608	4.248	This work
Fluorene	1.588	1.060	0.000	0.250	6.922	1.3565	7.040	4.590	This work
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.403	4.453	21
<i>trans</i> -Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	7.785	5.005	This work
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	3.196	2.606	This work
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	3.919	3.099	This work
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	4.341	3.271	This work
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.361	4.861	This work
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	10.280	4.877	This work
Benzoic acid	0.730	0.900	0.590	0.400	4.657	0.9317	7.079	1.939	This work
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.1059	9.264	2.364	21
3,5-Dinitrobenzoic acid	1.250	1.630	0.700	0.590	6.984	1.2801	10.734	2.434	This work
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.1313	8.209	1.409	21
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313	8.991	2.291	21
3,4-Dimethoxybenzoic acid	0.950	1.646	0.570	0.755	6.746	1.3309	10.066	1.796	22
4-Hydroxyacetanilide	1.060	1.630	1.040	0.860	6.430	1.1724	11.810	0.910	21
3-Chlorobenzoic acid	0.840	0.950	0.630	0.320	5.197	1.0541	7.988	2.838	This work
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	4.947	1.0541	7.844	3.044	21
3,5-Dinitro-2-methylbenzoic acid	1.310	2.120	0.750	0.650	8.040	1.4210	12.478	2.522	This work
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726	6.556	2.246	This work
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	4.819	1.0726	7.408	2.428	21
4-Chloro-3-nitrobenzoic acid	1.250	1.470	0.700	0.440	6.685	1.2283	10.108	2.898	This work
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	4.732	0.9904	7.686	2.326	This work
3-Hydroxybenzoic acid	0.910	0.880	0.860	0.580	4.860	0.9904	8.413	1.413	This work

Acetylsalicylic acid	0.781	1.690	0.710	0.670	6.279	1.2879	10.176	1.676	This work
3,4-Dichlorobenzoic acid	0.950	0.920	0.670	0.260	5.623	1.1766	8.336	3.596	23
Diphenyl sulfone	1.570	2.150	0.000	0.700	8.902	1.6051	10.365	2.975	This work
Benzoin	1.585	2.115	0.196	0.841	9.159	1.6804	11.346	2.615	19
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	8.659	3.789	This work
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	8.994	3.926	This work
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.0315	9.383	1.698	21
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	10.007	3.973	This work
2-Ethylanthraquinone	1.410	1.540	0.000	0.550	8.876	1.8106	9.536	4.722	This work

^a For solid solutes the tabulated values represent molar solubility ratios.

Figure 1

Figure 1. Comparison of experimental log K data versus back-calculated values based on Eqn. (1) for solutes dissolved in 2-propoxyethanol.

Figure 2. Comparison of experimental log P data versus back-calculated values based on Eqn. (6) for solutes dissolved in 2-propoxyethanol.

Figure 3

Figure 3. Comparison of experimental log K data versus back-calculated values based on Eqn. (7) for solutes dissolved in 2-isopropoxyethanol.

Figure 4

Figure 4. Comparison of experimental log P data versus back-calculated values based on Eqn. (8) for solutes dissolved in 2-isopropoxyethanol.

Equation coefficients are reasonable and in line with our expectations based on earlier studies involving 2-methoxyethanol [11], 2-ethoxyethanol [12] and 2-butoxyethanol [13]. For example we estimated the equation coefficients for 2-propoxyethanol [13]:

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.039 + 0.385 \mathbf{E} - 0.513 \mathbf{S} + 0.022 \mathbf{A} - 4.285 \mathbf{B} + 4.061 \mathbf{V} \quad (9)$$

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.087 - 0.281 \mathbf{E} + 1.289 \mathbf{S} + 3.540 \mathbf{A} + 0.661 \mathbf{B} + 0.878 \mathbf{L} \quad (10)$$

as the arithmetic average of the coefficients for the 2-ethoxyethanol and 2-butoxyethanol correlations. Our predicted correlations for 2-propoxyethanol are given by Eqns. (9) and (10). The derived $\log P$ correlation for 2-propoxyethanol (see Eqn. 5 above) is nearly identical to what we predicted earlier, and in the case of the $\log K$ five of the six predicted equation coefficients fall within the confidence interval of the coefficients given in Eqn. (6). Only the predicted b_K -coefficient falls slightly outside of the confidence interval.

4. Conclusion

Mathematical expressions have been derived for predicting the solubility and partitioning behavior of neutral, nonelectrolyte solutions into both 2-propoxyethanol and 2-isopropoxyethanol at 298 K based on the Abraham solvation parameter model. The derived mathematical expressions are expected to predict the solute transfer properties to alkoxyethanol solvents ($\log P$, $\log K$, $\log (C_{S,\text{organic}}/C_{S,\text{water}})$, and $\log (C_{S,\text{organic}}/C_{S,\text{gas}})$) for additional solutes to within 0.12 log units, provided that the solute descriptors fall within the following range of numerical values: from $\mathbf{E} = 0.000$ to $\mathbf{E} = 2.808$; from $\mathbf{S} = 0.000$ to $\mathbf{S} = 2.150$; from $\mathbf{A} = 0.000$ to $\mathbf{A} = 1.040$; from $\mathbf{B} = 0.000$ to $\mathbf{B} = 0.860$; $\mathbf{V} = 0.4042$ to $\mathbf{V} = 1.6804$; and from $\mathbf{L} = 1.696$ to $\mathbf{L} = 9.171$. Many solutes will have descriptor values that fall within this range. Readers are reminded that caution should be exercised in using Eqns. (5) - (8) to make predictions for solutes that fall outside of the above range of descriptor values. While we fully expect the correlations to provide reasonable $\log K$ and $\log P$ estimates for inorganic gases (e.g., helium, argon, neon, carbon monoxide, carbon dioxide, oxygen gas) and organic gases (e.g., methane, ethane, propane, butane, ethene,

acetylene) we would be remiss if we did not remind readers that the 2-propoxyethanol and 2-isopropoxyethanol data sets contained no gaseous solutes.

Our study has shown that two solvents, 2-propoxyethanol and 2-isopropoxyethanol, have very similar solvation properties. The confidence intervals for the respective coefficients of equations (5) and (7) or (6) and (8) overlap. The RMS between the values of $\log K$ in the two solvents for 50 studied solutes is 0.046, the largest deviation by absolute value is 0.147 $\log K$ units for 3,4-dimethoxybenzoic acid and the second largest is 0.095 for 2-methoxybenzoic acid.

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GRAPHIC ABSTRACT