

# ABRAHAM MODEL CORRELATIONS FOR SOLUTE TRANSFER INTO 2-ETHOXYETHANOL FROM WATER AND FROM THE GAS PHASE

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## Abstract

Infinite dilution activity coefficients ( $\gamma_\infty$ ) were measured at 298 K for 13 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 12 different aromatic compounds (benzene, alkylbenzenes, halobenzenes, naphthalene), and 2-chloro-2-methylpropane dissolved in 2-ethoxyethanol, along with solubilities for 11 crystalline organic compounds (xanthene, phenothiazine, acenaphthene, diphenyl sulfone, 3,5-dinitro-2-methylbenzoic acid, 3-chlorobenzoic acid, 2-methylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 3,5-dinitrobenzoic acid, benzil, and thioxanthen-9-one) dissolved in 2-ethoxyethanol at 298 K. The experimental values were converted to gas-to-2-ethoxyethanol partition coefficients, water-to-2-ethoxyethanol partition coefficients, and molar solubility ratios using standard thermodynamic relationships. The calculated partition coefficient data and molar solubility ratios, combined with published literature values, were used to derive Abraham model correlations for solute transfer into 2-

ethoxyethanol from both water and the gas phase. The derived Abraham model correlations predicted the observed values to within 0.15 log units (or less).

**KEY WORDS AND PHRASES:**

Partition coefficients; Infinite dilution activity coefficients; Solubility ratios; Headspace chromatographic measurements; Hydrogen-bonding; Solute transfer

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## 1. Introduction

Hydrogen-bonding has received considerable attention over the years due to its role in determining solubilities, molecular shapes and spectral properties of biomolecules dissolved in fluid solution. Hydrogen-bonding interactions can be intermolecular or intramolecular in nature, and generally results from the electrostatic attraction between a hydrogen atom bonded to a highly electronegative element (e.g., bonded to a nitrogen, oxygen or fluorine atom) and a lone electron pair residing on a nearby electronegative atom or group.  $\text{C-H} \cdots \text{Y}$  (Y = lone-pair electron donor) interactions have also been classified as hydrogen-bonds, with the strength increasing when the C-H bond is in close proximity of electronegative atoms that are capable of withdrawing electron density from the hydrogen atom. The first ever established  $\text{C-H} \cdots \text{Y}$  hydrogen-bond involved the participation of the acidic C-H group in the chloroform molecule. [1].

Differences in hydrogen-bonding interactions are important considerations in predicting solute transfer between water and hydrogen-bonding solvents such as alcohols and alkoxyalcohols. If the water-solute hydrogen bonds are stronger than the organic solvent-solute hydrogen bonds then solute transfer into the organic solvent is generally not favored. If on the other hand the organic solvent-solute interactions are the stronger of the hydrogen-bonding interactions, then one would predict a greater molar solute concentration in the organic solvent relative to that in the aqueous phase. Over the past two decades we have been demonstrating the applicability of the Abraham solvation parameter model to describe solute transfer into organic solvents of varying polarities and hydrogen-bonding character from both water and the gas phase. The Abraham model includes not only the effects from hydrogen-bonding interactions, but also contains contributions from the other types of solute-solute, solute-solvent and solvent-

solvent interactions as well. Neglect of these contributions can lead to significant errors in predicting solute transfer, particularly in the case of weak H-bonded molecular solute-solvent complexes.

To date we have published correlations for describing the solubility and partitioning behavior of solutes into inert solvents (hexane – hexadecane [2, 3], cyclohexane [2], methylcyclohexane [2], and isooctane [4]), into several alkylbenzene [2, 5, 6] and halobenzene [7] solvents, into several aprotic H-bond acceptor solvents (dibutyl ether [2], diethyl ether [2], diisopropyl ether [8], 1,4-dioxane [9], tetrahydrofuran [9], acetone [10], butanone [10], cyclohexanone [10], methyl acetate [11], ethyl acetate [11], butyl acetate [11], tributyl phosphate [12] and dimethyl sulfoxide [2]), and into several protic alcohol solvents (methanol – decanol [2, 13], 2-propanol [2, 14], 2-butanol [2, 14], 2-methyl-1-propanol [2, 14], 2-methyl-2-propanol [2, 14], ethylene glycol [2, 15] and propylene glycol [16]) that possess both H-bond donor and H-bond acceptor character. In total we have reported correlations for more than 80 common organic solvents [2], for more than 35 different ionic liquids [17-37], and for aqueous micellar sodium dodecylsulfate [38] and aqueous micellar cetyltrimethylammonium bromide [39] solvent media. In the present communication we are extending our considerations to include 2-ethoxyethanol, which contains both an ether (R-O-R) and hydroxyl (R-OH) functional group. Infinite dilution activity coefficients ( $\gamma_\infty$ ) were measured at 298 K for 13 different aliphatic hydrocarbons (alkanes, cycloalkanes, alkenes), 12 different aromatic compounds (benzene, alkylbenzenes, halobenzenes, naphthalene), and 2-chloro-2-methylpropane dissolved in 2-ethoxyethanol 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 xanthene,

phenothiazine, acenaphthene, diphenyl sulfone, 3,5-dinitro-2-methylbenzoic acid, 3-chlorobenzoic acid, 2-methylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 3,5-dinitrobenzoic acid, benzil, and thioxanthen-9-one dissolved in 2-ethoxyethanol at 298 K. The measured partition coefficients, combined with published infinite dilution activity coefficient data for liquid organic compounds [40-52], gas solubility data for 2-methylpropane [53] and hydrogen gas [54], and solubility data for crystalline nonelectrolyte organic compounds [55-66] dissolved in 2-ethoxyethanol, were used to derive Abraham model correlations for both water-to-2-ethoxyethanol partition coefficients (as  $\log P$ ) and gas-to-2-ethoxyethanol partition coefficients (as  $\log K$ ).

## 2. Experimental Methods

### 2.1 Gas Chromatographic Headspace Measurements

Limiting activity coefficients of low polar liquid organic compounds in 2-ethoxyethanol were measured using PerkinElmer Clarus 580 chromatograph with a headspace autosampler. The autosampler takes portions of equilibrium vapor phase from sealed thermostated vials (22 ml glass vials containing 5 ml of liquid). In two sequential experiments with pure liquid solute and its solution in 2-ethoxyethanol, the areas of the chromatographic peaks of the solute are proportional to its saturated vapor pressure  $p_{sat}$  and the vapor pressure  $p$  over solution respectively. The activity coefficient of the solute  $\gamma$  is given by  $\gamma = p / (p_{sat} \cdot x)$ , where  $x$  is the equilibrium molar fraction of a solute in the liquid phase. To obtain the value of  $x$ , we subtracted the quantity of solute evaporated into the equilibrium gas phase from the quantity of solute initially added into a vial [67]. To determine the limiting activity coefficient  $\gamma_{\infty}$ , we measured activity coefficients at 3–4 different concentrations of a solute in the range of 0.1–1.5

vol % and repeated 2 times for each concentration. Since the considered solutes form no dimers or other associates, it is likely that at such concentrations the solutions behave like infinitely diluted ones. This was confirmed experimentally by the absence of concentration dependence of the activity coefficients. Gas-to-liquid partition coefficients  $K$  can be calculated using a formula

$$\log K = \log \left( \frac{RT}{\gamma_{\infty} p_{\text{solute}}^{\circ} V_{\text{solvent}}} \right), \text{ where } p_{\text{solute}}^{\circ} \text{ is the saturated vapor pressure over pure dissolved}$$

compound (taken from [68, 69]) and  $V_{\text{solvent}}$  is the molar volume of 2-ethoxyethanol. The Gibbs free energy of solvation is calculated according to the equation  $\Delta_{\text{solv}} G = RT \ln(\gamma_{\infty} p_{\text{sat}})$ . Average values of  $\log K$  and  $\Delta_{\text{solv}} G$  calculated from all measurements for the same system were taken.

Results are presented in Table 1.

Comparison with the VLE data for the mixtures of hexane, heptane, and cyclohexane with 2-ethoxyethanol at 303 and 323 K (Carmona et al. [40]) shows that our limiting activity coefficients are 7-12% lower than the values extrapolated to 298K using the results of that study. However, the lowest concentrations of hydrocarbons at which authors conducted their measurements were 3 and 6 mol %. This corresponds to 3.3 – 9 vol % of a hydrocarbon, and is certainly not at infinite dilution. Extrapolation to zero concentration made by authors [40] is likely to lead to the overestimation of  $\gamma_{\infty}$ .

Comparison with the previously reported Gibbs free energies of solvation in 2-methoxyethanol at 298 K ( $\Delta_{\text{solv}} G^{A/MC}$ ) [70] shows a good correlation between the data in two solvents:

$$\Delta_{\text{solv}} G^{A/EC} = 0.951 \Delta_{\text{solv}} G^{A/MC} - 1.712$$

$$n = 25, \sigma = 0.62 \text{ kJ} \cdot \text{mol}^{-1}, R^2 = 0.9780.$$

This correlation is shown in Figure 1. For all the considered solutes the Gibbs free energy of solvation in 2-ethoxyethanol is lower than in 2-methoxyethanol, and for aliphatic compounds this difference is larger than for aromatic.

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

Solute	$\gamma_\infty$	$u(\gamma_\infty)$	Log $K$	$\Delta_{solv} G^b /$ (kJ·mol <sup>-1</sup> )
n-Hexane	7.65	0.4	2.22	1.1
n-Heptane	9.63	0.3	2.64	-1.3
n-Octane	12.16	0.3	3.05	-3.7
n-Nonane	14.70	0.6	3.47	-6.0
n-Decane	20.80	0.9	3.81	-8.0
n-Undecane	30.40	0.6	4.19	-10.1
Cyclohexane	5.47	0.3	2.56	-0.9
Methylcyclopentane	5.52	0.6	2.40	0.0
Methylcyclohexane	6.93	0.4	2.78	-2.1
Cyclooctane	8.70	0.2	3.60	-6.8
Cyclohexene	3.98	0.2	2.73	-1.9
1,7-Octadiene	5.38	0.5	3.20	-4.5
4-Vinyl-1-cyclohexene	4.53	0.2	3.43	-5.8
Benzene	1.91	0.1	3.03	-3.5
Toluene	2.42	0.15	3.45	-5.9
Fluorobenzene	1.52	0.1	3.21	-4.6
Chlorobenzene	1.69	0.1	3.98	-8.9
Bromobenzene	2.01	0.2	4.36	-11.1
o-Dichlorobenzene	2.00	0.4	4.85	-13.9
o-Xylene	3.18	0.15	3.96	-8.9
m-Xylene	3.36	0.2	3.84	-8.2
p-Xylene	3.38	0.15	3.81	-8.0

Ethylbenzene	3.16	0.1	3.80	-7.9
p-Cymene	5.46	0.3	4.38	-11.3
Naphthalene	9.97	1.4	5.36	-16.8
<i>tert</i> -Butyl chloride	2.30	0.55	2.43	-0.1

<sup>a</sup> Standard uncertainty for temperature  $u(T) = 0.2$  K.

<sup>b</sup> Standard state for the  $\Delta_{\text{solv}}G$  is a hypothetical ideal solution at unit mole fraction and a gas at 1 bar fugacity.  $\Delta_{\text{solv}}G$  calculated in this fashion are not the same as values calculated as  $\Delta_{\text{solv}}G = -RT\ln K$  where  $K$  is the equilibrium constant in the table.

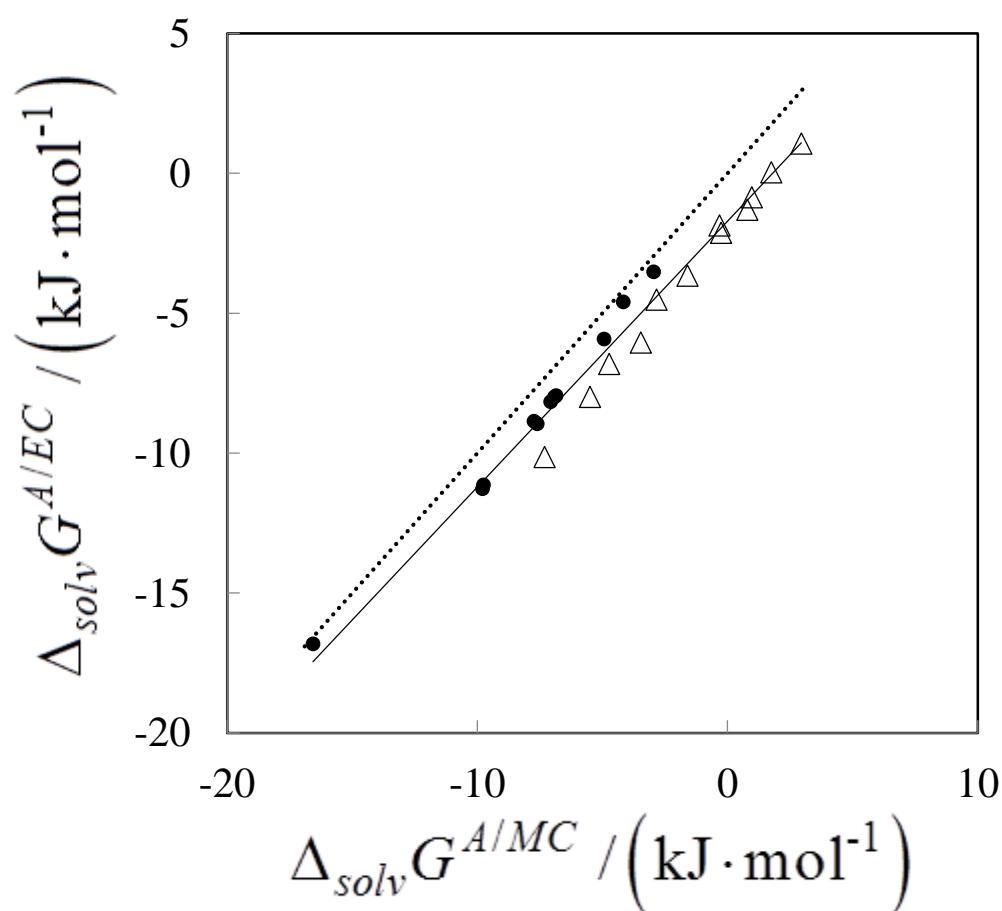


Figure 1. Comparison of the Gibbs free energies of solvation of low polar solutes in 2-ethoxyethanol (EC) and 2-methoxyethanol (MC) at  $T = 298.15$  K. Triangles are aliphatic, circles are aromatic solutes. Dotted line is  $y = x$ .



## 2.2 Solubility Measurements

Xanthene (Aldrich, 98 %), acenaphthene (Aldrich, 98 %), phenothiazine (Acros, 99 %), diphenyl sulfone (Aldrich, 97 %), 3,5-dinitro-2-methylbenzoic acid (Aldrich, 99+ %), 3-chlorobenzoic acid (Aldrich, 99 %), 2-methylbenzoic acid (Aldrich 99 %), 4-chloro-3-nitrobenzoic acid (Acros, 99.5 %), 3,5-dinitrobenzoic acid (Aldrich, 99+ %), benzil (Aldrich 97 %), and thioxanthen-9-one (Aldrich, 98 %) were purchased from commercial sources. Xanthene, acenaphthene, diphenyl sulfone, thioxanthen-9-one and benzil were recrystallized several times from anhydrous methanol prior to use. The remaining six solutes were used as received. 2-Ethoxyethanol (Aldrich, 99 %) was stored over molecular sieves and distilled shortly before use. Gas chromatographic analysis showed that the purity of 2-ethoxyethanol was 99.8 mass percent.

Excess solute and 2-ethoxyethanol were placed in amber glass bottles and allowed to equilibrate in a constant temperature water bath at  $298.15 \pm 0.1\text{K}$  for at least 3 days with periodic agitation. After equilibrium, the samples stood unagitated for several hours in the constant temperature bath to allow any finely dispersed particles to settle. Attainment of equilibrium was verified by both repetitive measurements the following day (or sometimes after 2 days) and by approaching equilibrium from supersaturation by pre-equilibrating the solution at a slightly higher temperature.

Aliquots of the respective saturated solutions were transferred through a coarse filter into a tared volumetric flask to determine the amount of sample and diluted quantitatively with methanol (or 2-propanol) for spectrophotometric analysis on a Milton Roy Spectronic 1001 Plus spectrophotometer. Concentrations of the diluted solutions were determined from a Beer–Lambert law absorbance versus concentration working curve for nine standard solutions of

known concentration. The analysis wavelengths and concentration ranges used for each solute have been reported in earlier solubility publications [71-79].

Experimental molar concentrations were converted to (mass/mass) solubility fractions by multiplying by the molar mass of the solute, volume(s) of the volumetric flasks used and any dilutions required to place the measured absorbances on the Beer–Lambert law absorbance versus concentration working curve, and then dividing by the mass of the saturated solution analyzed. Mole fraction solubilities were computed from solubility mass fractions using the molar masses of the solutes and 2-ethoxyethanol. Experimental mole fraction solubilities,  $X_S^{\text{exp}}$ , are tabulated in Table 2 for the 11 organic solutes for which solubility measurements were made. Numerical values represent the average of between four and eight independent determinations, and were reproducible to within  $\pm 1.5\%$ .

Table 2. Experimental mole fraction solubilities of crystalline nonelectrolyte solutes dissolved in 2-ethoxyethanol at 298.15 K

Solute	$X_S^{\text{exp}}$
Xanthene	0.04299
Acenaphthene	0.04561
Thioxanthen-9-one	0.002795
Phenothiazine	0.08050
Diphenyl sulfone	0.03087
3,5-Dinitrobenzoic acid	0.1361
4-Chloro-3-nitrobenzoic acid	0.08320
2-Methylbenzoic acid	0.2194
3-Chlorobenzoic acid	0.1612
3,5-Dinitro-2-methylbenzoic acid	0.09944
Benzil	0.06654

## Results and Discussion

The Abraham solvation parameter model is among the more popular of the quantitative structure-property relationships (QSPRs) and linear free energy relationships (LFERs) proposed in the last 25 years. Unlike many of the other models proposed models that use a different set of solute descriptors for different partitioning processes, the Abraham model uses a common set of solute descriptors (**E**, **S**, **A**, **B**, **V** and **L**) for all types solute transfer processes, including solute transfer into an organic solvent from water, from another organic solvent, and from the gas phase. The basic model consists of two LFERs that describe solute transfer of electrically neutral molecules between two condensed phases:

$$SP = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \quad (1)$$

and solute transfer into a condensed phase from the gas phase:

$$SP = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L}, \quad (2)$$

where  $SP$  denotes some property of a series of solutes in a given solvent, a given partitioning system, or a given biological or pharmaceutical process.

In the present communication  $SP$  refers to the logarithm of the solute's water-to-organic solvent ( $\log P$ ), or the logarithm of the ratio of the solute's molar solubility in two solvents or phases,  $\log (C_{S,\text{organic}}/C_{S,\text{water}})$  (eqn. 1) and the gas-to-organic solvent ( $\log K$ ) partition coefficient  $\log (C_{S,\text{organic}}/C_{S,\text{gas}})$  (eqn. 2). In these equations,  $C_{S,\text{organic}}$  and  $C_{S,\text{water}}$  are the solute's molar solubility in the organic solvent and water, respectively, and  $C_{S,\text{gas}}$  is a molar gas phase concentration calculable from the solute's vapor pressure. In other published studies  $SP$  has

referred to the logarithm of the solute's blood-to-body organ/tissue partition coefficient [80-84] and logarithm of the solute's gas-to-body organ/tissue partition coefficient [80-84], median lethal concentration of an organic compound in aquatic toxicity studies [85-87], enthalpy of solvation of the solute in water and in organic solvents [88-90], biological responses (eye irritation [91, 92], nasal pungency [91, 93], minimum alveolar concentration on inhalation anesthesia in rats [94], and convulsant activity of gases and vapors [95]) and skin permeation of organic solvents and pharmaceutical compounds from aqueous solution [96, 97].

Equations 1 and 2 contain product terms that represent the various types of solute-solvent interactions believed to be present in the solution. The product terms contain a solute property (**E**, **S**, **A**, **B**, **V** and **L**) and the complementary process property (e, s, a, b, v and l). The six solute properties are defined as: the excess molar refraction descriptor (**E**); the dipolarity/polarizability descriptor (**S**); the solute hydrogen-bond acidity descriptor (**A**); the solute hydrogen-bond basicity descriptor (**B**); the McGowan characteristic volume descriptor (**V**); and the logarithm of the solute's gas-to-hexadecane partition coefficient at 25 °C (**L**). Solute descriptors are independent of the system properties, and once calculated can be used to describe the various solute transfer processes noted above.

The complementary process constants/coefficients represent the ability of the system to participate in lone electron pair interactions (e), in dipole-type interactions (s), as a hydrogen-bond type base (a), as a hydrogen-bond type acid (b), and in interactions involving formation of the solvent cavity needed for solute transfer between condensed phases (v) or for solute transfer from the gas phase (l). The  $v_p \cdot \mathbf{V}$  and  $l_k \cdot \mathbf{L}$  terms may also contain dispersion interactions that do not cancel in the representative solute transfer process. Positive numerical values of the product terms facilitate solute transfer to the destination phase, while negative product terms

keep the solute in the origination phase. For example, in the case of solute transfer to an organic solvent from water, stronger hydrogen-bonding interactions between the solute and organic solvent lead to a positive  $a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B}$  sum term and larger water-to-organic solvent partition coefficient,  $P$ . Weak solute-organic solvent hydrogen-bonding interactions lead to a negative  $a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B}$  sum term, which would tend to keep the solute in the aqueous phase.

Assembled in Table 3 are the experimental partition coefficients and solubility ratios for a chemically diverse set of 76 solutes dissolved in 2-ethoxyethanol. For hexane, heptane, and cyclohexane we have elected to use our measured  $\log K$  values at 298 K in the data treatment rather than the extrapolated values based on the published  $\log K$  data of Carmona et al. [40]. As noted above, the data of Carmona et al. was measured at a slightly higher temperature, and to remove any uncertainty associated with extrapolating the values to a slightly lower temperature we have chosen to use the values that were measured at 298 K. In the case of the liquid solutes, the experimental partition coefficients were calculated from measured infinite dilution activity coefficient data ( $\gamma_{\text{solute}}^\infty$ ) using standard thermodynamic relationships:

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

$$\log P = \log K - \log K_w \quad (4)$$

where  $R$  is the universal gas constant,  $T$  is the system temperature,  $P_{\text{solute}}^\circ$  is the vapor pressure of the solute at  $T$ , and  $V_{\text{solvent}}$  is the molar volume of the solvent. This definition of  $K$  is the same as  $K = C_{\text{s solvent}}/C_{\text{s gas}}$  so if concentrations are measured in the same units in solution and the gas phase, say in mol/L, then  $K$  is dimensionless. 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.

In the case of crystalline solutes, the tabulated numerical values in Table 3 represent the logarithm of the molar solubility ratios,  $\log (C_{S,\text{organic}}/C_{S,\text{water}})$  (eqn. 1) and  $\log (C_{S,\text{organic}}/C_{S,\text{gas}})$  (eqn. 2). Several authors reported their experimental solubility data in units of mole fraction. Measured mole fraction solubilities were converted to molar solubilities by dividing  $X_{S,\text{organic}}^{\text{exp}}$  by the ideal molar volume of the saturated solution (i.e.,  $C_{S,\text{organic}}^{\text{exp}} \approx X_{S,\text{organic}}^{\text{exp}}/[X_{S,\text{organic}}^{\text{exp}} V_{\text{Solute}} + (1 - X_{S,\text{organic}}^{\text{exp}}) V_{\text{Solvent}}]$ ). 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 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 at 298.15 K for solutes dissolved in 2-ethoxyethanol are listed in the last two columns of Table 3. Also given in Table 3 are the molecular solute descriptors for all solutes considered in this study. The tabulated values came from our solute descriptor database and are all based on experimental partition coefficient, molar solubility ratios, and chromatographic retention factor data.

Table 3. 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 Anhydrous 2-Ethoxyethanol 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	-1.243	0.477	54
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.061	2.761	53
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.220	4.040	This work
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	2.640	4.600	This work
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.050	5.160	This work
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	3.470	5.620	This work
Decane	0.000	0.000	0.000	0.000	4.686	1.5180	3.810	6.130	This work
Undecane	0.000	0.000	0.000	0.000	5.191	1.6590	4.190	6.570	This work
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	2.560	3.460	This work
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.8454	2.400	3.570	This work
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	2.780	3.990	This work
Cyclooctane	0.413	0.100	0.000	0.000	4.329	1.1272	3.600	4.370	This work
Cyclohexene	0.395	0.200	0.000	0.070	3.021	0.8024	2.730	3.000	This work

1,7-Octadiene	0.191	0.200	0.000	0.100	3.415	1.1498	3.200	4.160	This work
4-Vinyl-1-cyclohexene	0.450	0.330	0.000	0.170	3.708	1.0412	3.430	3.500	This work
<i>tert</i> -Butyl chloride	0.142	0.300	0.000	0.030	2.273	0.7946	2.430	3.230	This work
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	3.179	-0.561	42,52
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	3.346	-0.324	43,52
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.5900	3.910	0.350	44,52
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900	3.571	0.091	45,52
Methyl formate	0.192	0.680	0.000	0.380	1.285	0.4648	2.256	0.216	46,51
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	2.703	0.403	47,51
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	3.037	0.877	48,51
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	3.450	1.400	49,51
Ethyl propanoate	0.087	0.580	0.000	0.450	2.807	0.8875	3.360	1.390	50,51
2-Ethoxyethanol	0.237	0.550	0.290	0.820	2.719	0.7896	4.569	-0.341	Unity
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.030	2.400	This work
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.450	2.800	This work
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	3.800	3.220	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	3.840	3.230	This work
<i>p</i> -Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	3.810	3.220	This work
4-Isopropyltoluene	0.607	0.490	0.000	0.190	4.590	1.2800	4.380	3.880	This work
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.360	3.630	This work
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	7.864	4.834	59
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.135	5.635	60
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	6.562	4.202	This work
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.409	4.459	55
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.7341	3.210	2.620	This work
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	3.980	3.160	This work
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.9612	4.850	3.950	This work
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.8914	4.360	3.290	This work
Xanthene	1.502	1.070	0.000	0.230	7.153	1.4152	7.344	4.844	This work
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.4789	10.399	4.996	This work
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.1059	9.366	2.466	55
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.1313	8.427	1.627	55
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313	9.120	2.420	55
3,4-Dimethoxybenzoic acid	0.950	1.646	0.570	0.755	6.746	1.3309	10.429	1.982	56
4-Hydroxyacetanilide	1.060	1.630	1.040	0.860	6.430	1.1724	12.034	1.134	55
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	4.947	1.0541	7.895	3.095	55
3,5-Dinitro-2-methylbenzoic acid	1.310	2.120	0.750	0.650	8.040	1.4210	12.543	2.587	This work
3-Chlorobenzoic acid	0.840	0.950	0.630	0.320	5.197	1.0541	8.004	2.854	This work
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726	6.689	2.389	This work
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	4.819	1.0726	7.432	2.452	55
4-Chloro-3-nitrobenzoic acid	1.250	1.470	0.700	0.440	6.685	1.2283	10.129	2.919	This work
3,5-Dinitrobenzoic acid	1.250	1.630	0.700	0.590	6.984	1.2801	10.842	2.542	This work
4-Aminobenzoic acid	1.075	1.650	0.940	0.600	5.916	1.0315	11.105	1.675	62
Diphenyl sulfone	1.570	2.150	0.000	0.700	8.902	1.6051	10.522	3.132	This work
Benzoin	1.585	2.115	0.196	0.841	9.159	1.6804	11.544	2.813	58
3,4-Dichlorobenzoic acid	0.950	0.920	0.670	0.260	5.623	1.1766	8.373	3.633	57

2,3-Dimethyl-2,3-dinitrobutane	0.430	1.410	0.040	0.590	5.717	1.3624	7.089	2.389	61
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	8.729	3.859	This work
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.065	3.997	This work
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.0315	9.543	1.858	55
Methyl 4-hydroxybenzoate	0.930	1.460	0.710	0.460	5.914	1.1313	9.461	2.221	62
Testosterone	1.540	2.560	0.320	1.170	11.690	2.3827	14.949	3.759	62
Phosphorous compd 1 <sup>b</sup>	2.080	2.440	0.000	1.860	13.672	2.6903	15.595	2.465	64
Phosphorous compd 2 <sup>c</sup>	1.130	1.070	1.210	1.160	6.175	1.2380	11.950	0.380	64
Phosphorous compd 3 <sup>d</sup>	2.020	2.100	0.000	1.170	13.536	2.7354	15.130	6.240	64
Phosphorous compd 4 <sup>e</sup>	2.070	2.780	0.000	1.900	14.442	2.7941	16.980	2.880	64
Phosphorous compd 5 <sup>f</sup>	2.330	2.180	0.360	1.910	11.644	2.3127	14.890	1.250	65
Phosphorous compd 6 <sup>g</sup>	1.040	1.250	0.860	0.860	5.543	1.0384	9.760	0.440	66
Phosphorous compd 7 <sup>h</sup>	0.930	1.390	0.750	0.960	6.0100	1.1793	10.040	0.460	66
Phosphorous compd 8 <sup>i</sup>	0.850	1.180	0.000	0.500	7.236	1.6676	7.950	4.460	66
Phosphorous compd 9 <sup>j</sup>	4.290	2.290	0.000	2.200	24.707	4.9122	24.270	10.480	66
Phosphorous compd 10 <sup>k</sup>	1.500	1.500	0.870	1.230	8.380	1.6462	12.605	1.565	63

<sup>a</sup> For solid solutes the tabulated values represent molar solubility ratios, except for naphthalene.

<sup>b</sup> Phosphorous compd 1 is 3,9-diphenoxy-2,4,8,10-tetraoxa-3,9-diphosphaspiro-[5.5]-undecane-3,9-dioxide.

<sup>c</sup> Phosphorous compd 2 is hydroxymethylphenylphosphinic acid.

<sup>d</sup> Phosphorous compd 3 is tri(4-methoxyphenyl)phosphine.

<sup>e</sup> Phosphorous compd 4 is tri(4-methoxyphenyl)phosphine oxide.

<sup>f</sup> Phosphorous compd 5 is (2,5-dihydroxyphenyl)diphenylphosphine oxide.

<sup>g</sup> Phosphorous compd 6 is phenylphosphinic acid.

<sup>h</sup> Phosphorous compd 7 is methylphenylphosphinic acid.

<sup>i</sup> Phosphorous compd 8 is hexachlorocyclotriphosphazene.

<sup>j</sup> Phosphorous compd 9 is hexaphenoxycyclotriphosphazene.

<sup>k</sup> Phosphorous compd 10 is diphenylphosphinic acid.

Regression analysis of the 76 experimental log *P* values and 76 log *K* values in Table 3 yielded the following two Abraham model correlations.

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.133(0.049) + 0.392(0.050) \mathbf{E} - 0.419(0.056) \mathbf{S} + 0.125(0.068) \mathbf{A} \\ - 4.200(0.073) \mathbf{B} + 3.888(0.056) \mathbf{V} \quad (5)$$

$$(\text{with } N = 76, \text{SD} = 0.149, R^2 = 0.994, F = 2153)$$

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.064(0.032) - 0.257(0.049) \mathbf{E} + 1.452(0.047) \mathbf{S} + 3.672(0.055) \mathbf{A} \\ + 0.662(0.060) \mathbf{B} + 0.843(0.012) \mathbf{L} \quad (6)$$

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



where the standard error in each calculated equation coefficients is given in parentheses immediately after the respective coefficient. The statistical information associated with each correlation includes the number of experimental data points used in the regression analysis (N), the standard deviation (SD), the squared correlation coefficient ( $R^2$ ) and the Fisher F-statistic (F).

The Abraham model correlations given by eqns. 5 and 6 are statistically very good with standard deviations of 0.149 log units and 0.126 log units, respectively. Figure 2 compares the observed log ( $K$  or  $C_{S,organic}/C_{S,gas}$ ) values against the back-calculated values based on eqn. 6. The experimental data covers a range of approximately 25.51 log units, from log  $K = -1.24$  for hydrogen gas to log ( $C_{S,organic}/C_{S,gas}$ ) = 24.27 for hexaphenoxycyclotriphosphazene. A comparison of the back-calculated versus measured log ( $P$  or  $C_{S,organic}/C_{S,water}$ ) data is depicted in Figure 3 for values that cover a range of about 11.04 log units. As expected the standard deviation for the log ( $P$  or  $C_{S,organic}/C_{S,water}$ ) correlation is slightly larger than that of the log ( $K$  or  $C_{S,organic}/C_{S,gas}$ ) correlations because the log ( $P$  or  $C_{S,organic}/C_{S,water}$ ) values contain the additional experimental uncertainty in the gas-to-water partition coefficients used in the log ( $K$  or  $C_{S,organic}/C_{S,gas}$ ) to log ( $P$  or  $C_{S,organic}/C_{S,water}$ ) conversion.

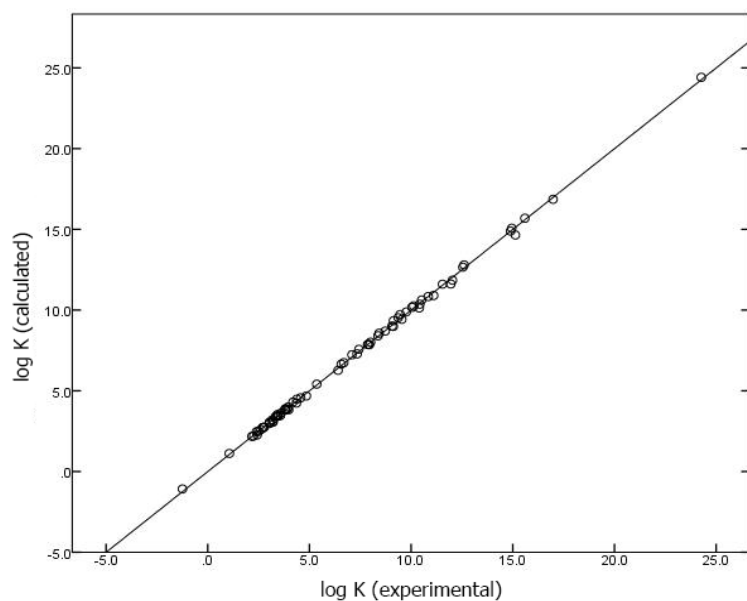


Figure 2. Comparison between experimental  $\log K$  data and calculated values based on eqn. 6.

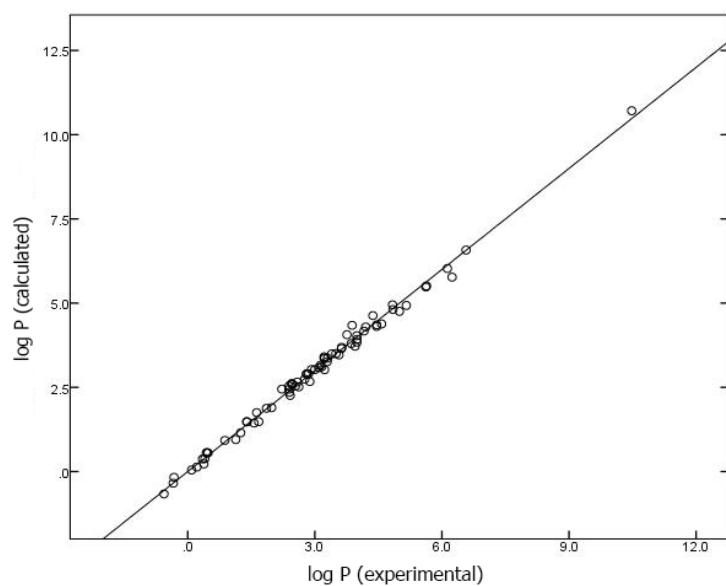


Figure 3. Comparison between experimental  $\log P$  data and calculated values based on eqn. 5.

The  $\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$  and  $\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$  databases for 2-ethoxyethanol contain experimental values for only 76 different solutes. It would be difficult to obtain a good training set correlation by using only half of the experimental values. To assess the

predictive ability of Eq. 7 the parent data points were divided into three subsets (A, B, and C) as follows: the 1st, 4th, 7th, etc. data points comprise the first subset (A); the 2nd, 5th, 8th, etc. data points comprise the second subset (B); and the 3rd, 6th, 9th, etc. data points comprise the third subset (C). Three training sets were prepared as combinations of two subsets (A and B), (A and C), and (B and C). For each training set, a correlation was derived:

**(Training Set A and B)**

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.092(0.057) + 0.316(0.061) \mathbf{E} - 0.363(0.064) \mathbf{S} + 0.157(0.077) \mathbf{A} \\ - 4.277(0.086) \mathbf{B} + 3.964(0.065) \mathbf{V} \quad (7)$$

$$(\text{with } N = 51, SD = 0.138, R^2 = 0.995, F = 1931)$$

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.079(0.041) - 0.229(0.070) \mathbf{E} + 1.462(0.060) \mathbf{S} + 3.722(0.071) \mathbf{A} \\ + 0.628(0.082) \mathbf{B} + 0.842(0.016) \mathbf{L} \quad (8)$$

$$(\text{with } N = 51, SD = 0.133, R^2 = 0.999, F = 11191)$$

**(Training Set A and C)**

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.126(0.061) + 0.392(0.063) \mathbf{E} - 0.399(0.070) \mathbf{S} + 0.124(0.089) \mathbf{A} \\ - 4.227(0.099) \mathbf{B} + 3.880(0.071) \mathbf{V} \quad (9)$$

$$(\text{with } N = 51, SD = 0.153, R^2 = 0.993, F = 1331)$$

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.087(0.038) - 0.317(0.059) \mathbf{E} + 1.508(0.056) \mathbf{S} + 3.644(0.068) \mathbf{A} \\ + 0.599(0.077) \mathbf{B} + 0.851(0.014) \mathbf{L} \quad (10)$$

$$(\text{with } N = 51, SD = 0.122, R^2 = 0.999, F = 13882)$$

**(Training Set B and C)**

$$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}}) = 0.128(0.070) + 0.472(0.063) \mathbf{E} - 0.490(0.080) \mathbf{S} + 0.128(0.085) \mathbf{A} \\ - 4.118(0.085) \mathbf{B} + 3.864(0.077) \mathbf{V} \quad (11)$$

$$(\text{with } N = 50, SD = 0.146, R^2 = 0.992, F = 1147)$$

$$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}}) = -0.049(0.042) - 0.219(0.055) \mathbf{E} + 1.430(0.070) \mathbf{S} + 3.669(0.065) \mathbf{A} \\ + 0.693(0.067) \mathbf{B} + 0.836(0.016) \mathbf{L} \quad (12)$$

(with N = 50, SD = 0.116, R<sup>2</sup> = 0.999, F = 10238)

Each validation computation gave a training set correlation equation having coefficients not too different from that obtained from the parent 76 compound database. The training set equations were then used to predict  $\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$  and  $\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$  values for the compounds in the respective test sets (A, B and C). The standard deviations, average absolute errors (AAEs) and average errors (AEs) for the test set computations are reported in Table 4 for eqns. 7 – 12. Examination of the numerical AE values in the last column of Table 4 shows that there is very little bias associated with the derived training set correlations. The training and test set analyses were performed three more times with very similar results. Each time the large 76 compound database was randomized prior to separating the compounds into the smaller A, B, and C datasets.

Table 4. Statistic Test Set Results for Abraham Model Training Set Eqns. 7 - 12

Property	Test Set	N	SD	AAE	AE
$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$	A	26	0.171	0.123	−0.013
$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$	A	26	0.146	0.106	−0.011
$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$	B	25	0.136	0.110	0.035
$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$	B	25	0.136	0.099	0.041
$\log (P \text{ or } C_{S,\text{organic}}/C_{S,\text{water}})$	C	25	0.175	0.139	−0.030
$\log (K \text{ or } C_{S,\text{organic}}/C_{S,\text{gas}})$	C	25	0.114	0.093	−0.031

It is expected that Abraham model eqns. 5 and 6 will provide reasonably accurate predictions of the water-to-2-ethoxyethanol partition coefficients, gas-to-2-ethoxyethanol partition coefficients, and molar solubilities of additional solutes dissolved in anhydrous 2-

ethoxyethanol provided that the solutes stay within the predictive area of chemical space defined the compounds used in determining eqns. 5 and 6. The numerical values of the solute descriptors for the 76 compounds in the 2-ethoxyethanol database ranged from:  $E = 0.000$  to  $E = 4.290$ ;  $S = 0.000$  to  $S = 2.780$ ;  $A = 0.000$  to  $A = 1.210$ ,  $B = 0.000$  to  $B = 2.200$ ;  $V = 0.1086$  to  $V = 4.9122$  and  $L = -1.200$  and  $L = 24.707$ . As noted previously the 76 compounds were chemically diverse and included several liquid and crystalline nonelectrolyte organic compounds, plus hydrogen gas and 2-methylpropane gas. Experimental-based solute descriptors have been determined for more than 5,000 different organic, organometallic and inorganic compounds, plus several ions and ionic species.

It is possible to compare the regression coefficients of eq 6 for 2-ethoxyethanol with the previously reported coefficients in similar equations for other solvents. 1-Butanol has the same number of carbon atoms and one OH-group as 2-ethoxyethanol, and is different from it by one oxygen atom. As can be seen from Table 5, 5 of the 6 coefficients of eq 6 are very similar for 1-butanol and 2-ethoxyethanol, the only one that is significantly different is the  $s$ -coefficient, which corresponds to polar interactions. It is obvious that addition of electronegative oxygen atom increases these polar interactions. On the other hand, 2-ethoxyethanol is a derivative of ethylene glycol, which has a hydroxyl group instead of ethoxy group in its molecule. The  $a$ - and  $b$ -coefficients are much larger for ethylene glycol than for 2-ethoxyethanol, which means that the diol engages in much stronger hydrogen bonding interactions than 2-ethoxyethanol with both solute hydrogen bond acids and solute hydrogen bond bases, because of the additional OH group.

Table 4. Regression coefficients of eq 6 for different solvents

Solvent	$c_k$	$e_k$	$s_k$	$a_k$	$b_k$	$l_k$
2-Ethoxyethanol	-0.064	-0.257	1.452	3.672	0.662	0.843

1-Butanol [13]	-0.004	-0.285	0.768	3.705	0.879	0.800
Ethylene glycol [15]	-0.887	0.132	1.657	4.457	2.355	0.500

## Conclusion

The mathematical correlations derived in this study further document the applicability of the Abraham solvation parameter model to describe solute transfer between two condensed phases and solute transfer to a condensed phase from the vapor phase. The derived  $\log (GSR \text{ or } K)$  and  $\log (SR \text{ or } P)$  expressions for solutes dissolved in anhydrous 2-ethoxyethanol should provide reasonably accurate solubility ratio, GSR and SR, and partition coefficient predictions for additional organic solutes that fall in the area of predictive chemical space defined by hydrogen gas and the various organic solutes given in Table 3. Solutes used in deriving the two Abraham model correlations cover a wide range of chemical diversity as evidenced by the different functional groups present on the molecules, and the range of numerical values encompassed by the solute descriptors.

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