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Correlation of Solute Transfer Into Toluene and Ethylbenzene from Water and from the Gas Phase Based on the Abraham Model

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Abstract: Experimental data have been compiled from the published literature on the partition coefficients of solutes and vapors into ethylbenzene and toluene at 298 K. The logarithms of the water-to-ethylbenzene and water-to-toluene partition coefficients, log *P*, and gas-to-ethylbenzene and gas-to-toluene partition coefficients, log *K*, were correlated with the Abraham solvation parameter model. The derived mathematical expressions described the observed log *P* and log *K* data for the two aromatic hydrocarbon solvents to within average deviations of 0.13 log units or less.

Keywords: Partition coefficients, infinite dilution activity coefficients, toluene, ethylbenzene, Abraham model correlations.

INTRODUCTION

Extraction provides a convenient experimental method for removing phenolic compounds, flavonoids and anthocyanidins from medicinal plants, for pre-concentrating trace chemical pollutants from environmental samples prior to chemical analysis, and for isolating active pharmaceutical ingredients and metabolites from tissue samples. Extraction methods are based on the equilibrium solute partitioning in a biphasic system containing both a liquid and condensed phase, or in the case of liquid-liquid extraction containing two or more liquid solvents having limited mutual solubility. Molecular interactions between the dissolved solute(s) and surrounding extraction solvents determine the solute's affinity for a given phase, which in turn affects both the solute recovery factor and chemical separation efficiency. Design of an effective extraction method requires complete (or nearly complete) solute recovery and large separation efficiency. Considerable effort has been given in recent years to developing solution models to enable researchers to select the best extraction solvent to achieve a desired chemical separation.

Our efforts in this regard have been directed towards deriving Abraham model correlations for predicting the logarithms of the gas-to-organic solvent partition coefficients (log *K*), logarithms of the water-to-organic solvent partition coefficients (log *P*), and logarithms of molar solubility ratios (log $C_{solute,organic}/C_{solute,water}$ and $C_{solute,organic}/C_{solute,gas}$) defined as the solute's molar solubility in the given organic solvent ($C_{solute,organic}$) divided by the solute's molar solubility in water ($C_{solute,water}$) or solute's molar solubility in the vapor phase ($C_{solute,gas}$). The latter quantity is calculable from the equilibrium vapor pressure of the solute above its pure condensed phase. To date we and other research groups have determined Abraham model correlations for more than 70 common organic solvents [1-8], as well as the partition coefficient data for solutes dissolved in 30 room temperature ionic liquids [9-15] and in human and cow milk [16], for solutes adsorbed onto (partitioned into) polydimethylsiloxane [17, 18], polyoxymethylene [19] and polyacrylate fibers [20], and for solutes in two 1,2-dichloroethane/polar organic solvent [21,22], in ten alkane/polar organic solvent [21, 23-29], and in four diisopentyl ether/polar organic solvent [21-23, 29] biphasic partitioning systems. The latter biphasic organic systems are needed for compounds that are not stable in an aqueous environment, or are too insoluble in water to enable an accurate measurement of the water-to-organic solvent partition coefficient which might used in calculating solute descriptors for future log *P* predictions.

The Abraham solvation parameter model depends on two linear free energy relationships, the first for transfer processes between two condensed phases [2, 4-8, 30, 31]:

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

and the second process involving solute transfer from the gas phase:

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

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The dependent variables in eqns. 1 and 2 are the logarithm of partition coefficients and solubility ratios for a series of solutes in a given solvent or biphasic partition system. The upper case letters denote the solute properties as follows: **E** corresponds the solute excess molar refraction descriptor in $cm^3\ mol^{-1}/10$, **S** is to the solute dipolarity/ polarizability descriptor, **A** and **B** represent the overall solute hydrogen bond acidity and overall solute hydrogen bond basicity descriptors, respectively, **V** is McGowan's characteristic molecular volume in $cm^3\ mol^{-1}/100$ and **L** refers to the logarithm of the gas-to-hexadecane partition coefficient measured at 298 K. The lower case regression coefficients and constants (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) in Eqns. 1 and 2 are computed through a multiple linear regression analysis of experimental partition coefficient data for a specific biphasic system. Once the equation coefficients have been determined for a given biphasic partition system, further values of log *P*, log *K*, log $C_{solute,organic}/C_{solute,water}$ and log $C_{solute,organic}/C_{solute,air}$ can be estimated with known values for the solute descriptors. Numerical values of the solute descriptors are available for several thousand neutral organic and organometallic compounds [2, 4, 5, 30, 32, 33]. The list of available solute descriptors continues to grow as values for more complex molecules are added. Solute descriptors have also been computed for a select ions and ionic species [34-38] and for a few ion pairs [39].

We continue to publish Abraham model expressions for additional organic and ionic liquid solvents, and to revise several of our older, existing correlation equations that were based on experimental partition coefficient databases that included small numbers of solute molecules. It is important to periodically update our published log *P* and log *K* equations to take into account new experimental data. As noted in several previous papers [6, 8, 40] our published log *P* and log *K* Abraham model correlations should give reasonably accurate predictions, provided that the compound's five solute descriptors fall within the predictive area of chemical space covered by the derived Abraham model equation. The predictive area is determined by the maximum and minimum numerical values of each of the five solute descriptors in the Abraham model correlation.

In the present communication we report Abraham model correlations for the partitioning of solutes into ethylbenzene both from the gas phase (log *K* data) and from water (log *P* data). As part of the present study we have updated the log *P* and log *K* correlations that we had previously reported for toluene [41]:

$$\log P = 0.143 + 0.527\ \mathbf{E} - 0.720\ \mathbf{S} - 3.010\ \mathbf{A} - 4.824\ \mathbf{B} + 4.545\ \mathbf{V} \qquad (3)$$

$(N = 151.\ SD = 0.130,\ R^2 = 0.9968,\ F = 4566)$

$$\log K = 0.121 - 0.222\ \mathbf{E} + 0.938\ \mathbf{S} + 0.467\ \mathbf{A} + 0.099\ \mathbf{B} + 1.012\ \mathbf{L} \qquad (4)$$

$(N = 121,\ SD = 0.111,\ R^2 = 0.9988,\ F = 9968)$

Statistical information includes: the number of solutes, N, the correlation coefficient, R, the standard deviation, SD, and the Fisher F-statistic, F. The databases used in constructing eqns. 3 and 4 were never published, and it is not possible to ascertain the predictive area of chemical space over which each expression is valid. The updated Abraham model log *P* and log *K* correlations presented here for toluene are based on 204 log *P* (SD = 0.124) and 194 log *K* (SD = 0.120) data points. Each correlation has been validated on a training set and verified with test set analyses.

DATA SETS AND COMPUTATION METHODOLOGY

Through a search of the published chemical and engineering literature [42-85] we were able to gather Raoult's law infinite dilution activity coefficient, γ_{solute}^{∞}, Henry's law constants (solute concentrations are in mole fraction), K_{Henry}, or solubilities for nonelectrolye organic solutes and gases dissolved in ethylbenzene and toluene. In order to apply the Abraham model, the γ_{solute}^{∞} and K_{Henry} data were converted to gas-to-organic solvent partition coefficients (*K* values) through standard thermodynamic expressions, Eqns. 5 and 6, as described in several of our earlier publications [2, 4-8]:

$$K = \left(\frac{RT}{\gamma_{solute}^{\infty} P_{solute}^{o} V_{solvent}}\right) \qquad (5)$$

$$K = \left(\frac{RT}{K_{Henry}\ V_{solvent}}\right) \qquad (6)$$

or to water-to-organic solvent (or log *P*) values for partition from water to solvent through Eqn. 7, where K_w is the solute's gas-to-water partition coefficient.

$$P = K \times (1/K_w) \quad \text{or} \quad \log P = \log K - \log K_w \qquad (7)$$

The numerical constants, solute and solvent properties in Eqns. 5 and 6 are defined as follows: R is the universal gas constant, T is the system temperature, P_{solute}^{o} is the vapor pressure of the solute at the temperature of the activity coefficient and/or Henry constant measurement, *T*, and $V_{solvent}$ is the molar volume of the solvent. The calculation of log *P* from gas-to-organic solvent partition coefficient data requires knowledge of the solute's gas phase partition coefficient into water, K_w, which is available for most of the solutes being studied.

Our experimental databases also contain solubility data for several polycyclic aromatic hydrocarbons, several carboxylic acids and other miscellaneous crystalline solutes in both ethylbenzene and toluene [86-113]. The independent variable in the case of crystalline organic solutes is the molar solubility ratio, which is defined as the solute's molar solubility in the organic solvent under consideration divided by the solute's aqueous molar solubility (i.e., $C_{solute,organic}/C_{solute,water}$) as discussed above. Molar solubilities can also be used in the log *K* correlation, provided that the equilibrium vapor pressure of the solute above crystalline solute, P_{solute}^{o}, at 298 K is also available. P_{solute}^{o} can be transformed into the gas phase concentration, $C_{solute,gas}$, and the $C_{solute,organic}/C_{solute,air}$ obtained through the following equation

$$C_{solute,organic}/C_{solute,air} = (C_{solute,organic}/C_{solute,water}) \times K_w \quad (8)$$

where $K_w = C_{solute,water}/C_{solute,air}$. The vapor pressure, log K_w and aqueous solubility data needed for these calculations are reported in our previous publications.

Several published papers reported experimental partition coefficient data for substituted phenols [114-122], substituted benzenediols [123], substituted anilines [124, 125] and a few miscellaneous organic compounds [126-139]. These latter values pertain to practical partitioning studies where the aqueous and ethylbenzene (or toluene) phases were in direct contact with each other. Our previous studies [7, 8] have shown that the practical partition coefficients, log *P* values, are nearly identical to calculated solubility ratios, $C_{solute,organic}/C_{solute,water}$, whenever the organic solvent and water are "completely" immiscible or "near completely immiscible" with each other. Given the small mole fraction solubilities of water in ethylbenzene ($x_{water} = 2.60 \times 10^{-3}$ [140]) and toluene ($x_{water} = 2.80 \times 10^{-3}$ [140]), and the small mole fraction solubilities of both aromatic hydrocarbon solvents in water ($x_{ethylbenzene} = 3.18 \times 10^{-5}$ [140] and $x_{toluene} = 1.12 \times 10^{-4}$ [140]), we elected to combine the "dry" and "wet" data sets. Water and the two aromatic hydrocarbon solvents are "almost" completely immiscible with each other at 298 K. The experimental log *K* and log *P* values at 298 K for ethylbenzene and toluene are listed in Tables **1** and **2**, respectively. Also included in the two tables are the literature references pertaining to the log *K* and log *P* data, and the numerical values of the solute descriptors for the different compounds considered in the present study. The tabulated values are from our solute descriptor database, and were obtained using various types of experimental data, including water-to-solvent partitions, gas-to-solvent partitions, molar solubilities and chromatographic retention data [9-11, 15, 16].

RESULTS AND DISCUSSION

We have listed in Table **1** experimental data for the partitioning for 77 solutes between the gas phase and ethylbenzene, and partitioning data for 78 solutes between water and ethylbenzene at 298 K. The solutes considered cover a reasonably wide range of polar and nonpolar compounds, molecular sizes and shapes, and descriptor values. The experimental partition coefficient data were analyzed in accordance with the Abraham solvation parameter model to give the following two mathematical expressions:

$$\log P = 0.093(0.053) + 0.467(0.060)\,\mathbf{E} - 0.723(0.073)\,\mathbf{S} - 3.001(0.067)\,\mathbf{A} - 4.844(0.084)\,\mathbf{B} + 4.514(0.063)\,\mathbf{V} \quad (9)$$

(N = 78, SD = 0.137, R^2 = 0.995, F = 3114)

and

$$\log K = 0.059(0.043) - 0.295(0.071)\,\mathbf{E} + 0.924(0.078)\,\mathbf{S} + 0.537(0.071)\,\mathbf{A} + 0.098(0.088)\,\mathbf{B} + 1.010(0.019)\,\mathbf{L} \quad (10)$$

(N = 77, SD = 0.143, R^2 = 0.996, F = 3857)

All experimental data points were included in the regression analysis. Equation coefficients and statistical information were calculated using SPSS statistical software. The standard errors in the calculated coefficients are given in parenthesis after the respective equation coefficient. The statistics of both correlations are quite good as documented by the near unity values of the squared correlation coefficients and by the small standard deviations of SD = 0.137 and SD = 0.143 log units. The maximum deviation between the observed and predicted values was 0.40 log units for both the log *P* (for 2,2,4-trimethylpentane) and the log *K* (for 2-chlorophenol and pyrene) correlations. See Figs. (**1** and **2**) for a graphical depiction of the calculated log *P* and log *K* values based on Eqns. 9 and 10 against observed partition coefficient data. The experimental log *P* and log *K* values cover ranges of about 9.5 and 12.7 log units, respectively.

In order to assess the predictive ability of the two ethylbenzene correlation equations, Eqns. 9 and 10 we divided the observed data points into a training set and a test set by allowing the SPSS software to randomly select half of the experimental values. The selected data points became the training sets and the remaining half of the compounds served as the test sets. Analysis of the experimental data in the log *P* and log *K* training sets gave:

$$\log P = 0.039(0.075) + 0.492(0.100)\,\mathbf{E} - 0.747(0.124)\,\mathbf{S} - 2.954(0.127)\,\mathbf{A} - 4.816(0.160)\,\mathbf{B} + 4.557(0.086)\,\mathbf{V} \quad (11)$$

(N = 39, SD = 0.155, R^2 = 0.995, F = 3114)

and

$$\log K = 0.036(0.058) - 0.367(0.048)\,\mathbf{E} + 0.901(0.162)\,\mathbf{S} + 0.641(0.157)\,\mathbf{A} + 0.028(0.127)\,\mathbf{B} + 1.016(0.021)\,\mathbf{L} \quad (12)$$

(N = 39, SD = 0.140, R^2 = 0.997, F = 2048)

Careful examination of Eqns 9-12 reveals that there is very little difference in the equation coefficients for the full dataset and the training dataset correlations, thus showing that both training sets of compounds are representative samples of the total log *P* and log *K* data sets. The derived training set equations were then used to predict the respective partition coefficients for the compounds in the test sets. For the predicted and experimental values, we found SD = 0.122 (Eqn. 11) and SD = 0.145 (Eqn. 12), AAE (Average Absolute Error) = 0.093 (Eqn. 11) and AAE = 0.098 (Eqn. 12), and AE (Average Error) = –0.013 (Eqn. 11) and AE = 0.039 (Eqn. 12). There is therefore very little bias in using Eqns. 11 and 12 with AE equal to –0.013 and 0.039 log units. The training and test set analyses were performed five more times with similar results.

The toluene database considered in the present study contains 204 experimental log *P* values and 194 experimental log *K* data points. Analysis of the experimental partition

Table 1. Experimental log *P* and log *K* Data for Solutes Dissolved in Ethylbenzene at 298 K

Solute	E	S	A	B	L	V	Log K_{obs}	Log P_{obs}	Ref.
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-1.187	0.533	[53]
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.615	0.895	[52, 53]
Chlorine	0.360	0.320	0.100	0.000	1.193	0.3534	1.609	1.429	[50]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.336	0.416	[53]
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.185	2.625	[44]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.787	4.607	[48]
Heptane	0.000	0.000	0.000	0.000	3.130	1.0949	3.299	5.259	[48, 49]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.640	5.950	[48]
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	4.826	7.146	[48]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	3.006	3.906	[54]
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863	3.340	4.590	[49]
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358	3.190	5.310	[49]
Tetrachloromethane	0.458	0.380	0.000	0.000	2.823	0.7391	3.105	3.295	[49, 51]
1-Chlorohexane	0.201	0.390	0.000	0.090	3.708	1.0764	4.229	4.229	[55]
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	3.054	0.504	[58]
1,4 Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	3.452	-0.259	[58]
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	3.018	0.298	[59]
Methanol	0.278	0.440	0.430	0.470	0.970	0.3080	1.704	-2.036	[57]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	2.214	-1.456	[49]
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.701	-0.859	[57]
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	3.246	-0.214	[47, 49]
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.8718	3.800	0.450	[47]
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	2.763	-0.537	[46]
2-Methylpropan-2-ol	0.180	0.300	0.310	0.600	1.963	0.7309	2.564	-0.716	[45]
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	2.988	-0.402	[47]
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	3.011	0.8718	3.580	0.340	[47]
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	4.323	0.973	[131]
Heptan-1-ol	0.211	0.420	0.370	0.480	4.115	1.1536	5.033	1.803	[131]
2-Chloroethanol	0.419	0.770	0.390	0.500	2.435	0.5715	3.409	-1.325	[47]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.181	2.551	[49]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.724	3.074	[59]
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	4.197	3.617	unity
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	8.218	5.188	This work
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.741	3.981	[106, 107]
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.358	5.858	[86]
trans-Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	8.207	5.427	[109]

Table 1. contd….

Solute	**E**	**S**	**A**	**B**	**L**	**V**	**Log K_{obs}**	**Log P_{obs}**	**Ref.**
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	6.184	4.264	[111]
Iodine	1.398	0.670	0.280	0.000	3.681	0.6250	4.435	2.575	[87]
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	4.947	0.097	[122]
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	5.798	0.945	[114]
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	6.114	0.954	[114]
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	5.464	1.814	[114]
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	5.440	1.380	[124]
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	5.370	1.280	[124]
2-Nitroaniline	1.180	1.370	0.300	0.360	5.627	0.9904	7.001	1.591	[125]
4-Nitroaniline	1.220	1.920	0.460	0.350	6.042	0.9904	7.925	0.745	[125]
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	6.000	-2.350	[123]
1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	6.541	-0.889	[123]
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	5.730	1.230	[122]
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	11.499	0.949	[133]
2,4-Dimethylphenol	0.843	0.790	0.520	0.400	4.770	1.0569	5.531	1.121	[121]
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	5.660	1.320	[116]
3,4-Dimethylphenol	0.830	0.900	0.550	0.380	4.980	1.0569	5.910	1.140	[121]
3,5-Dimethylphenol	0.830	0.860	0.550	0.370	4.856	1.0569	5.841	1.241	[121]
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	5.548	2.188	[117]
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	7.264	0.204	[117]
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	7.623	-0.187	[117]
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	4.206	0.326	[115]
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.652	1.312	[122]
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	5.271	1.561	[115]
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5451	3.060	0.240	[43, 51]
Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	3.014	-0.096	[56]
Ethylamine	0.236	0.350	0.160	0.610	1.677	0.4902	1.902	-1.398	[134]
Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	2.521	-0.699	[134]
Butylamine (wet)	0.224	0.350	0.160	0.610	2.618	0.7720	2.943	-0.167	[134]
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7720	2.843	-0.147	[51]
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	4.092	3.272	[42, 51]
Monuron	1.140	1.500	0.470	0.780	7.180	1.4768	8.379	0.749	[104]
Diuron	1.280	1.600	0.570	0.700	8.060	1.5992	9.507	1.537	[105]
2,4-Dinitrophenol	1.200	1.490	0.090	0.560	5.981	1.1235	7.386	1.806	[118]
1-Naphthol	1.520	1.100	0.660	0.340	6.284	1.1441	7.592	1.722	[129]
2-Naphthol	1.520	1.080	0.610	0.400	6.200	1.1441	7.497	1.547	[129]

Table 1. contd….

Solute	E	S	A	B	L	V	Log K_{obs}	Log P_{obs}	Ref.
2,4-Dinitro-6-aminophenol	1.750	1.850	0.210	0.800	7.466	1.2233	9.201	0.851	[135]
2-Amino-6-chloro-4-nitrophenol	1.370	1.210	0.570	0.700	6.264	1.1715	7.519	0.079	[135]
Acetylacetone	0.412	0.780	0.000	0.630	3.326	0.8445	4.173	0.633	[136]
2-Furaldehyde	0.690	1.130	0.000	0.450	3.318	0.6962	4.292	0.462	[132]
5-Methylfurfural	0.744	1.110	0.000	0.520	3.933	0.8339	4.944	0.914	[132]
2-Iodophenol	1.360	1.000	0.400	0.350	4.964	1.0333		1.772	[115]

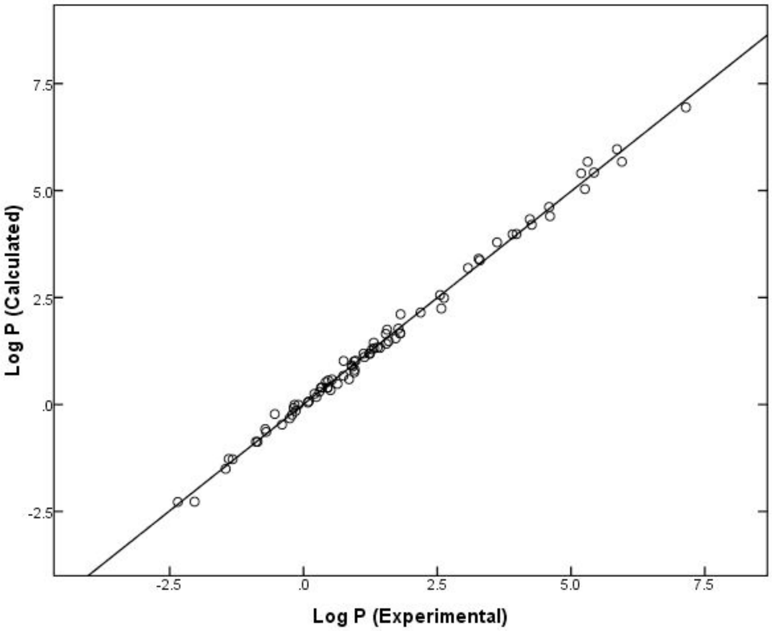

Fig. (1). Comparison of observed log *P* data for solutes dissolved in ethylbenzene and predicted values based on Eqn. 9.

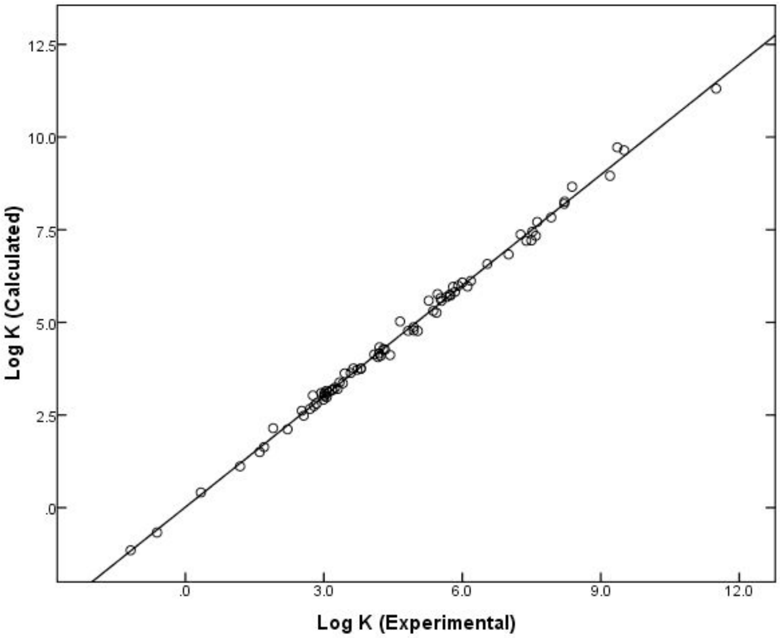

Fig. (2). Comparison of observed log *K* data for solutes dissolved in ethylbenzene and predicted values based on Eqn. 10.

Table 2. Experimental log *P* and log *K* Data for Solutes Dissolved in Toluene at 298 K

Solute	E	S	A	B	L	V	Log K_{obs}	Log P_{obs}	Ref.
Helium	0.000	0.000	0.000	0.000	-1.741	0.0680	-1.650	0.370	[60]
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.492	0.468	[60]
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.603	0.867	[60]
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-0.111	1.099	[60]
Xenon	0.000	0.000	0.000	0.000	0.378	0.3290	0.530	1.500	[65]
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-1.162	0.558	[53]
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.686	0.824	[63]
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.2222	-0.881	0.919	[63]
Nitric oxide	0.370	0.020	0.000	0.090	-0.590	0.2026	-0.595	0.735	[76]
Carbon monoxide	0.000	0.000	0.000	0.040	-0.836	0.2220	-0.740	0.880	[63]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.370	0.450	[63]
Chlorine	0.360	0.320	0.100	0.000	1.193	0.3534	1.669	1.489	[50]
Bromine	0.918	0.500	0.230	0.000	2.326	0.4586		1.630	[131]
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.259	1.201	[63]
Ethane	0.000	0.000	0.000	0.000	0.492	0.3904	0.551	1.891	[66]
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.177	2.617	[62]
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.744	3.264	[62]
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.550	3.250	[62]
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	2.305	4.005	[61]
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.821	4.641	[61]
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540	2.653	4.493	[61]
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	3.335	5.295	[61]
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949	2.964	5.044	[61]
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.853	5.963	[61]
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.2358	3.476	5.496	[61]
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358	3.540	5.420	[61]
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	4.346	6.496	[61]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	3.056	3.956	[61]
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272	3.918	5.498	[61]
Ethene	0.107	0.100	0.000	0.070	0.289	0.3474	0.503	1.443	[66]
Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.208	2.178	[62]
1-Butene	0.100	0.080	0.000	0.070	1.529	0.6292	1.765	2.775	[62]
cis 2-Butene	0.140	0.080	0.000	0.050	1.737	0.6292	1.925	2.915	[62]
trans-2-Butene	0.126	0.080	0.000	0.050	1.664	0.6292	1.871	2.851	[62]
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.7700	2.277	3.507	[68]
Hex-1-ene	0.080	0.080	0.000	0.070	2.572	0.9110	2.843	4.003	[69]
Isobutene (2-Methylpropene)	0.120	0.080	0.000	0.080	1.579	0.6292	1.752	2.612	[62]

Table 2. contd….

Solute	**E**	**S**	**A**	**B**	**L**	**V**	**Log K_{obs}**	**Log P_{obs}**	**Ref.**
Isopentene (3-methyl-1-butene)	0.063	0.060	0.000	0.050	1.933	0.7701	2.149	3.489	[68]
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	1.868	2.318	[62]
2-Methylbuta-1,3-diene	0.313	0.230	0.000	0.100	2.101	0.7271	2.429	2.929	[68]
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.799	1.491	[63]
Dichloromethane	0.387	0.570	0.100	0.050	2.019	0.4940	2.670	1.710	[68]
Trichloromethane	0.430	0.490	0.150	0.020	2.480	0.6167	3.122	2.332	[68]
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.7391	3.173	3.363	[68]
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	2.178	1.718	[62]
1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.6537	2.682	2.422	[68]
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946	3.187	3.067	[70]
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	2.689	3.489	[68]
1-Chlorohexane	0.201	0.390	0.000	0.090	3.708	1.0764	4.306	4.306	[55]
Bromoethane	0.370	0.400	0.000	0.120	2.120	0.5654	2.575	2.035	[68]
Iodomethane	0.676	0.430	0.000	0.120	2.106	0.5077	2.573	1.923	[68]
Iodoethane	0.640	0.400	0.000	0.150	2.573	0.6486	3.086	2.546	[68]
1,1-Difluoroethane	-0.250	0.470	0.040	0.070	0.570	0.4258	1.282	1.202	[62]
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	1.586	0.186	[62]
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7310	2.440	1.150	[71]
Di-isopropyl ether	-0.060	0.160	0.000	0.580	2.530	1.0127	2.920	1.870	[71]
Di-n-butyl ether	0.000	0.250	0.000	0.450	3.924	1.2945	4.368	3.678	[82]
Methyl t-butyl ether	0.024	0.220	0.000	0.590	2.380	0.8718	2.690	1.100	[71]
Ethyl t-butyl ether	-0.020	0.180	0.000	0.590	2.699	1.0127	3.010	1.740	[71]
Methyl t-pentyl ether	0.050	0.210	0.000	0.600	2.916	1.0127	3.300	1.705	[71]
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223	3.218	0.668	[72]
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	3.611	-0.099	[73]
Butanal	0.187	0.650	0.000	0.450	2.270	0.6879	2.935	0.605	[81]
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	2.581	-0.249	[68]
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	3.147	0.427	[73]
Pentan-2-one	0.143	0.680	0.000	0.510	2.755	0.8288	3.679	1.099	[67]
Hexan-2-one	0.136	0.680	0.000	0.510	3.286	0.9697	4.105	1.695	[67]
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.1106	4.618	2.368	[67]
3,3-Dimethylbutan-2-one	0.106	0.620	0.000	0.510	2.928	0.9697	3.665	1.385	[67]
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057	2.660	0.360	[65]
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	3.164	1.004	[68]
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.8875	3.665	1.615	[67]
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.0284	4.083	2.143	[67]
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.1693	4.698	2.858	[67]

Table 2. contd….

Solute	E	S	A	B	L	V	Log K_{obs}	Log P_{obs}	Ref.
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7466	3.386	1.236	[67]
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.0284	4.141	2.261	[67]
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.1693	4.676	2.846	[67]
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	2.679	-0.171	[68]
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450	3.144	0.324	[68]
Methylamine	0.250	0.350	0.160	0.580	1.300	0.3493	1.942	-1.398	[67]
n-Propylamine	0.225	0.350	0.160	0.610	2.141	0.6311	2.580	-0.640	[65]
n-Butylamine	0.224	0.350	0.160	0.610	2.618	0.7720	3.247	0.137	[67]
Dimethylamine	0.189	0.300	0.080	0.660	1.600	0.4902	1.964	-1.186	[67]
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.7720	2.749	-0.241	[67]
Dipropylamine	0.124	0.300	0.080	0.690	3.351	1.0538	3.841	1.161	[67]
Trimethylamine	0.140	0.200	0.000	0.670	1.620	0.6311	1.986	-0.364	[67]
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	3.450	1.090	[65]
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	3.096	0.146	[73]
Nitroethane	0.270	0.950	0.020	0.330	2.414	0.5646	3.388	0.668	[75]
Nitropropane	0.242	0.950	0.000	0.310	2.894	0.7055	3.848	1.398	[67]
Water	0.000	0.450	0.820	0.350	0.260	0.1673	1.239	-3.401	[67]
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082	1.776	-1.964	[68]
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	2.202	-1.468	[68]
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.746	-0.814	[79]
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	3.326	-0.134	[47]
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	3.077	-0.313	[47]
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	3.086	-0.214	[47]
2-Methylpropan-2-ol	0.180	0.300	0.310	0.600	1.963	0.7309	2.739	-0.541	[80]
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	3.860	0.510	[65]
3-Methylbutan-1-ol	0.192	0.390	0.370	0.480	3.011	0.8718	3.667	0.427	[47]
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	4.520	1.290	[65]
Heptan-1-ol	0.211	0.420	0.370	0.480	4.115	1.1536	4.947	1.870	[67]
2-Chloroethanol	0.419	0.770	0.390	0.500	2.435	0.5715	3.420	-1.180	[47]
Carbon disulfide	0.876	0.260	0.000	0.030	2.370	0.4905	2.590	2.740	[68]
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	-0.109	2.111	[83]
Tetramethyltin	0.324	0.110	0.000	0.100	2.651	1.0431	2.764	4.294	[77]
Mercury	0.850	0.430	0.000	0.040	1.721	0.3400	2.070	1.610	[64]
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.268	2.638	[68]
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.786	3.136	Unity
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982	4.233	3.653	[78]
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.9982	4.485	3.825	[78]

Table 2. contd….

Solute	**E**	**S**	**A**	**B**	**L**	**V**	**Log K_{obs}**	**Log P_{obs}**	**Ref.**
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	4.347	3.757	[78]
trans-Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	8.327	5.540	[109]
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.3242	6.770	4.820	[107]
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.760	4.030	[106, 107]
Fluoranthene	2.377	1.550	0.000	0.240	8.827	1.5850	9.380	5.930	[86]
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	8.297	5.267	[110]
Phenanthrene	2.055	1.290	0.000	0.290	7.632	1.4544	8.272	5.472	[110]
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.436	5.936	[86]
Fluorene	1.588	1.060	0.000	0.240	6.922	1.3565	7.513	5.063	[113]
1,4-Dibromobenzene	1.150	0.860	0.000	0.040	5.324	1.0660	5.856	4.416	[112]
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753	3.730	0.290	[65]
9-Fluorenone	1.600	1.490	0.000	0.350	7.474	1.3722	8.513	4.313	[89, 95]
1-Nitronaphthalene	1.600	1.590	0.000	0.290	7.056	1.2600	8.284	4.088	[88]
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.6512	10.713	4.679	[94]
Benzil	1.445	1.590	0.000	0.620	7.611	1.6374	8.970	4.150	[90]
p-Chloro-1-phenyl-3,3-dimethylurea	1.140	1.500	0.470	0.780	7.180	1.4768	8.610	0.970	[104]
2,4-Dichloro-1-phenyl-3,3-dimethylurea	1.280	1.600	0.570	0.700	8.060	1.5992	9.550	1.660	[91, 105]
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	6.272	4.352	[111]
4-Nitropyridine N-oxide	0.934	1.920	0.210	0.760	5.271	0.9082	7.518	-0.602	[93]
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	5.011	0.160	[119]
2-Methylphenol	0.840	0.860	0.520	0.300	4.218	0.9160	5.446	1.136	[67]
m-Cresol	0.822	0.880	0.570	0.340	4.310	0.9160	5.385	0.786	[120]
p-Cresol	0.820	0.870	0.570	0.310	4.312	0.9160	5.372	0.872	[120]
2,4-Dimethylphenol	0.843	0.790	0.520	0.400	4.770	1.0569	5.665	1.255	[121]
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	5.771	1.431	[121]
3,4-Dimethylphenol	0.830	0.900	0.550	0.380	4.980	1.0569	5.998	1.228	[121]
3,5-Dimethylphenol	0.830	0.860	0.550	0.370	4.856	1.0569	5.892	1.292	[121]
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	5.779	1.279	[122]
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	4.336	0.456	[115]
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.709	1.369	[114]
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	5.899	1.049	[114]
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	6.239	1.079	[114]
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	5.523	1.873	[114]
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	5.323	1.613	[115]
2-Methoxyphenol	0.837	0.910	0.220	0.520	4.449	0.9747	5.350	1.260	[65]
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	5.620	2.260	[117]
3-Nitrophenol	1.050	1.570	0.790	0.230	5.692	0.9493	7.402	0.342	[117]

Table 2. contd….

Solute	E	S	A	B	L	V	Log K_{obs}	Log P_{obs}	Ref.
4-Nitrophenol	1.070	1.720	0.820	0.260	5.876	0.9493	7.750	-0.060	[117]
2,4-Dinitrophenol	1.200	1.490	0.090	0.560	5.981	1.1235	7.520	1.940	[118]
1-Naphthol	1.520	1.100	0.660	0.340	6.284	1.1441	7.667	1.797	[129]
2-Naphthol	1.520	1.080	0.610	0.400	6.200	1.1441	7.635	1.685	[129]
2-Nitroaniline	1.180	1.370	0.300	0.360	5.627	0.9904	7.061	1.651	[125]
4-Nitroaniline	1.220	1.920	0.460	0.350	6.042	0.9904	7.993	0.813	[125]
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	6.180	-2.170	[65]
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162	4.970	0.890	[65]
1-Naphthylamine	1.670	1.260	0.200	0.570	6.490	1.1852	7.662	2.322	[126]
2-Naphthylamine	1.670	1.280	0.220	0.550	6.540	1.1852	7.802	2.332	[126]
Benzonitrile	0.742	1.110	0.000	0.330	4.039	0.8711	5.283	2.193	[85]
Catechol	0.970	1.100	0.880	0.470	4.450	0.8338	5.940	-1.260	[123]
Hydroquinone	1.063	1.270	1.060	0.570	4.827	0.8338	6.721	-2.149	[123]
1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	6.685	-0.745	[123]
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.291	4.223	[92]
Acetone oxime	0.390	0.660	0.370	0.560	2.557	0.6499	3.504	-0.960	[74]
Cyclohexanone oxime	0.580	0.900	0.330	0.610	4.432	0.9609	5.423	0.308	[74]
Benzoylacetone	0.766	0.990	0.010	0.580	5.647	1.3114	6.604	2.914	[136]
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	5.540	1.480	[124]
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	5.420	1.330	[124]
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	11.626	1.076	[133]
2-Furaldehyde	0.690	1.130	0.000	0.450	3.318	0.6962	4.443	0.613	[132]
5-Methylfurfural	0.744	1.110	0.000	0.520	3.933	0.8339	5.008	0.978	[132]
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	8.250	-1.150	[127]
16-Crown-5	0.410	1.170	0.000	1.760	7.276	1.8434	8.580	-0.600	[127]
Benzo 15-Crown-5	1.055	1.940	0.000	1.590	9.403	2.0285	11.470	0.920	[127]
18-Crown-6	0.410	1.470	0.000	2.100	8.228	2.0430	9.840	-1.590	[127]
Dibenzo-18-Crown-6	1.690	2.730	0.000	1.780	13.384	2.6950	16.150	2.770	[127]
Dibenzo-24-Crown-8	1.680	3.400	0.000	2.340	16.414	3.3760	20.310	2.930	[127]
AC-Benzo-18-Crown-6^{a}	0.684	2.650	0.000	1.850	11.100	2.4776	14.357	1.307	[128]
3-Chlorobenzoic acid	0.840	0.950	0.630	0.320	5.197	1.0541	6.270	1.120	[96]
4-Chlorobenzoic acid	0.840	1.020	0.630	0.270	4.947	1.0540	5.960	1.260	[102]
3-Nitrobenzoic acid	0.990	1.130	0.730	0.530	5.535	1.1059	7.020	0.138	[98]
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.1059	7.405	0.620	[99]
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.0726	5.530	1.230	[100]
2-Methyoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.1313	7.250	0.398	[97]
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.1313	7.240	0.484	[97]

Table 2. contd….

Solute	**E**	**S**	**A**	**B**	**L**	**V**	**Log K_{obs}**	**Log P_{obs}**	**Ref.**
Ibuprofen	0.730	0.695	0.565	0.790	7.184	1.7771	8.184	2.848	[108]
2-Hydroxybenzoic acid	0.900	0.850	0.730	0.370	4.732	0.9904	5.739	0.389	[139]
4-Methylbenzoic acid	0.730	0.930	0.620	0.420	4.890	1.0726	5.954	0.654	[138]
8-Hydroxyquinoline	1.450	1.020	0.060	0.560	5.812	1.1030	6.770	2.250	[137]
Dehydrodivanillin	2.320	2.170	0.800	1.290	12.000	2.1540	14.390	1.040	[3]
Diapocynin	2.000	2.430	0.320	1.770	12.700	2.4358	15.240	1.160	[3]
Apocyanin	1.000	1.480	0.370	0.750	6.329	1.2722	7.940	0.630	[3]
Pentanoic acid	0.205	0.600	0.600	0.450	3.227	0.8875	4.320	-0.200	[65]
Chlorotrifluoromethane	-0.250	-0.050	0.000	0.000	0.209	0.4250	0.303	1.953	[84]
Dichlorodifluoromethane	0.037	0.040	0.000	0.040	0.998	0.5297	1.014	2.154	[84]
Vanilllin	0.990	1.300	0.310	0.680	5.727	1.1313		0.700	[3]
Thalidomide	1.920	2.810	0.360	1.190		1.7479		0.319	[101]
N-Methylthalidomide	1.982	2.430	0.000	1.280		1.8888		1.978	[101]
N-Propylthalidomide	1.894	2.450	0.000	1.280		2.1706		3.076	[101]
N-Pentylpthalidomide	1.868	2.440	0.000	1.260		2.4524		4.600	[101]
Sudan I (Z-form)	1.945	1.350	0.060	0.320		1.9085		7.220	[103]
Sudan I (Q-form)	1.945	1.360	0.020	0.500		1.9085		6.370	[103]
Nicotine	0.865	0.750	0.000	1.140		1.3710		0.860	[65]
Phenylacetic acid	0.730	0.970	0.600	0.610		1.0700		0.090	[65]

[a] 1,2-*bis*[2-(2-methoxyethoxy)ethoxy]benzene.

coefficient values tabulated in Table **2** yielded the following two Abraham model expressions:

$$\log P = 0.125(0.021) + 0.431(0.030)\,\mathbf{E} - 0.644(0.036)\,\mathbf{S} - 3.002(0.036)\,\mathbf{A} - 4.748(0.041)\,\mathbf{B} + 4.524(0.033)\,\mathbf{V} \qquad (13)$$

$$(N = 204,\ SD = 0.124,\ R^2 = 0.996,\ F = 8965)$$

and

$$\log K = 0.085(0.015) - 0.400(0.034)\,\mathbf{E} + 1.063(0.039)\,\mathbf{S} + 0.501(0.035)\,\mathbf{A} + 0.154(0.041)\,\mathbf{B} + 1.011(0.009)\,\mathbf{L} \qquad (14)$$

$$(N = 194,\ SD = 0.120,\ R^2 = 0.999,\ F = 27911)$$

Both correlations provide a reasonably accurate mathematical description of the experimental partition coefficient data as graphically shown in Figs. (**3** and **4**) for datasets that span ranges of 10.6 log units (log *P*) and 22.0 log units (log *K*), respectively. The maximum deviation between the observed and predicted values was 0.35 log units for the log *P* (for 3,3-dimethylbutan-2-one) and 0.41 log units for the log *K* (for 2-chlorophenol and fluoranthene) correlations. As noted in the introduction, Abraham model log *P* and log *K* correlations were derived previously for toluene. The earlier correlations were based on much smaller data sets. In the log *K* data set, we were able to increase the number of experimental values by more than 50 %, from N = 121 (Eqn. 4) to N = 194 (Eqn. 14).

Equations 13 and 14 were validated as before by allowing the SPSS software to randomly divide the total data points into training and test sets as before. Analyses of the experimental data in the two training sets yielded:

$$\log P = 0.093(0.027) + 0.408(0.039)\,\mathbf{E} - 0.652(0.047)\,\mathbf{S} - 2.981(0.048)\,\mathbf{A} - 4.789(0.054)\,\mathbf{B} + 4.596(0.042)\,\mathbf{V} \qquad (15)$$

$$(N = 102,\ SD = 0.113,\ R^2 = 0.997,\ F = 5762)$$

and

$$\log K = 0.084(0.020) - 0.427(0.054)\,\mathbf{E} + 1.104(0.064)\,\mathbf{S} + 0.450(0.057)\,\mathbf{A} + 0.174(0.062)\,\mathbf{B} + 1.005(0.012)\,\mathbf{L} \qquad (16)$$

$$(N = 97,\ SD = 0.118,\ R^2 = 0.999,\ F = 13844)$$

Careful examination of Eqns. 13 versus 15, and Eqns. 14 versus 16 reveals that there is very little difference in the equation coefficients for the full dataset and the training

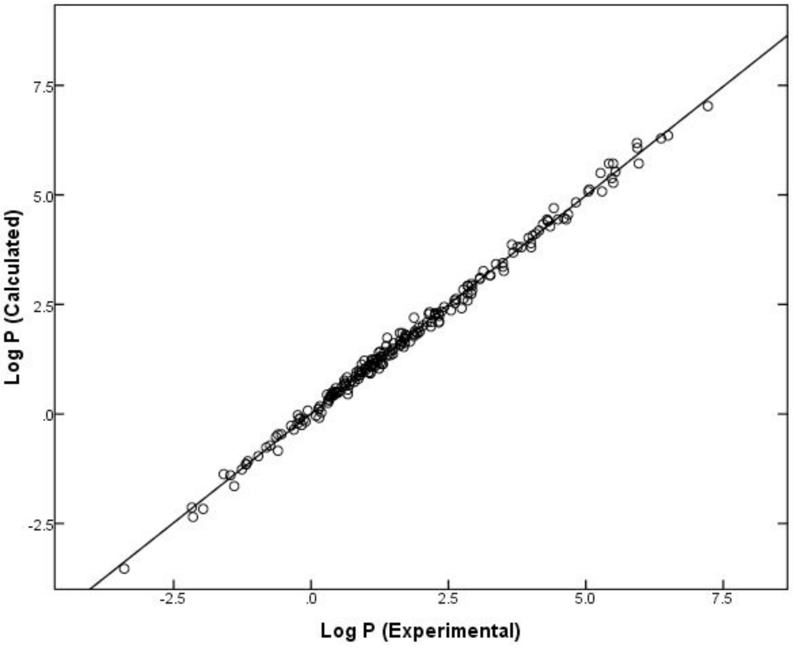

Fig. (3). Comparison of observed log *P* data for solutes dissolved in toluene and predicted values based on Eqn. 13.

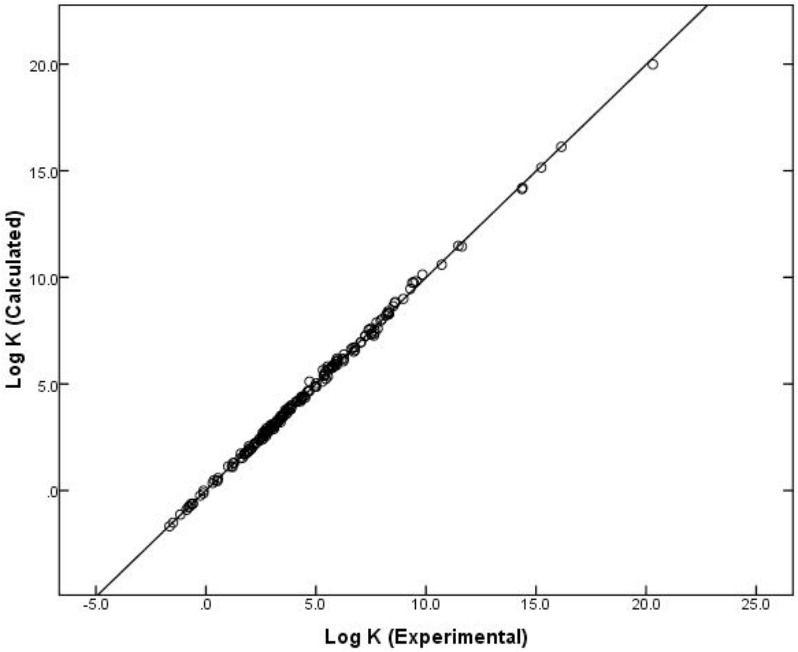

Fig. (4). Comparison of observed log *K* data for solutes dissolved in toluene and predicted values based on Eqn. 14.

dataset correlations. Both training sets of compounds are representative samples of the total log *P* and log *K* data sets. The derived training set equations were then utilized to estimate the respective partition coefficients for the compounds in the test sets. For the estimated and experimental values, we found SD = 0.138 (Eqn. 15) and SD = 0.125 (Eqn. 16), AAE = 0.102 (Eqn. 15) and AAE = 0.092 (Eqn. 16), and AE = –0.008 (Eqn. 15) and AE = 0.025 (Eqn. 16). There is therefore very little bias in using Eqns. 15 and 16 with AE equal to –0.008 and 0.025 log units.

The present study documents that the correlations based on the Abraham solvation parameter model provide reasonably accurate mathematical descriptions of solute transfer at 298 K from both water and from the gas phase into both ethylbenzene and toluene. The derived correlations should provide reasonably accurate estimations of the water-to-ethylbenzene, water-to-toluene, gas-to-ethylbenzene and gas-to-toluene partition coefficients at 298 K for additional organic compounds and gases, provided that each of the compound’s solute descriptors falls within the range of predictive chemical space defined by the respective correlation equation. The estimated partition coefficients can be converted to infinite dilution activity coefficients, $\gamma_{\text{solute}}^{\infty}$, through the standard thermodynamic relationships given by Eqns. 5 – 7. Partition coefficients calculated using Eqns. 9, 10, 13 and 14 pertain to 298 K. Standard thermodynamic relationships enable the predicted log K and log P values to be extrapolated to other temperatures [141]. In this regard, Mintz *et al*. published enthalpy of solvation correlations, $\Delta H_{solvation}$, for organic gases and gaseous solutes into water [141] and toluene [142]. The published $\Delta H_{solvation}$ correlations allow one to extrapolate predicted water-to-toluene and gas-to-toluene partition coefficients based on Eqs. 13 and 14 to other temperatures not too far removed from 298 K.

CONFLICT OF INTEREST

None declared.

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NOMENCLATURE

English Symbols

a = Solvent coefficient in the Abraham model representing hydrogen-bond basicity of the solvent

A = Abraham model solute descriptor representing hydrogen-bond acidity

AAE = Absolute average error

AE = Absolute error

b = Solvent coefficient in the Abraham model representing hydrogen-bond acidity of the solvent

B = Abraham model solute descriptor representing hydrogen-bond basicity

c = Constant in the Abraham model correlation equation

C = Concentration of the solute expressed in units of moles per liter

e = Solvent equation coefficient in the Abraham model measuring the solvent's interaction with π- and nonbonding electrons on the solute

E = Abraham model solute descriptor describing excess molar refraction

F = Fisher F-statistic

K = Gas-to-liquid partition coefficient of the solute

K_{Henry} = Henry's constant of the solute in the given solvent

K_w = Gas-to-water partition coefficient of the solute

l = Solvent equation coefficient in the Abraham model describing dispersion forces

L = Abraham model solute descriptor defined as the logarithm of the solute's gas-to-hexadecane partition coefficient at 298 K

N = Number of experimental data points

P = Water-to-solvent partition coefficient

$P_{\text{solute}}^{\text{o}}$ = Vapor pressure of the solute at temperature of the activity coefficient measurement

R = Correlation coefficient for the derived correlation model, also used as the gas constant in Eqns. 5 and 6

s = Solvent equation coefficient in the Abraham model measuring dipolarity/polarizability of the solvent

S = Abraham model solute descriptor describing polarity/polarizability

SD = Standard deviation

T = Temperature

v = Solvent equation coefficient in the Abraham model

V = McGowan volume of the solute

V_{solvent} = Molar volume of the solvent

x = Mole fraction

Greek symbols

γ_{solute}^{∞} = Infinite dilution activity coefficient of solute

$\Delta H_{solvation}$ = Enthalpy of solvation of the solute in the given solvent

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