

ABRAHAM MODEL CORRELATIONS FOR SOLUTE PARTITIONING INTO *o*-XYLENE,
m-XYLENE AND *p*-XYLENE FROM BOTH WATER AND THE GAS PHASE

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Abstract

Experimental data have been compiled from the published literature on the partition coefficients of solutes and vapors into *o*-xylene, *m*-xylene and *p*-xylene at 298 K. The logarithms of the water-to-xylene partition coefficients, $\log P$, and gas-to-xylene 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 three xylene isomers to within average deviations of 0.14 log units or less.

Key words and phrases

Partition coefficients, xylene solvents, Abraham model correlations

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1. Introduction

Liquid-liquid extraction affords a convenient experimental means for separating synthesized organic materials from reaction solvent media, and for pre-concentrating chemicals in unknown liquid samples prior to quantitative analyses. Extraction methods are based on solute partitioning in a biphasic liquid system containing two or more solvents having limited mutual solubility. Molecular interactions between the dissolved solute(s) and surrounding extraction solvents determine the solute recovery factor and separation efficiency. Considerable attention has been given in recent years to developing methods for selecting the best biphasic partitioning system to achieve a desired chemical separation.

In many previous studies [1-8], we have shown that two general linear free energy Abraham model correlations, equations 1 and 2, can be used to mathematically describe the transfer of neutral solutes from water to organic solvents and from the gas phase to organic solvents

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

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

The dependent variables in eqns. 1 and 2 are the [logarithm of the water-to-organic solvent partition coefficient, \$\log P\$, and the logarithm of the gas-to-organic solvent partition coefficient, \$\log K\$, for a series of solutes](#). The independent variables, or solute descriptors, are properties of the neutral solutes as follows: [9,10] \mathbf{E} is the solute excess molar refraction in $\text{cm}^3 \text{mol}^{-1}/10$, \mathbf{S} is the solute dipolarity/polarizability, \mathbf{A} is the overall solute hydrogen bond acidity, \mathbf{B} is the overall solute hydrogen bond basicity, \mathbf{V} is McGowan's characteristic molecular volume in $\text{cm}^3 \text{mol}^{-1}/100$ and \mathbf{L} is the logarithm of the gas to hexadecane partition coefficient measured at 298 K. The 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) are obtained

by multiple linear regression analysis of experimental partition coefficient data for a specific biphasic system. In the case of processes involving two condensed solvent phases, the c_p , e_p , s_p , a_p , b_p and v_p coefficients represent differences in the solvent phase properties. For any fully characterized system/process (those with calculated values for the equation coefficients), further values of the water-to-organic solvent partition coefficient, P , and gas-to-organic solvent partition coefficient, K , can be estimated with known values for the solute descriptors.

To date we have reported equation coefficients describing more than 70 different organic solvents, including both “anhydrous” organic solvents and “wet” organic solvents that are saturated with water [1-8, 11-14]. The $\log P$ values for anhydrous solvents correspond to a hypothetical partitioning process involving solute transfer where the aqueous and organic phases are not in physical contact with each other. Partition coefficients for the hypothetical processes are calculated as a ratio of the solute’s measured molar solubility in the organic solvent divided by the solute’s molar solubility in water [15], or in the case of liquid and gaseous solutes, calculated using the solute’s measured infinite dilution activity coefficient, $\gamma_{\text{Solute}}^{\infty}$, and measured gas-to-water partition coefficient, K_w , in accordance to established thermodynamic principles [17].

Published studies [1, 12-14] have shown that partition coefficients calculated as molar solubility ratios are not the same as measured partition coefficients obtained from partitioning studies between water (saturated with the organic solvent) and organic solvent (saturated with water) in the case of solvents that are partially/fairly miscible with water (*i.e.*, 1-butanol, ethyl acetate, butyl acetate and diethyl ether). Presence of water in the organic phase, and/or presence of organic solvent in the aqueous phase, affects the solute’s affinity for the two respective liquid phases. For such solvents, one must be careful not to confuse the two sets of $\log P$ equation

coefficients. No confusion is possible for solvents that are completely miscible with water, such as methanol and N,N-dimethylformamide. Only one set of log P equation coefficients have been reported, and here the calculated log P values must refer to the hypothetical partitioning process between the two solvents. In the case of solvents that are “almost” totally immiscible with water, such as alkanes, chlorinated alkanes and many aromatic solvents, published studies have shown the calculated molar solubility ratio of $C_{\text{solute,organic solvent}}/C_{\text{solute,water}}$ to be nearly identical to the measured partition coefficient from direct partitioning studies [5, 6, 8]. The direct and hypothetical partitioning processes are denoted as “wet” and “dry”, respectively, in our recent publications [1-8, 11-14] and recent equation coefficient tabulation [11].

The aim of the present work is to collect experimental data from the published literature on the partition coefficients of neutral solutes from water and from air into *o*-xylene, *m*-xylene and *p*-xylene, and to derive Abraham model log P and log K correlations for the three organic solvents. The derived Abraham model correlations will be available for planned future studies involving the development of predictive log P equations for ionic species into more organic solvents, and the determination of solute descriptors for ion-pairs from measured partition coefficient data.

2. Data Sets and Computation Methodology

Most of the experimental data [18-44] that we were able to retrieve from the published literature pertained either to the Raoult’s law infinite dilution activity coefficient, $\gamma_{\text{solute}}^{\infty}$, Henry’s law constants (solute concentrations are in mole fraction), K_{Henry} , or solubilities for solutes dissolved in *o*-xylene, *m*-xylene and *p*-xylene. In order to apply the Abraham model, the infinite dilution activity coefficients and Henry’s law constants needed to be converted to log K values through Eqns. 4 and 5

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

$$\log K = \log \left(\frac{RT}{K_{Henry} V_{solvent}} \right) \quad (4)$$

or to log P values for partition from water to solvent through Eqn. 6 where K_w is the gas to water partition coefficient.

$$\log P = \log K - \log K_w \quad (5)$$

In Eqns. 3 and 4, R is the universal gas constant, T is the system temperature, P_{solute}° is the vapor pressure of the solute at T , and $V_{solvent}$ is the molar volume of the solvent. The calculation of log P requires knowledge of the [solute's gas phase partition coefficient into water, \$K_w\$](#) , which is available for most of the solutes being studied.

Our experimental databases also contain measured solubility data [45-57] for several crystalline solutes dissolved in the three xylenes and in water. The solubility data were taken largely from our previously published solubility studies. In the case of crystalline solutes, the partition coefficient between water and the anhydrous organic solvent is calculated as a solubility ratio

$$P = C_{solute,organic\ solvent} / C_{solute,water} \quad (6)$$

of the solute's molar solubilities ([in units of moles per liter](#)) in the organic solvent, [C_{solute,organic solvent}](#), and in water, [C_{solute,water}](#). Molar solubilities can also be used to calculate log K values, provided that the equilibrium vapor pressure of the solute above crystalline solute, P_{solute}° , at 298 K is also available. P_{solute}° can be transformed into the gas phase concentration, $C_{solute,gas}$, and the gas-to-water and gas-to-organic solvent partitions, K_w and K , can be obtained through the following equations

$$K_W = C_{\text{solute,water}}/C_{\text{solute,gas}} \quad \text{or} \quad K = C_{\text{solute,organic solvent}}/C_{\text{solute,gas}} \quad (7)$$

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

Several published articles reporting experimental partition coefficient data for crown ethers [58], substituted phenols [59-64], substituted anilines [65], substituted benzenediols [66] and a few miscellaneous organic compounds [67-69] were also found. These latter values pertain to practical partitioning studies where the aqueous and xylene phases were in direct contact with each other. Given the small mole fraction solubilities of water in the xylenes ($x_{\text{water}} = 2.60 \times 10^{-3}$ for *o*-xylene, $x_{\text{water}} = 2.60 \times 10^{-3}$ for *m*-xylene and $x_{\text{water}} = 2.70 \times 10^{-3}$ for *p*-xylene) [70] and the small mole fraction solubilities of the three xylenes in water ($x_{\text{o-xylene}} = 3.61 \times 10^{-5}$, $x_{\text{m-xylene}} = 2.70 \times 10^{-5}$ and $x_{\text{p-xylene}} = 2.73 \times 10^{-5}$) [70], we elected to combine the “dry” and “wet” data sets. Water and the xylene solvents are “almost” completely immiscible with each other at 298 K. The experimental $\log K$ and $\log P$ values at 298 K for *o*-xylene, *m*-xylene and *p*-xylene are listed in Tables 1-3, respectively. Also included in the tables are the literature references pertaining to the $\log K$ and $\log P$ data, and the numerical values for the solute descriptors for all of the compounds considered in the present study. The tabulated values came from our solute descriptor database, and were obtained using various types of experimental data, including water-to-solvent partitions, gas-to-solvent partitions, solubility and chromatographic data [9-11, 15, 16].

3. Results and Discussion

We have assembled in Table 1 $\log K$ and $\log P$ values for the partitioning of 59 solutes between the gas phase and *o*-xylene, and between water and *o*-xylene at 298 K. The solutes

considered cover a reasonably wide range of compound type and descriptor values. Preliminary analysis of the experimental log *K* data yielded a correlation equation having very small b_k coefficients, would be expected from the molecular structure considerations. *o*-Xylene does not have an acidic hydrogen. The b_k -coefficients were set equal to zero, and the final regression analyses performed to give:

$$\log P = 0.083(0.041) + 0.518(0.065) \mathbf{E} - 0.813(0.087) \mathbf{S} - 2.884(0.064) \mathbf{A} - 4.821(0.121) \mathbf{B} + 4.559(0.082) \mathbf{V} \quad (8)$$

$$(N = 59, SD = 0.104, R^2 = 0.997, F = 3055)$$

and

$$\log K = 0.064(0.027) - 0.296(0.070) \mathbf{E} + 0.934(0.092) \mathbf{S} + 0.647(0.069) \mathbf{A} + 1.010(0.019) \mathbf{L} \quad (9)$$

$$(N = 59, SD = 0.120, R^2 = 0.998, F = 8943)$$

All regression analyses were performed using SPSS statistical software. The standard errors in the calculated coefficients are given in parenthesis. Here and elsewhere, *N* corresponds to the number of solutes, *R* denotes the correlation coefficient, *SD* is the standard deviation and *F* corresponds to the Fisher *F*-statistic. The statistics of both correlations are quite good as evidenced by the near unity values of the squared correlation coefficients and by the small standard deviations of *SD* = 0.104 and *SD* = 0.120 log units. [The maximum deviation between the observed and predicted values was 0.40 log units for both the log *P* \(for iodine\) and the log *K* \(for iodine\) correlations.](#) See Figures 1 and 2 for plots of the calculated log *P* and log *K* values based on Eqns. 8 and 9 against observed data. The experimental log *P* and log *K* values cover ranges of about 8.2 and 12.5 log units, respectively.

The predictive ability of Eqns. 8 and 9 was assessed through a training set and test analysis. The parent data points were divided into three subsets (A–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); 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). Each validation computation gave a training set correlation equation having coefficients not too different from that obtained from the parent 59 compound database. The training set equations were then used to predict $\log P$ and $\log K$ values for the compounds in the respective test sets (A–C). The statistical information for the three test set predictions are summarized in Table 3. For the three test sets the average values of S.D. = 0.116, AAE (average absolute error) = 0.083, and AE (average error) = 0.003 were obtained for the water-to-*o*-xylene $\log P$ correlation, and average values of S.D. = 0.119, AAE = 0.080, and AE = 0.013 were obtained for the gas-to-*o*-xylene $\log K$ correlation. We conclude that there is very little bias in the predictions based on the derived Abraham model correlations, and that Eqs. 8 and 9 can be used to predict further values with an S.D. of about 0.12 log units.

The predictive ability was further examined using the leave-one-out method. The first data point was removed from the training data set and the correlation model was calibrated on the remaining data points, which in the present case are 58 experimental values. The value for the left-out data point was then predicted with the derived mathematical correlation, and the deviation between the predicted and observed $\log P$ (or $\log K$) was computed. The data point was returned to data set, the second data point was removed, and the process repeated until every experimental value had been removed once. The computed deviations were then averaged to obtain an indication of the predictive ability of the respective $\log P$ and $\log K$ correlation models.

Calculated average errors of $AAE = 0.085$ and $AAE = 0.092$ log units were obtained for the respective $\log P$ and $\log K$ predictions.

The data set for *m*-xylene contains experimental $\log P$ and $\log K$ values for 79 organic solutes and gases. Regression analysis of the tabulated experimental values in Table 2 gave the following two mathematical expressions:

$$\log P = 0.122(0.025) + 0.377(0.048) \mathbf{E} - 0.603(0.070) \mathbf{S} - 2.981(0.053) \mathbf{A} - 4.961(0.064) \mathbf{B} + 4.535(0.031) \mathbf{V} \quad (10)$$

$$(N = 79, SD = 0.120, R^2 = 0.998, F = 7216)$$

and

$$\log K = 0.071(0.023) - 0.423(0.038) \mathbf{E} + 1.068(0.048) \mathbf{S} + 0.552(0.055) \mathbf{A} + 1.014(0.008) \mathbf{L} \quad (11)$$

$$(N = 79, SD = 0.130, R^2 = 0.999, F = 17946)$$

The b_k coefficient in the $\log K$ correlation was found to be negligible, and was removed from the final correlation. Both correlations provide a reasonably accurate mathematical description of the experimental water-to-*m*-xylene partition coefficient data (Eqn. 10) and gas-to-*m*-xylene partition coefficient data (Eqn. 11) for experimental values that cover ranges of about 20.4 and 21.7 log units, respectively. [The maximum deviation between the observed and predicted values was 0.48 log units for the \$\log P\$ correlation and 0.50 log units for the \$\log K\$ correlation. The solute in both cases was iodine.](#) Graphical comparisons of predicted versus observed values are given in Figures S1 and S2 (Supporting Information).

In order to assess the predictive ability of Eqns. 10 and 11 we divided the data points into a training set and a test set by allowing the SPSS software to randomly select half of the experimental data points. The selected data points became the training sets and the remaining

compounds that were left served as the test sets. Analysis of the experimental data in the log P and log K training sets gave:

$$\log P = 0.091(0.043) + 0.316(0.058) \mathbf{E} - 0.596(0.104) \mathbf{S} - 2.934(0.079) \mathbf{A} - 5.015(0.096) \mathbf{B} + 4.603(0.096) \mathbf{V} \quad (12)$$

$$(N = 40, SD = 0.100, R^2 = 0.997, F = 266.8)$$

and

$$\log K = 0.094(0.031) - 0.467(0.048) \mathbf{E} + 1.063(0.098) \mathbf{S} + 0.546(0.078) \mathbf{A} + 1.012(0.023) \mathbf{L} \quad (13)$$

$$(N = 40, SD = 0.115, R^2 = 0.999, F = 7199)$$

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 $SD = 0.147$ (Eqn. 12) and $SD = 0.153$ (Eqn. 13), $AAE = 0.101$ (Eqn. 12) and $AAE = 0.098$ (Eqn. 13), and $AE = 0.019$ (Eqn. 12) and $AE = -0.023$ (Eqn. 13). There is therefore very little bias in using Eqns. 12 and 13 with AE equal to 0.019 and -0.023 log units. The training and test set analyses were performed five more times with similar results.

In [Table 3](#) are collected values of the logarithms of the partition coefficients of 91 organic solutes and gases in *p*-xylene. Regression analyses of the experimental log P and log K data in accordance with the Abraham model yielded:

$$\log P = 0.166(0.032) + 0.477(0.060) \mathbf{E} - 0.812(0.094) \mathbf{S} - 2.939(0.071) \mathbf{A} - 4.874(0.096) \mathbf{B} + 4.532(0.033) \mathbf{V} \quad (14)$$

(N = 91, SD = 0.137, R² = 0.997, F = 6720)

and

$$\log K = 0.113(0.023) - 0.302(0.052) \mathbf{E} + 0.826(0.070) \mathbf{S} + 0.651(0.061) \mathbf{A} + 1.011(0.007) \mathbf{L} \quad (15)$$

(N = 91, SD = 0.120, R² = 0.998, F = 10227)

The b_k coefficient in the log K correlation was again found to be negligible, and was removed from the final correlation. Both equations are statistically very good with standard deviations of 0.137 and 0.120 log units for data sets that cover ranges of about 21.0 and 15.8 log units, respectively (See Figures S3 and S4 in the Supporting Information for a graphical comparison of observed versus predicted values). [The maximum deviation between the observed and predicted values was 0.40 log units for the log \$P\$ correlation \(for iodine\) and 0.40 log units for the log \$K\$ correlation \(for iodine and vinyl acetylene\).](#) The robustness of each correlation was determined through a training set and test set analyses as before by splitting the large data set in half. To conserve journal space we give only the test results. The training set correlations predicted the 45 experimental log P values in the test set to within SD = 0.172, AAE = 0.130 and AE = 0.020, and the 45 experimental log K values in the test set to within SD = 0.144, AAE = 0.096 and AE = -0.010. The training and test set analyses were performed five more times with similar results.

The present study shows that the correlations derived from 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 each of the three xylene isomers. [The derived correlations pertain to 298 K.](#) Careful examination of the three sets of log P correlations and three sets of log K correlations reveals that for each transfer process the equation coefficients are nearly identical as would be expected from the very similar molecular structures. The location of

the two methyl functional groups on the aromatic ring does not significantly affect the solvent's molecular interactions with dissolved solute molecules.

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Table 1. Experimental $\log P^a$ and $\log K^a$ Data for Solutes Dissolved in *o*-Xylene 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	-1.735	0.295	21
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.564	0.396	21
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.660	0.810	21
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-0.165	1.045	21
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.646	0.864	27
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.314	0.394	21
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.888	1.402	21
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	-0.200	2.020	21
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.294	1.166	21
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.116	2.556	43
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.692	3.212	43
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.495	3.195	43
1-Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.144	2.114	43
1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	1.695	2.705	43
<i>cis</i> 2-Butene	0.140	0.080	0.000	0.050	1.737	0.6292	1.863	2.853	43
<i>trans</i> 2-Butene	0.126	0.080	0.000	0.050	1.664	0.6292	1.812	2.792	43
2-Methylprop-1-ene	0.120	0.080	0.000	0.080	1.579	0.6292	1.692	2.552	43
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	1.805	2.255	43
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	2.099	1.639	43
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943	2.627	1.667	19
Tetrachloromethane	0.458	0.380	0.000	0.000	2.823	0.7391	3.183	3.373	31, 32
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352	3.238	1.964	33, 34
1,1-Difluoroethane	-0.250	0.470	0.040	0.070	0.570	0.4258	1.186	1.106	43
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	1.493	0.093	43
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	2.460	-0.330	18

Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	3.272	-0.188	22
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	3.068	-0.322	22
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	3.011	0.8718	3.621	0.381	22
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	3.816	0.466	22
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.0127	4.332	1.102	22
2-Chloroethanol	0.419	0.770	0.390	0.500	2.435	0.5715	3.474	-1.260	22
<i>o</i> -Xylene	0.663	0.560	0.000	0.160	3.939	0.9982	4.363	3.623	Unity
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	4.098	3.278	39, 40
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	8.406	5.376	49
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.757	4.027	54
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	7.171	4.811	53
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.428	5.928	51
<i>trans</i> -Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	8.265	5.485	50
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	6.207	4.287	52
Iodine	1.398	0.670	0.280	0.000	3.681	0.6250	4.570	2.710	46
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	5.017	0.167	59
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	5.918	1.068	60
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	6.213	1.053	60
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	5.601	1.951	60
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.325	4.257	47
Chlorine	0.360	0.320	0.100	0.000	1.193	0.3534	1.527	1.347	44
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	5.418	1.358	65
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	5.331	1.241	65
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	6.103	-2.247	66
Catechol	0.970	1.100	0.880	0.470	4.450	0.8338	5.879	-1.321	66
Hydroquinone	1.063	1.270	1.060	0.570	4.827	0.8338	6.511	-2.359	66
Benzidine	1.882	2.450	0.400	0.800	9.230	1.5238	11.483	1.053	68

1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	6.632	-0.798	66
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	5.772	1.272	64
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	11.458	0.908	69
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	5.720	1.380	61
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	4.371	0.491	62
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.702	1.352	62
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	5.290	1.580	62

^a Estimated uncertainties in the experimental log P and log K data are believed to be on the ± 0.05 log units based on the data for two or three solutes for which independent measurements had been made two research groups. The papers from which the experimental data was taken reported much smaller uncertainties of less than 5 %, which corresponds to less than ± 0.02 log units.

Table 2. Experimental $\log P^a$ and $\log K^a$ Data for Solutes Dissolved in *m*-Xylene 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	-1.690	0.330	21
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.485	0.475	21
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.628	0.842	21
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-0.142	1.068	21
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.1086	-1.089	0.631	21
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.624	0.886	27
Nitric Oxide	0.370	0.020	0.000	0.086	-0.590	0.2026	-0.580	0.747	20
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.328	0.408	21
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.827	1.461	21
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	-0.142	2.078	21
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.269	1.191	21
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.190	2.630	43
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.713	3.233	43
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.518	3.218	43
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	2.279	3.979	28
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.821	4.641	28
Octacosane	0.000	0.000	0.000	0.000	13.780	4.0536	14.109	18.449	57
Ethene	0.107	0.100	0.000	0.070	0.289	0.3470	0.447	1.387	29
1-Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.158	2.128	43
1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	1.688	2.698	43
<i>cis</i> 2-Butene	0.140	0.080	0.000	0.050	1.737	0.6292	1.881	2.871	43
<i>trans</i> 2-Butene	0.126	0.080	0.000	0.050	1.664	0.6292	1.829	2.809	43
2-Methylprop-1-ene	0.120	0.080	0.000	0.080	1.579	0.6292	1.709	2.569	43
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	1.815	2.265	43
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110	2.738	3.898	28
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	2.106	1.646	43
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943	2.624	1.664	28

Tetrachloromethane	0.458	0.380	0.000	0.000	2.823	0.7391	3.144	3.334	31, 32
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352	3.264	1.994	33, 34
1,1-Difluoroethane	-0.250	0.470	0.040	0.070	0.570	0.4258	1.197	1.117	43
1,1,2-Trichlorotrifluoroethane	0.100	0.130	0.000	0.000	2.210	0.8107	2.472	3.772	28
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	1.501	0.101	43
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309	2.410	1.120	28
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	2.493	-0.297	28
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	2.997	0.277	28
Methanol	0.278	0.440	0.430	0.470	0.970	0.3080	1.777	-1.963	28
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	2.201	-1.469	28
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.728	-0.832	28
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	3.209	-0.251	22
Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.5900	2.443	-1.037	28
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	3.007	-0.293	22
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	3.032	-0.358	22
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	3.011	0.8718	3.615	0.375	22
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.8718	3.822	0.472	22
2-Chloroethanol	0.419	0.770	0.390	0.500	2.435	0.5715	3.438	-1.162	22
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.182	2.552	30
<i>m</i> -Xylene	0.623	0.520	0.000	0.160	3.839	0.9982	4.255	3.645	Unity
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	8.270	5.240	49
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.764	4.034	56
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.397	5.897	51
<i>trans</i> -Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	8.234	5.454	50
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	6.168	4.248	52
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	3.045	0.885	28
Iodine	1.398	0.670	0.280	0.000	3.681	0.6250	4.585	2.725	46
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	4.970	0.120	59
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	5.899	1.049	60

4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	6.151	0.991	60
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	5.540	1.890	60
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.258	4.190	47
15-Crown-5	0.410	1.200	0.000	1.750	6.779	1.7025	8.030	-1.370	58
16-Crown-5	0.410	1.170	0.000	1.760	7.276	1.8434	8.390	-0.790	58
Benzo 15-Crown-5	1.055	1.940	0.000	1.590	9.403	2.0285	10.850	0.300	58
18-Crown-6	0.410	1.470	0.000	2.100	8.228	2.0430	9.480	-1.950	58
Dibenzo-18-Crown-6	1.690	2.730	0.000	1.780	13.384	2.6950	15.930	2.550	58
Dibenzo-24-Crown-8	1.680	3.400	0.000	2.340	16.414	3.3760	19.990	2.610	58
AC-Benzo-18-Crown-6	0.684	2.650	0.000	1.850	11.100	2.4776	14.056	1.006	58
2-Methylaniline	0.966	0.920	0.230	0.450	4.442	0.9571	5.367	1.307	65
4-Methylaniline	0.923	0.950	0.230	0.450	4.452	0.9571	5.323	1.233	65
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	6.104	-2.246	66
Catechol	0.970	1.100	0.880	0.470	4.450	0.8338	5.842	-1.358	66
Hydroquinone	1.063	1.270	1.060	0.570	4.827	0.8338	6.512	-2.538	66
1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	6.633	-0.797	66
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	5.743	1.243	64
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	11.395	0.845	69
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	5.690	1.350	61
2-Nitrophenol	1.015	1.050	0.050	0.370	4.760	0.9493	5.663	2.303	63
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	4.319	0.439	62
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.709	1.369	62
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	5.330	1.620	62

^a Estimated uncertainties in the experimental log *P* and log *K* data are believed to be on the ± 0.05 log units based on the data for two or three solutes for which independent measurements had been made two research groups. The papers from which the experimental data was taken reported much smaller uncertainties of less than 5 %, which corresponds to less than ± 0.02 log units.

Table 3. Experimental $\log P^a$ and $\log K^a$ Data for Solutes Dissolved in *p*-Xylene 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	-1.674	0.346	21
Neon	0.000	0.000	0.000	0.000	-1.575	0.0850	-1.521	0.439	21
Argon	0.000	0.000	0.000	0.000	-0.688	0.1900	-0.608	0.862	21
Krypton	0.000	0.000	0.000	0.000	-0.211	0.2460	-0.125	1.085	21
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.1830	-0.609	0.901	27
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.2809	0.332	0.340	21
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.3203	-0.814	1.476	21
Sulfur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.4643	-0.141	2.079	21
Methane	0.000	0.000	0.000	0.000	-0.323	0.2495	-0.244	1.216	21
Propane	0.000	0.000	0.000	0.000	1.050	0.5313	1.146	2.586	43
Butane	0.000	0.000	0.000	0.000	1.615	0.6722	1.709	3.229	43
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.6722	1.509	3.209	43
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131	2.303	4.003	23, 26
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540	2.818	4.638	26
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949	3.336	5.296	26
Octane	0.000	0.000	0.000	0.000	3.677	1.2358	3.839	5.949	24, 25, 26
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767	4.329	6.479	26
Decane	0.000	0.000	0.000	0.000	4.686	1.5176	4.897	7.219	36
Octacosane	0.000	0.000	0.000	0.000	13.780	4.0536	14.167	18.507	58
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.9540	2.651	4.801	26
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.0949	2.962	5.042	26
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.2358	3.472	5.492	26
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.2358	3.541	5.421	26
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454	3.062	3.962	26
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272	3.901	5.481	26
1-Propene	0.100	0.080	0.000	0.070	0.946	0.4883	1.161	2.131	43

1-Butene	0.100	0.080	0.000	0.070	1.491	0.6292	1.710	2.720	43
<i>cis</i> 2-Butene	0.140	0.080	0.000	0.050	1.737	0.6292	1.870	2.860	43
<i>trans</i> 2-Butene	0.126	0.080	0.000	0.050	1.664	0.6292	1.821	2.801	43
2-Methylprop-1-ene	0.120	0.080	0.000	0.080	1.579	0.6292	1.700	2.560	43
1,3-Butadiene	0.320	0.230	0.000	0.100	1.543	0.5862	1.799	2.249	43
Isopentene	0.063	0.060	0.000	0.050	1.933	0.7701	2.430	3.450	23
Pent-1-ene	0.093	0.080	0.000	0.070	2.047	0.7701	2.278	3.508	23
Acetylene	0.190	0.470	0.120	0.050	0.070	0.3474	0.590	0.590	38
Vinyl acetylene	0.327	0.260	0.180	0.010	1.467	0.5432	2.249	2.279	37
Chloroethane	0.227	0.400	0.000	0.100	1.678	0.5128	2.078	1.618	43
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.4943	2.602	1.642	23
Tetrachloromethane	0.458	0.380	0.000	0.000	2.823	0.7391	3.190	3.380	23, 31
1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.6537	2.626	2.386	23
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.7946	2.626	3.426	23
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.6352	3.234	1.964	32-34
Bromoethane	0.366	0.400	0.000	0.120	2.120	0.5654	2.502	1.962	23
Iodomethane	0.676	0.430	0.000	0.120	2.106	0.5077	2.544	1.894	23
Iodoethane	0.640	0.400	0.000	0.150	2.573	0.6486	3.034	2.494	23
1,1-Difluoroethane	-0.250	0.470	0.040	0.070	0.570	0.4258	1.191	1.111	43
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.4491	1.488	0.088	43
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810	3.497	-0.213	25
Propanone	0.179	0.700	0.040	0.490	1.696	0.5470	2.485	-0.305	23
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879	3.096	0.376	24, 25
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.0538	3.314	0.954	23
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4042	2.522	-0.328	23
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237	3.000	0.050	25
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491	2.224	-1.446	25
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.5900	2.736	-0.824	22
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.7309	3.289	-0.171	22

Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.5900	2.486	-0.994	22
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.7309	3.115	-0.185	22
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.7309	3.104	-0.286	22
2-Methylpropan-2-ol	0.180	0.300	0.310	0.600	1.963	0.7309	2.466	-0.814	41, 42
3-Methyl-1-butanol	0.192	0.390	0.370	0.480	3.011	0.8718	3.612	0.372	22
2-Chloroethanol	0.419	0.770	0.390	0.500	2.435	0.5715	3.496	-1.104	22
Carbon disulfide	0.876	0.260	0.000	0.030	2.370	0.4905	2.600	2.750	23
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164	3.200	2.570	23, 35
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573	3.735	3.085	25
<i>p</i> -Xylene	0.613	0.520	0.000	0.160	3.839	0.9982	4.233	3.643	Unity
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.8388	4.050	3.230	39, 40
Anthracene	2.290	1.340	0.000	0.280	7.568	1.4544	8.231	5.201	48
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854	5.778	4.048	54
Acenaphthene	1.604	1.050	0.000	0.220	6.469	1.2586	7.015	4.655	55
Pyrene	2.808	1.710	0.000	0.280	8.833	1.5846	9.381	5.881	51
<i>trans</i> -Stilbene	1.450	1.050	0.000	0.340	7.520	1.5630	8.279	5.499	50
Ferrocene	1.350	0.850	0.000	0.200	5.622	1.1209	6.185	4.265	52
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466	3.083	0.923	23
Iodine	1.398	0.670	0.280	0.000	3.681	0.6250	4.551	2.691	46
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751	4.960	0.110	59
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.8975	5.845	0.995	60
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.8975	6.079	0.919	60
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	1.0199	5.555	1.905	64
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.5357	9.248	4.180	47
Chlorine	0.360	0.320	0.100	0.000	1.193	0.3534	1.535	1.355	44
Methyl 2-hydroxybenzoate	0.850	0.820	0.010	0.480	4.961	1.1313	5.601	2.631	67
Resorcinol	0.980	1.110	1.090	0.520	4.618	0.8338	6.118	-2.232	66
Catechol	0.970	1.100	0.880	0.470	4.450	0.8338	5.831	-1.369	66
Hydroquinone	1.063	1.270	1.060	0.570	4.827	0.8338	6.458	-2.412	66

1,2-Dihydroxy-4-methylbenzene	0.950	1.220	0.850	0.490	5.135	0.9747	6.631	-0.799	66
4-Ethylphenol	0.800	0.900	0.550	0.360	4.737	1.0569	5.755	1.255	64
Bisphenol A	1.607	1.560	0.990	0.910	9.603	1.8643	11.363	0.813	69
2,5-Dimethylphenol	0.840	0.830	0.500	0.380	4.774	1.0569	5.660	1.320	61
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.7928	4.294	0.414	62
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.8975	4.668	1.328	62
2-Bromophenol	1.037	0.850	0.350	0.300	4.802	0.9501	5.266	1.556	62

^a Estimated uncertainties in the experimental $\log P$ and $\log K$ data are believed to be on the ± 0.05 log units based on the data for two or three solutes for which independent measurements had been made two research groups. The papers from which the experimental data was taken reported much smaller uncertainties of less than 5 %, which corresponds to less than ± 0.02 log units.

Table 4. Summary of Training Set and Test Set Computations for *o*-Xylene

Training Set	Test Set	Predictions (log units)		
		S.D.	AAE	AE
log <i>P</i> correlation				
A + B	C	0.098	0.080	0.017
A + C	B	0.097	0.066	-0.028
B + C	A	<u>0.152</u>	<u>0.103</u>	<u>0.021</u>
Average		0.116	0.083	0.003
log <i>K</i> correlation				
A + B	C	0.079	0.061	-0.001
A + C	B	0.118	0.073	0.018
B + C	A	<u>0.160</u>	<u>0.105</u>	<u>0.022</u>
Average		0.119	0.080	0.013

Figure 1 – log P for o-xylene

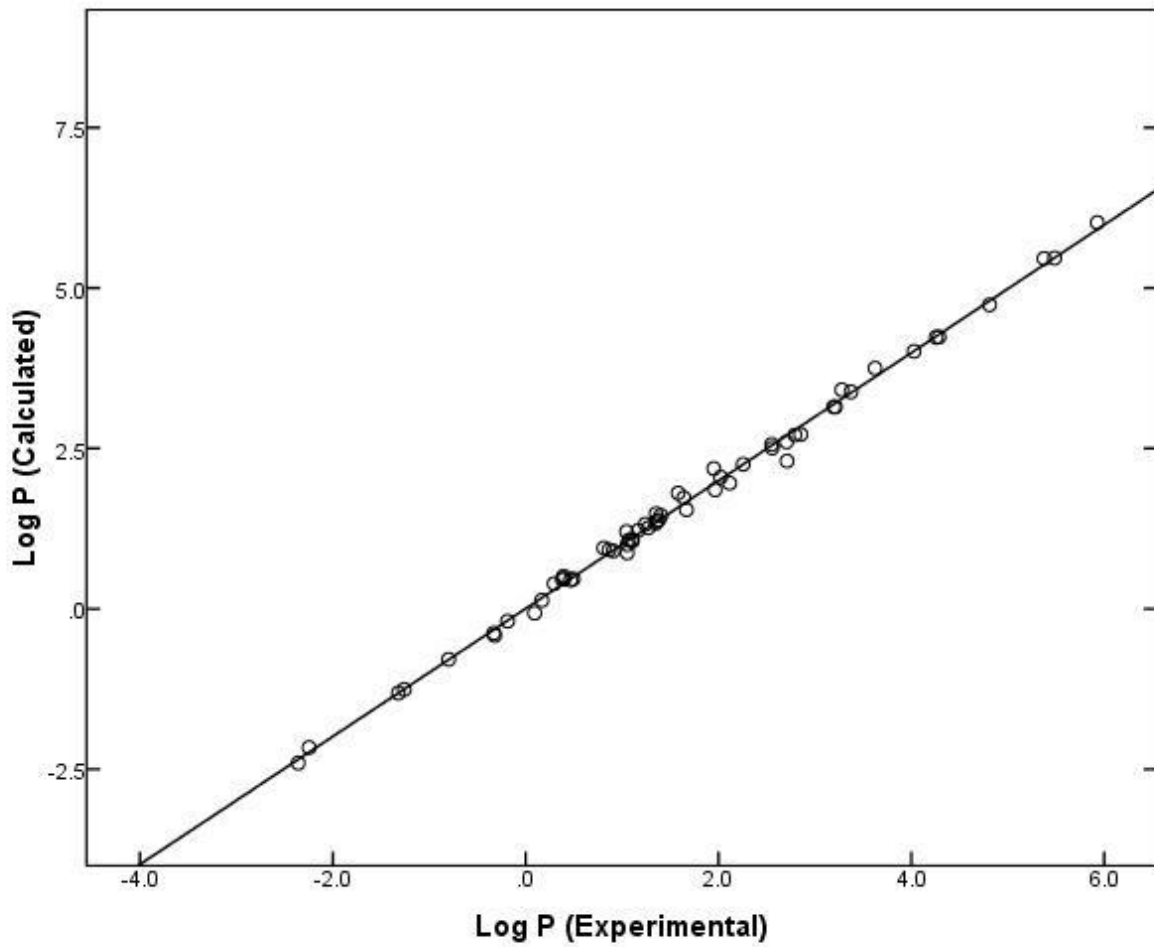


Figure 1. Comparison of observed $\log P$ data for solutes dissolved in *o*-xylene and predicted values based on Eqn. 8

Figure 2 – log K for o-xylene

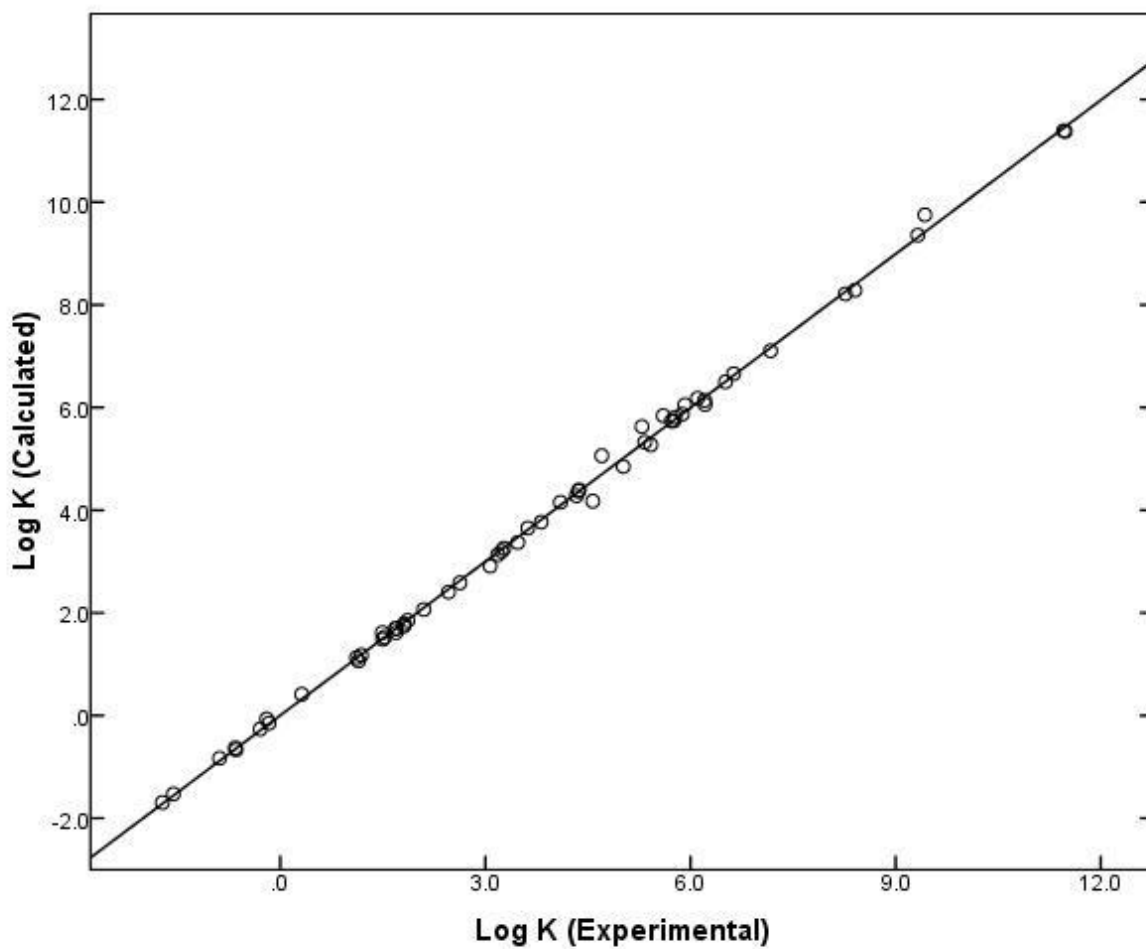


Figure 2. Comparison of observed log K data for solutes dissolved in *o*-xylene and predicted values based on Eqn. 9.