



# DETERMINATION OF THE SOLUBILIZING CHARACTER OF 1-(2-HYDROXYETHYL)-1-METHYLIMIDAZOLIUM TRIS(PENTAFLUOROETHYL)TRIFLUOROPHOSPHATE BASED ON THE ABRAHAM SOLVATION PARAMETER MODEL

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Chromatographic retention factor data were measured for a chemically diverse set of thirty-seven organic solutes on a 1-(2-hydroxyethyl)-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>) ionic liquid stationary phase at both 323 K and 353 K. The measured retention factors were combined with published gas-to-liquid partition coefficient data for solutes dissolved in ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>) and with published gas-to-water partition coefficient data to yield gas-to-anhydrous ionic liquid and water-to-anhydrous ionic liquid partition coefficients. The three sets of partition coefficients were correlated with the Abraham solvation parameter model. The derived Abraham model correlations describe the experimental gas-to-ionic liquid and water-to-ionic liquid partition coefficient data to within an average standard deviation of 0.12 log units.

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## Introduction

Ionic liquids (ILs) have been used as solvent media in chemical synthesis and chemical separations, and as solvent coatings in sensor arrays. For example, Yao, Pitner and Anderson<sup>1</sup> showed that ILs containing the tris(pentafluoroethyl)trifluorophosphate anion exhibited both high selectivity and sensitivity in extracting polycyclic aromatic hydrocarbon solutes from aqueous samples using single drop microextraction. Li et al.<sup>2</sup> successfully demonstrated the application of ILs as solvents in the extraction and pre-concentration of deoxyribonucleic acids using a separation method involving *in situ* liquid-liquid micro-extraction. Extraction efficiencies exceeding 97 % were observed, and metal ions did not interfere in the DNA extraction. More recently, Toniolo and coworkers<sup>3</sup> showed that ILs could be employed as sensing layers for estimating food quality from their odor analysis by quartz crystal microbalance measurements. The authors constructed an array of quartz crystals coated with a combination of 1,3-dialkylimidazolium, 1,1-dialkylpyrrolidinium and tetraalkylphosphonium ILs having different alkyl chain lengths and counter-anions. The sensor array was able to discriminate the headspace vapor above cinnamon samples of two

different botanical varieties (*cinnamon zeylanicum* and *cinnamon cassia*). Additional examples can be found in recent review articles and book chapters.<sup>4-9</sup> The aforementioned applications are facilitated by the IL's unique physical and solubilizing properties. At the present time more than 500 ionic liquids are known from the many different possible specific cation-anion pair combinations.

It is not possible to experimentally determine the solubilizing properties of every known or possible ionic liquid. The solvation parameter model, developed by Abraham and co-workers,<sup>10,11</sup> has been used successfully to describe the solubilizing properties of traditional organic solvents,<sup>12-17</sup> binary aqueous-ethanol solvent mixtures,<sup>18</sup> aqueous-micellar surfactant solutions,<sup>19,20</sup> and several different classes of ILs.<sup>21-33</sup> For IL solvents, Sprunger *et al.*<sup>34-36</sup> expressed the logarithm of the water-to-ionic liquid partition coefficient, log *P*:

$$\log P = c_{p,cation} + c_{p,anion} + (e_{p,cation} + e_{p,anion})E + (s_{p,cation} + s_{p,anion})S + (a_{p,cation} + a_{p,anion})A + (b_{p,cation} + b_{p,anion})B + (v_{p,cation} + v_{p,anion})V \quad (1)$$

and logarithm of the gas-to-ionic liquid partition coefficient, log *K*:

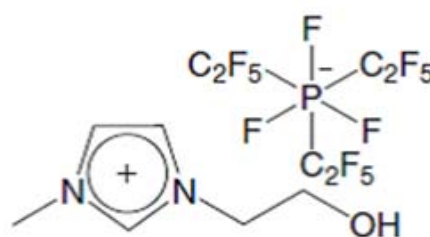
$$\log K = c_{k,cation} + c_{k,anion} + (e_{k,cation} + e_{k,anion})E + (s_{k,cation} + s_{k,anion})S + (a_{k,cation} + a_{k,anion})A + (b_{k,cation} + b_{k,anion})B + (l_{k,cation} + l_{k,anion})L \quad (2)$$

to include ion-specific equation coefficients. Numerical values of the two sets of equation coefficients are calculated as a paired cation-anion sum (e.g.,  $c_{p,cation} + c_{p,anion}$ ,  $e_{p,cation} + e_{p,anion}$ , etc.) through regression analyses of measured  $\log P$  and  $\log K$  values for a series of solutes (with known solute descriptors) dissolved in the desired partitioning system in accordance with Eqns. 1 and 2. The solute descriptors are the capitalized quantities in the  $\log P$  and  $\log K$  expressions. To calculate equation coefficients for an individual ion, one must know the equation coefficients for the other ion in the IL. In other words, to calculate  $c_{p,cation}$  the value of  $c_{p,anion}$  must be known, and *vice versa*. Numerical values of the first sets of ion-specific equation coefficients were obtained by setting the six coefficients of the [Tf<sub>2</sub>N]<sup>-</sup> anion equal to zero. In many respects this is analogous to setting a reference point for calculating thermodynamic properties of single ions. To date equation coefficients have been published for 27 different cations and 14 different anions. The equation coefficients can also be calculated from available group and fragment values,<sup>37</sup> and there are provisions for incorporating a temperature dependency into the model if one wishes to describe  $\log P$  and  $\log K$  values measured at different temperatures.<sup>38-41</sup>

The solute descriptors are the capitalized quantities in Eqns. 1 and 2, and describe how the solute interacts with surrounding solvent molecules based on its size, polarity and hydrogen-bonding character. Solute descriptors are defined as follows: **E** refers to the solute excess molar refraction in units of cm<sup>3</sup> mol<sup>-1</sup>/10 computed from the solute's refractive index; **S** represents to a combined dipolarity/polarizability descriptor; **A** and **B** quantify the overall hydrogen-bond donor and acceptor properties of the solute, respectively; **V** denotes the McGowan characteristic molecular volume in units of cm<sup>3</sup> mol<sup>-1</sup>/100; and **L** is the logarithm of the solute's gas-to-hexadecane partition coefficient measured at 298 K. Solute descriptors were devised to reflect particular solute-solvent interactions, and when multiplied by the complementary solvent equation coefficient will encode quantitative information on the extent to which a given solute-solvent interaction influences the partitioning process. For example, the  $(a_{p,cation} + a_{p,anion})\mathbf{A}$  and  $(a_{k,cation} + a_{k,anion})\mathbf{A}$  terms in Eqns. 1 and 2 describe the hydrogen-bonding interactions between the H-bond donor sites on the solute and the H-bond acceptor sites on the solvent, while the  $(b_{p,cation} + b_{p,anion})\mathbf{B}$  and  $(b_{k,cation} + b_{k,anion})\mathbf{B}$  terms involve interactions between the solute H-bond acceptor sites and solvent H-bond donor sites. Positive numerical values of  $(a_{p,cation} + a_{p,anion})\mathbf{A}$  and  $(b_{p,cation} + b_{p,anion})\mathbf{B}$  result in larger water-to-IL partition coefficients and greater solute partitioning into the IL from the aqueous phase. Negative  $(a_{p,cation} + a_{p,anion})\mathbf{A}$  and  $(b_{p,cation} + b_{p,anion})\mathbf{B}$  values, on the other hand, means less solute transfer into the IL phase.

In the present study, we report gas-liquid chromatographic retention factor data for a wide range of organic solutes on 1-(2-hydroxyethyl)-3-methylimidazolium *tris*(pentafluoroethyl)trifluorophosphate, ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>), stationary phases at 323 K and 353 K. See Figure 1 for the molecular structure of the ionic liquid solvent. Results of the chromatographic measurements, combined with published gas-to-liquid partition coefficient data from two published studies<sup>42,43</sup> for volatile solutes dissolved in

([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>) were used to derive Abraham model  $\log K$  and  $\log P$  correlations at 298 K and 323 K. We note that authors of both of the earlier studies correlated their experimental with the Abraham model. Marciniak and Wlazlo<sup>42</sup> previously reported on Abraham model correlations for ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>) at 318, 328, 338, 348, 358 and 368 K based on 65 experimental data points. The datasets used in deriving the published correlations included only one acidic carboxylic acid solute (e.g., acetic acid) and none of the lesser volatile organic compounds considered in the present study. Orfao *et al.*<sup>43</sup> performed measurements from 318 K to 353 K, and their dataset of 30 contained only volatile organic compounds. Alcoholic solutes were the most acidic compounds studied by Orfao *et al.* As a result the predictive area of chemical space encompassed by the published Abraham model correlations is significantly less than that achieved by the correlations derived here as our data set also contains propanoic acid and two acidic phenolic solutes (phenol and *p*-cresol). The predictive area of chemical space is important in that one should not use the derived equations to estimate  $\log P$  and  $\log K$  values for compounds whose solute descriptors fall outside of the range of solute descriptors used in obtaining the predictive equations. Several of the IL-specific Abraham model correlations that have been reported in the published literature were based on datasets containing only fairly volatile and nonacidic organic solutes. Correlation equations derived from such data sets do need to be updated as experimental data for more diverse chemical solutes become available in order to provide better  $\log K$  and  $\log P$  predictions for a wider range of compounds.



**Figure 1.** Molecular structure of 1-(2-hydroxyethyl)-1-methylimidazolium *tris*(pentafluoroethyl)trifluorophosphate ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>)

## 2. Experimental Methods and Partition Coefficient Datasets

The sample of 1-(2-hydroxyethyl)-1-methylimidazolium *tris*(pentafluoroethyl)trifluorophosphate examined in this study was kindly donated as a gift from Merck KGaA (Darmstadt, Germany). The IL stationary phase was coated onto untreated fused silica capillary columns (5 m x 0.25 mm) obtained from Supelco (Bellefonte, PA). The IL coating solutions were prepared in dichloromethane using a 0.45% (w/v) concentration of [EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>.

Thirty-seven (37) probe molecules were selected for the characterization of the [EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup> stationary phase. The names of the solutes, along with the chemical suppliers and chemical purities, are listed in Table 1. All solute molecules were used as received. The presence of trace impurities in these probes should in no way affect our

results because the main chromatographic peak is easily discernible from any impurity peak that might be present by its much greater intensity.

Chromatographic retention factors,  $k$ , were determined on a [EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup> stationary phase at 323 K and 353 K as part of the present study. The percentage relative standard deviation (% RSD) in experimental retention times for all solutes included in this study was less than 1%. The stationary phase's integrity during the duration of the experimental measurements was established by periodically monitoring the retention factor and efficiency of naphthalene separation. The experimental log  $k$  values are tabulated in the second and third columns of Table 2. The extrapolated 298 K log  $k$  values obtained through a log  $k$  versus  $1/T$  linear plot of the measured data at 323 K and 353 K are given in the table's last column.

**Table 1.** List of organic solutes, chemical suppliers and chemical purities

Solute	Supplier <sup>a</sup>	Purity
Acetic acid	Supelco	99.7%
Acetophenone	Sigma-Aldrich	99%
Aniline	Sigma-Aldrich	99.5%
Benzaldehyde	Sigma-Aldrich	99+%
Benzene	Sigma-Aldrich	99.8%
Benzonitrile	Sigma-Aldrich	99%
Benzyl alcohol	Sigma-Aldrich	99%
1-Bromohexane	Sigma-Aldrich	98%
1-Bromooctane	Sigma-Aldrich	99%
Butyraldehyde	Acros Organics	99%
1-Butanol	Fisher Scientific	99.9%
2-Chloroaniline	Sigma-Aldrich	98%
1-Chlorobutane	Sigma-Aldrich	99%
1-Chlorohexane	Sigma-Aldrich	99%
1-Chlorooctane	Sigma-Aldrich	99%
<i>p</i> -Cresol	Fluka	99%
Cyclohexanol	J.T. Baker	99%
Cyclohexanone	Sigma-Aldrich	99.8%
1,2-Dichlorobenzene	Sigma-Aldrich	99%
Ethyl acetate	Fisher Scientific	99.9%
Ethylbenzene	Eastman Kodak Co	95+%
Methyl caproate	Supelco	98%
Naphthalene	Supelco	98%
1-Nitropropane	Sigma-Aldrich	99%
1-Octanol	Sigma-Aldrich	99+%
Octylaldehyde	Sigma-Aldrich	99%
1-Pentanol	Sigma-Aldrich	99+%
2-Pentanone	Sigma-Aldrich	99+%
Phenetole	Sigma-Aldrich	99%
Phenol	Sigma-Aldrich	99+%
Propionitrile	Sigma-Aldrich	99%
<i>m</i> -Xylene	Fluka	99.5%
<i>o</i> -Xylene	Fluka	99.5%
<i>p</i> -Xylene	Fluka	99.5%
Propanoic acid	Supelco	99%
1-Decanol	Sigma-Aldrich	99+%
2-Propanol	Fisher Scientific	99.6%

<sup>a</sup> Fluka (Steinheim, Germany); Eastman Kodak Company (Rochester, NY, USA); Supelco (Bellefonte, PA, USA); Acros Organics (Morris Plains, NJ, USA); J.T. Baker (Phillipsburg, NJ,

USA), Sigma-Aldrich (St. Louis, MO, USA); and Fisher Scientific (Pittsburgh, PA, USA).

The thermodynamic gas-to-IL partition coefficient,  $K$ , can be computed from isothermal gas-liquid chromatographic measurements through  $K = V_N/V_L$ , where  $V_N$  is the volume of the carrier gas required to elute the solute, and  $V_L$  is the volume of liquid present as the stationary phase.<sup>44</sup> The retention factor,  $k$ , is defined as<sup>44</sup>  $k = (t_r - t_m)/t_m$  where  $t_r$  is the retention time of a solute and  $t_m$  is the "void" retention time for an unretained solute. Since  $t_r - t_m$ , the corrected retention time, is proportional to  $V_N$ , the corrected elution volume, it follows that gas-to-liquid partition coefficients and retention factors are interrelated,

$$K = P^* \cdot k \quad \text{or} \quad \log K = \log P^* + \log k \quad (3)$$

The proportionality constant,  $P^*$ , is the phase ratio and depends only upon the chromatographic conditions. The value of  $P^*$  should remain essentially constant for a given column during the time the experimental measurements are performed.

Thermodynamic gas-to-IL partition coefficients are required to calculate the proportionality constants needed in Eqn. 3 for converting the measured log  $k$  data in Table 2 to log  $K$  values. Marciniak and Wlazlo<sup>42</sup> reported infinite dilution activity coefficients and gas-to-liquid partition coefficients of 65 solutes dissolved in [EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup> in the 318 to 368 K temperature range. Uncertainties in the measured  $K$  and  $\gamma_{\text{solute}}^\infty$  values were reported to be on the order of 2 to 3%. The published experimental data were extrapolated to 298 K and 323 K by assuming a linear ln  $K$  versus  $1/T$  relationship. A linear extrapolation should be valid as the measurements were performed not too far removed from the desired temperatures (less than 20 K in most instances). The log  $P$  values for partition from water to the anhydrous IL can be calculated via Eqn. 4

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

The conversion of log  $K$  data to log  $P$  requires a prior knowledge of the solute's gas phase partition coefficient into water,  $K_w$ , which is available for most of the solutes being studied. As noted above, water-to-anhydrous IL partition coefficients (more formally called Gibbs energy of solute transfer when multiplied by  $-2.303 RT$ ) calculated through Eqn. 4 refer to a hypothetical partitioning process involving solute transfer from water to the anhydrous IL. Log  $P$  values calculated in this fashion are still useful because the predicted log  $P$  values can be used to estimate the solute's infinite dilution activity coefficient in the IL.

The proportionality constants needed in Eqn. 3; log  $P^* = 2.642$  (298 K) and log  $P^* = 2.564$  (323 K) for [EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup> were the calculated average differences between the measured log  $k$  and log  $K$  values for the 12 common compounds (i.e., acetic acid, benzene, 1-butanol, butyraldehyde, ethyl acetate, ethylbenzene, 1-nitropropane, 2-pentanone, 2-propanol, *m*-xylene, *o*-xylene and *p*-xylene) in the IL's data set that had been studied by us and by Marciniak and Wlazlo.<sup>42</sup> The calculated log  $K$  and log  $P$  values are compiled in Table 3 for solutes dissolved in [EtOHMIM]<sup>+</sup>[FAP]<sup>-</sup>. Log  $P$  values are tabulated only for 298 K as we do not have experimental values for the

solutes' gas-to-water partition coefficients,  $\log K_w$ , at 323 K. The  $\log K_w$  values that we have compiled to date pertain to gas-to-water partitioning at 298 K<sup>45</sup> and 310 K,<sup>46</sup> or for gas-to-physiological saline partitioning at 310 K.<sup>46</sup> For the convenience of the reader, we have compiled the numerical values of solute descriptors for the 90 organic compounds considered in the present study in Table 4. The solute

descriptors are of experimental origin, and were retrieved from the Abraham database. The numerical values were deduced from experimental solubility data, gas-liquid and high-performance liquid chromatographic retention factor measurements and water-to-solvent partition determinations as discussed in several of our earlier papers.<sup>11,12,47-49</sup>

**Table 2.** Chromatographic retention factor data for organic solutes on 1-(2-hydroxyethyl)-3-methylimidazolium *tris*(pentafluoroethyl)trifluorophosphate, ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>), stationary phase at 298, 323 and 353 K

Solute	$\log k$ (323 K)	$\log k$ (353 K)	$\log k$ (298 K)
Acetic acid	0.867	0.266	1.461
Acetophenone	2.254	1.526	2.973
Aniline	2.175	1.427	2.913
Benzaldehyde	1.674	1.040	2.301
Benzene	-0.248	-0.689	0.187
Benzonitrile	1.806	1.172	2.433
Benzyl alcohol	2.316	1.520	3.102
1-Bromooctane	0.579	0.004	1.146
1-Butanol	0.459	-0.107	1.018
Butyraldehyde	0.219	-0.261	0.694
2-Chloroaniline	2.048	1.345	2.741
1-Chlorobutane	-0.872		
1-Chlorohexane	-0.250	-0.723	0.216
1-Chlorooctane	0.328	-0.226	0.876
<i>p</i> -Cresol	2.064	1.316	2.803
Cyclohexanol	1.246	0.586	1.896
Cyclohexanone	1.697	1.058	2.328
1,2-Dichlorobenzene	0.694	0.194	1.188
Ethyl acetate	0.355	-0.152	0.855
Ethylbenzene	0.259	-0.233	0.745
Methyl caproate	1.006	0.396	1.607
Naphthalene	1.866	1.199	2.525
1-Nitropropane	0.908	0.409	1.401
1-Octanol	1.465	0.745	2.175
Octylaldehyde	1.208	0.588	1.820
1-Pentanol	0.730	0.136	1.315
2-Pentanone	0.837	0.295	1.372
Phenetole	1.089	0.498	1.672
Phenol	1.789	1.093	2.477
Propionitrile	0.774	0.300	1.242
<i>m</i> -Xylene	0.333	-0.156	0.815
<i>o</i> -Xylene	0.450	-0.052	0.947
<i>p</i> -Xylene	0.303	-0.188	0.788
2-Propanol	0.076	-0.435	0.580
1-Bromohexane	0.013	-0.448	0.468
Propanoic acid	1.099	0.454	1.735
1-Decanol	1.939	1.123	2.743

**Table 3.** Logarithm of the gas-to-anhydrous IL partition coefficient,  $\log K$ , and logarithm of the water-to-anhydrous IL partition coefficient,  $\log P$ , for organic solutes dissolved in [EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup> at 298 K and 323 K

Solute	$\log K$ (298 K)	$\log K$ (323 K)	$\log P$ (298 K)
Based on Thermodynamic Data			
Pentane	0.658	0.425	2.358
Hexane	0.982	0.696	2.802
3-Methylpentane	0.940	0.681	2.780
2,2-Dimethylbutane	0.798	0.557	2.638
Heptane	1.286	0.955	3.246
Octane	1.600	1.216	3.710
2,2,4-Trimethylpentane	1.313	0.988	3.433
Nonane	1.905	1.476	4.055

**Table 3.** (cont.)

Decane	2.226	1.736	4.546
Cyclopentane	1.090	0.831	1.970
Cyclohexane	1.405	1.094	2.305
Methylcyclohexane	1.561	1.233	2.811
Ethylcyclohexane	1.742	1.427	3.332
Cycloheptane	1.858	1.496	2.438
Cyclooctane	2.271	1.858	3.041
1-Pentene	0.983	0.713	2.213
1-Hexene	1.303	0.981	2.463
Cyclohexene	1.780	1.421	2.050
1-Heptene	1.609	1.235	2.829
1-Octene	1.909	1.487	3.319
1-Decene	2.500	1.982	4.140
1-Pentyne	1.632	1.292	1.642
1-Hexyne	1.942	1.549	2.152
1-Heptyne	2.238	1.801	2.678
1-Octyne	2.527	2.047	3.047
Benzene	2.783	2.318	2.153
Toluene	3.117	2.600	2.467
Ethylbenzene	3.359	2.803	2.779
<i>o</i> -Xylene	3.581	3.001	2.921
<i>m</i> -Xylene	3.447	2.877	2.837
<i>p</i> -Xylene	3.408	2.842	2.818
Styrene	3.790	3.188	2.840
$\alpha$ -Methylstyrene	3.942	3.308	2.982
Methanol	2.853	2.336	-0.887
Ethanol	3.097	2.548	-0.573
1-Propanol	3.380	2.786	-0.180
2-Propanol	3.209	2.631	-0.272
1-Butanol	3.707	3.062	0.247
2-Butanol	3.481	2.856	0.091
2-Methyl-1-propanol	3.506	2.883	0.206
<i>tert</i> -Butanol	3.299	2.687	0.019
Acetic acid	4.026	3.334	-0.884
Thiophene	2.837	2.376	1.797
Tetrahydrofuran	3.462	2.883	0.912
1,4-Dioxane	4.239	3.570	0.529
Methyl <i>tert</i> -butyl ether	2.743	2.199	1.123
Ethyl <i>tert</i> -butyl ether	2.645	2.085	1.375
Methyl <i>tert</i> -amyl ether	3.013	2.425	1.543
Diethyl ether	2.338	1.854	1.168
Dipropyl ether	2.668	2.114	1.778
Diisopropyl ether	2.601	2.030	1.551
Dibutyl ether	3.212	2.575	2.522
Acetone	3.616	3.063	0.826
Butanone	3.794	3.247	1.074
2-Pentanone	4.093	3.448	1.513
3-Pentanone	4.026	3.395	1.426
Methyl acetate	3.297	2.761	0.997
Ethyl acetate	3.523	2.949	1.363
Methyl propanoate	3.521	2.940	1.371
Methyl butanoate	3.739	3.123	1.659
Propanal	3.056	2.567	0.536
Butyraldehyde	3.318	2.799	0.988
Acetonitrile	3.763	3.236	0.913
Pyridine	4.888	4.138	1.448
Nitromethane	3.678	3.209	0.728
1-Nitropropane	4.109	3.517	1.659

**Table 3.** (cont.)

Based on Chromatographic Retention Factor Data

Acetic Acid	4.103	3.431	-0.807
Acetophenone	5.615	4.818	2.256
Aniline	5.555	4.739	1.473
Benzaldehyde	4.943	4.238	1.993
Benzene	2.829	2.316	2.199
Benzonitrile	5.075	4.370	1.985
Benzyl alcohol	5.744	4.880	0.884
1-Bromooctane	3.788	3.143	4.168
Butyraldehyde	3.660	2.783	1.330
1-Butanol	3.336	3.023	-0.124
2-Chloroaniline	5.383	4.612	1.783
1-Chlorobutane		1.692	
1-Chlorohexane	2.858	2.314	2.858
1-Chlorooctane	3.518	2.892	3.708
<i>p</i> -Cresol	5.445	4.629	0.945
Cyclohexanol	4.538	3.810	0.528
Cyclohexanone	4.970	4.261	1.370
1,2-Dichlorobenzene	3.830	3.258	2.930
Ethyl acetate	3.497	2.919	1.337
Ethylbenzene	3.387	2.823	2.807
Methyl caproate	4.249	3.570	2.419
Naphthalene	5.169	4.430	3.437
1-Nitropropane	4.043	3.472	1.593
1-Octanol	4.817	4.029	1.817
Octylaldehyde	4.462	3.772	2.782
1-Pentanol	3.957	3.294	0.607
2-Pentanone	4.014	3.401	1.434
Phenetole	4.314	3.653	2.684
Phenol	5.119	4.353	0.260
2-Propanol	3.222	2.640	-0.258
Propionitrile	3.884	3.338	1.064
<i>m</i> -Xylene	3.457	2.897	2.847
<i>o</i> -Xylene	3.589	3.014	2.929
<i>p</i> -Xylene	3.430	2.867	2.840
1-Bromohexane	3.110	2.577	3.240
Propanoic acid	4.377	3.663	-0.363
1-Decanol	5.385	4.503	2.715

**Table 4.** Abraham model solute descriptors of the organic compounds considered in the present study

Solute	<i>E</i>	<i>S</i>	<i>A</i>	<i>B</i>	<i>L</i>	<i>V</i>
Pentane	0.000	0.000	0.000	0.000	2.162	0.8131
Hexane	0.000	0.000	0.000	0.000	2.668	0.9540
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.9540
2,2-Dimethylbutane	0.000	0.000	0.000	0.000	2.352	0.9540
Heptane	0.000	0.000	0.000	0.000	3.173	1.0949
Octane	0.000	0.000	0.000	0.000	3.677	1.2358
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.2358
Nonane	0.000	0.000	0.000	0.000	4.182	1.3767
Decane	0.000	0.000	0.000	0.000	4.686	1.5176
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.7045
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.8454
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.9863
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.1272
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.9863
Cyclooctane	0.413	0.100	0.000	0.000	4.329	1.1272
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.7701
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.9110

**Table 4.** (cont.)

Cyclohexene	0.395	0.280	0.000	0.090	2.952	0.8204
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.0519
1-Octene	0.094	0.080	0.000	0.070	3.568	1.1928
1-Decene	0.093	0.080	0.000	0.070	4.554	1.4746
1-Pentyne	0.172	0.230	0.120	0.120	2.010	0.7271
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.8680
1-Heptyne	0.160	0.230	0.120	0.100	3.000	1.0089
1-Octyne	0.155	0.220	0.090	0.100	3.521	1.1498
Benzene	0.610	0.520	0.000	0.140	2.786	0.7164
Toluene	0.601	0.520	0.000	0.140	3.325	0.8573
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.9982
<i>o</i> -Xylene	0.663	0.560	0.000	0.160	3.939	0.9982
<i>m</i> -Xylene	0.623	0.520	0.000	0.160	3.839	0.9982
<i>p</i> -Xylene	0.613	0.520	0.000	0.160	3.839	0.9982
Styrene	0.849	0.650	0.000	0.160	3.908	0.9550
$\alpha$ -Methylstyrene	0.851	0.640	0.000	0.190	4.290	1.0960
Methanol	0.278	0.440	0.430	0.470	0.970	0.3082
Ethanol	0.246	0.420	0.370	0.480	1.485	0.4491
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.5900
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.5900
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.7310
2-Butanol	0.217	0.360	0.330	0.560	2.338	0.7310
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.7310
<i>tert</i> -Butanol	0.180	0.300	0.310	0.600	1.963	0.7310
Thiophene	0.687	0.570	0.000	0.150	2.819	0.6411
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.6223
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.6810
Methyl <i>tert</i> -butyl ether	0.024	0.220	0.000	0.550	2.372	0.8718
Ethyl <i>tert</i> -butyl ether	-0.020	0.160	0.000	0.600	2.720	1.0127
Methyl <i>tert</i> -amyl ether	0.050	0.210	0.000	0.600	2.916	1.0127
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.7309
Dipropyl ether	0.008	0.250	0.000	0.450	2.954	1.0127
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.0127
Dibutyl ether	0.000	0.250	0.000	0.450	3.924	1.2945
Acetone	0.179	0.700	0.040	0.490	1.696	0.5470
Butanone	0.166	0.700	0.000	0.510	2.287	0.6879
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.8288
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.8288
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.6057
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.7466
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.7470
Methyl butanoate	0.106	0.600	0.000	0.450	2.943	0.8880
Propanal	0.196	0.650	0.000	0.450	1.815	0.5470
Butyraldehyde	0.187	0.650	0.000	0.450	2.270	0.6880
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.4040
Pyridine	0.631	0.840	0.000	0.520	3.022	0.6753
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.4237
1-Nitropropane	0.242	0.950	0.000	0.310	2.894	0.7055
Acetic Acid	0.265	0.640	0.620	0.440	1.816	0.4648
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.0139
Aniline	0.955	0.960	0.260	0.410	3.934	0.8162
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.8730
Benzonitrile	0.742	1.110	0.000	0.330	4.039	0.8711
Benzyl alcohol	0.803	0.870	0.330	0.560	4.221	0.9160
1-Bromooctane	0.339	0.400	0.000	0.120	5.143	1.4108
2-Chloroaniline	1.033	0.920	0.250	0.310	4.674	0.9390
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.7946
1-Chlorohexane	0.201	0.390	0.000	0.090	3.708	1.0764
1-Chlorooctane	0.191	0.400	0.000	0.090	4.708	1.3582

**Table 4.** (cont.)

<i>p</i> -Cresol	0.820	0.870	0.570	0.310	4.312	0.9160
Cyclohexanol	0.460	0.540	0.320	0.570	3.758	0.9040
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.8611
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.318	0.9612
1-Iodobutane	0.628	0.400	0.000	0.150	3.628	0.9304
Methyl caproate	0.080	0.600	0.000	0.450	3.874	1.1693
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.0854
1-Octanol	0.199	0.420	0.370	0.480	4.619	1.2950
Octylaldehyde	0.160	0.650	0.000	0.450	4.380	1.2515
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.8718
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.8288
Phenetole	0.681	0.700	0.000	0.320	4.242	1.0569
Phenol	0.805	0.890	0.600	0.300	3.766	0.7751
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450
1-Bromohexane	0.349	0.400	0.000	0.120	4.130	1.1290
Propionic acid	0.233	0.650	0.600	0.450	2.290	0.6057
1-Decanol	0.191	0.420	0.370	0.480	5.610	1.5763

## Results and Discussion

Tabulated in Table 3 are the experimental log *K* and log *P* values for a chemically diverse set of 90 organic compounds dissolved in ([EtOHMim]<sup>+</sup>[FAP]<sup>-</sup>). The organic solutes span a large range of molecular size and shape, polarity, and hydrogen-bonding characteristics. Preliminary analysis of the experimental data in Table 3 in accordance with Eqns. 1 and 2 of the Abraham general solvation parameter indicated that the ( $e_{k,cation} + e_{k,anion}$ ) equation coefficient [ $(e_{k,cation} + e_{k,anion}) = 0.005 \pm 0.073$  and  $(e_{k,cation} + e_{k,anion}) = 0.015 \pm 0.060$ ] was negligible in both the log *K* (298) and log *K* (323 K) correlations, and that the [ $(c_{p,cation} + c_{p,anion})$ ] equation coefficient [ $(c_{p,cation} + c_{p,anion}) = 0.038 \pm 0.078$ ] was negligible in the log *P* (298 K) correlation. The ( $e_{k,cation} + e_{k,anion}$ )·*E* and ( $c_{p,cation} + c_{p,anion}$ ) terms were consequently removed from the respective correlations, and the regression analyses were rerun to yield the following three Abraham model expressions:

$$\begin{aligned} \log K (298 \text{ K}) = & -0.400(0.052) + 2.494(0.049) S \\ & + 1.340(0.076) A + 2.272(0.079) B \\ & + 0.542 (0.014) L \\ (N = 102, SD = 0.120, R^2 = 0.990, F = 2445) \end{aligned} \quad (5)$$

$$\begin{aligned} \log K (323 \text{ K}) = & -0.489(0.043) + 2.307(0.041) S \\ & + 1.163(0.063) A + 1.878(0.065) B \\ & + 0.464 (0.012) L \\ (N = 103, SD = 0.099, R^2 = 0.992, F = 2827) \end{aligned} \quad (6)$$

$$\begin{aligned} \log P (298 \text{ K}) = & 0.111(0.079) E + 0.490(0.085) S \\ & - 2.383(0.093) A - 2.523(0.101) B \\ & + 2.858 (0.026) V \\ (N = 102, SD = 0.140, R^2 = 0.996, F = 4836) \end{aligned} \quad (7)$$

where the standard errors in the calculated equation coefficients are given in parentheses immediately after the coefficient. All regression analyses were performed using SPSS Statistics (Version 20) software. The statistical

information associated with each derived correlation includes the number of experimental data points (*N*), the standard deviation (*SD*), the squared correlation coefficient (*R*<sup>2</sup>), and the Fisher *F*-statistic (*F*). The number of data points used in the regression analyses are slightly larger than the number of solutes because the twelve solutes used in converting the chromatographic retention factors to gas-to-liquid partition coefficients (see Eqn. 3) appear twice in Table 3 – first in the thermodynamic dataset at the top of the table, and then later in the chromatographic retention factor dataset. No attempt is made to calculate the ion-specific equation coefficients. Numerical values of the [EtOHMim]<sup>+</sup>-specific and [FAP]<sup>-</sup>-specific equation coefficients have already been reported.<sup>50</sup> The experimental data given in Table 3 will be used at a later time to update the existing values for both the [EtOHMim]<sup>+</sup> and [FAP]<sup>-</sup> ions.

The Abraham model correlations given by Eqns. 5 – 7 are statistically quite good with standard deviations of less than 0.145 log units. Figure 2 compares the observed log *K* (298 K) values against the back-calculated values based on Eqn. 5. The experimental data covers a range of approximately 5.1 log units, from log *K* = 0.658 for pentane to log *K* = 5.744 for benzyl alcohol. A comparison of the back-calculated versus measured log *P* data is depicted in Figure 3. As expected the standard deviation for the log *P* correlation is slightly larger than that of the log *K* correlations because the log *P* values contain the additional experimental uncertainty in the gas-to-water partition coefficients used in the log *K* to log *P* conversion.

The equation coefficients in Eqn. 6 can be compared to those previously reported by Marciniak and Wlazlo<sup>42</sup> and by Orfao and coworkers.<sup>43</sup> As noted above Marciniak and Wlazlo determined log *K* correlations based on experimental gas-to-liquid partition coefficient data for 65 different compounds measured at temperatures of 318, 328, 338, 348, 358 and 368 K. While 323 K was not one of the temperatures studied by the authors by the authors, one should be able to reasonably assume that the log *K*

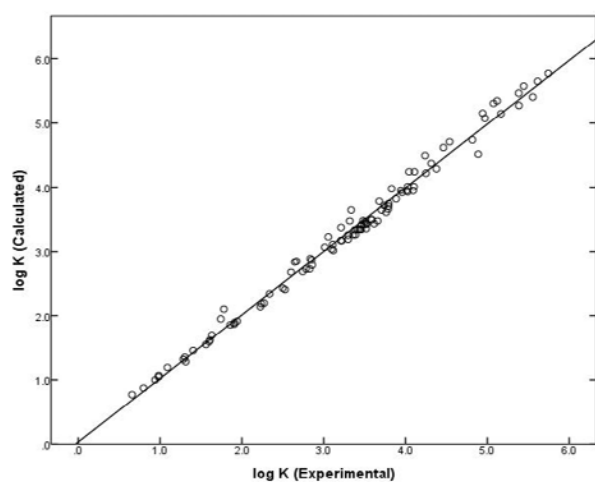


correlation for 323 K should fall somewhere between the reported correlations

$$\log K (318 \text{ K}) = -0.582(0.063) + 0.024(0.080) E + 2.48(0.08) S + 1.48(0.11) A + 1.82(0.08) B + 0.505 (0.019) L \quad (8)$$

$$\log K (328 \text{ K}) = -0.590(0.059) + 0.025(0.076) E + 2.41(0.07) S + 1.39(0.11) A + 1.66(0.08) B + 0.469 (0.018) L \quad (9)$$

for 318 K and 328 K. Comparison of Eqns. 6, 8 and 9 shows that our calculated equation coefficients for the 323 K correlation do fall in between those reported by Marciniak and Wlazlo for 318 K and 328 K when the combined standard errors in the calculated coefficients are taken into account. The slight difference between our coefficients and the arithmetic average of the coefficients of Eqns. 8 and 9 likely results from removal of the  $(e_{k,\text{cation}} + e_{k,\text{anion}}) \cdot E$  term in Eqn. 6 and the more diverse set of solutes used in deriving Eqn. 6. Our dataset (see Table 3) has 103 data points and includes one additional carboxylic acid (propanoic acid), two primary amine solutes (aniline and 2-chloroaniline), two phenolic compounds (phenol and *p*-cresol), several substituted aromatic benzene derivatives (benzointrile, acetophenone, benzaldehyde, 1,2-dichlorobenzene, and benzyl alcohol), and several halogenated alkanes (1-chlorobutane, 1-chlorohexane, 1-chlorooctane, 1-bromohexane, and 1-bromooctane), plus the solutes from both the Marciniak and Wlazlo study and Orfao *et al.* study. We also note that neither author reported a log K correlation for 298 K, nor did the authors correlate the water-to-anhydrous ionic liquid transfer properties.



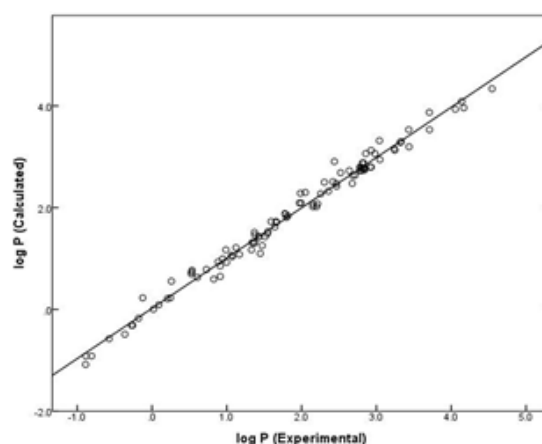
**Figure 2.** Comparison between experimental log K (298 K) and predicted values based on Eqn. 5

Orfao and coworkers<sup>43</sup> derived the following gas-to-anhydrous ionic liquid partition coefficient correlation:

$$\log K (323 \text{ K}) = -0.86(0.17) + 2.48(0.10) S + 1.18(0.23) A + 2.24(0.11) B + 0.54 (0.05) L \quad (10)$$

based on experimental data for 30 volatile organic solutes. Except for the first  $c_{k,\text{cation}} + c_{k,\text{anion}}$  term, the coefficients for Eqn. 10 are in reasonably good agreement with those of Eqn. 6. We prefer Eqn. 6 over Eqn. 10 because of the more diverse dataset used in regression analysis. As noted

previously, the dataset used by Orfao and coworkers did not contain the more acidic carboxylic acid and phenolic solutes, or any polar aromatic hydrocarbons. Benzene, toluene, ethylbenzene and *m*-xylene were the only aromatic hydrocarbons the authors studied.



**Figure 3.** Comparison between experimental log P (298 K) and predicted values based on Eqn. 7

In order to assess the predictive applicability and limitations of Eqns. 5 -7, we divided each of the three large datasets into training sets and test sets by permitting the SPSS software to randomly select half of the experimental data points. The selected data points became the training sets and the compounds that were not selected served as the test sets. Analysis of the measured log K and log P training sets yielded the following mathematical correlations:

$$\log K (298 \text{ K}) = -0.461(0.065) + 2.452(0.070) S + 1.543(0.139) A + 2.212(0.124) B + 0.564 (0.017) L \quad (11)$$

(N = 51, SD = 0.111, R<sup>2</sup> = 0.992, F = 1501)

$$\log K (323 \text{ K}) = -0.448(0.057) + 2.323(0.058) S + 1.224(0.101) A + 1.859(0.092) B + 0.448 (0.017) L \quad (12)$$

(N = 52, SD = 0.089, R<sup>2</sup> = 0.993, F = 1743)

$$\log P (298 \text{ K}) = 0.021(0.106) E + 0.517(0.119) S - 2.126(0.172) A - 2.620(0.164) B + 2.880 (0.032) V \quad (13)$$

(N = 51, SD = 0.134, R<sup>2</sup> = 0.997, F = 3111)

The  $(e_{k,\text{cation}} + e_{k,\text{anion}}) \cdot E$  and  $(c_{p,\text{cation}} + c_{p,\text{anion}})$  terms were removed from the correlations because the equation coefficients were small and the standard errors exceeded the calculated coefficients. Inspection of Eqns. 5-7 and Eqns. 11-13 indicate that to within the standard errors in the equation coefficients, the training set equation coefficients are identical to the equation coefficients for the full datasets. The training set expressions were then used to estimate the gas-to-anhydrous ionic liquid partition coefficients for the 51 solutes in the in the log K test sets, and the water-to-anhydrous ionic liquid partition coefficients for the 51 compounds in the log P test set. For the estimated and experimental values we found SD values of 0.139, 0.113 and 0.159; average absolute error (AAE) values of 0.105, 0.090, and 0.122; and average error (AE) values of 0.020,

0.001 and 0.008 for Eqns. 11-13, respectively. The small AE values suggest that there is very little bias in using Eqns. 11-13 predict partition coefficients of solutes into ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>). The training and test set analyses were performed three more times with very similar statistical results.

## Conclusion

Mathematical correlations based on the Abraham solvation parameter model have been derived for describing the partitioning behaviour of solutes dissolved in 1-(2-hydroxyethyl)-3-methylimidazolium tris(pentafluoroethyl)-trifluorophosphate ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>) from experimental partition coefficient data for 90 different organic compounds. The derived correlations are expected to provide reasonably accurate predictions for the partition coefficients of additional solutes in anhydrous ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>) provided that the solute's descriptor values fall within the range of values given in Table 4. Small gaseous solutes like nitrogen gas, carbon monoxide, carbon disulphide, sulphur dioxide, ethane, etc. would not be included in this descriptor range because their *V* and *L* solute descriptors are smaller than the values listed in Table 4. Lack of experimental solubility data for these small solutes dissolved in ([EtOHMIm]<sup>+</sup>[FAP]<sup>-</sup>) prevented their inclusion in the regression analyses.

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