

Thermochemical Investigations of Solute Transfer into Ionic Liquid Solvents: Updated
Abraham Model Equation Coefficients for Solute Activity Coefficient and Partition Coefficient
Predictions

Timothy W. Stephens^a, Vicky Chou^a, Amanda N. Quay^a, Connie Shen^a, Nishu Dabadge^a, Amy
Tian^a, Matthew Loera^a, Bria Willis^a, Anastasia Wilson^a, William E. Acree, Jr.^{a*}, Pamela Twu^b,
Jared L. Anderson^b and Michael H. Abraham^c

^a Department of Chemistry, University of North Texas, 1155 Union Circle Drive #305070,
Denton, TX 76203 (U.S.A.)

^b Department of Chemistry, University of Toledo, 2801 Bancroft Street MS 602, Toledo, OH
43606 (USA)

^c Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ
(UK)

Abstract

Experimental data have been compiled from the published chemical and engineering literature pertaining to the infinite dilution activity coefficients, gas solubilities and chromatographic retention factors for solutes dissolved in ionic liquid (IL) solvents. Included in the compilation are chromatographic retention factors for forty-five solutes on a 1-butyl-1-methylpyrrolidinium tricyanomethanide ionic liquid gas-liquid chromatographic stationary phase. The published experimental data were converted to gas-to-IL and water-to-IL partition coefficients, and correlated with the ion-specific equation coefficient version of the Abraham general solvation

model. Ion-specific equation coefficients were calculated for 40 different cations and 16 different anions. The calculated ion-specific equation coefficients describe the experimental gas-to-IL and water-to-IL partition coefficient data to within 0.123 and 0.149 log units, respectively.

Key Words and Phrases: ionic liquids, partition coefficients, activity coefficients, gas solubilities, predictive methods

Short running title: Solute Transfer into Ionic Liquid Solvents

* To whom correspondence should be addressed: e-mail: acree@unt.edu

Introduction

Task specific ionic liquids (ILs) can be designed by judicious selection of the cation-anion pair combination, or by functionalization of the cation/anion alkyl chain(s). Ionic liquid solvents have been designed that exhibit good selectivity in alkane/alkene and alkane/aromatic hydrocarbon separations [1], in removing sulfur and nitrogen compounds from petroleum products [2-7], in capturing carbon dioxide and sulfur dioxide from post-combustion gases [8-12], and in microfluidic “on-drop” separations and chemical sensing [13]. Predictive methods [14-19] have been developed to assist researchers in selecting a suitable cation-anion pair combination needed to achieve the desired chemical separation. In the case of functionalized ILs group contribution methods [20, 21] are available for ILs containing 1,3-dialkylimidazolium, N-alkylpyridinium, N,N-dialkylpyrrolidinium, tetraalkylammonium and tetrakisphosphonium cations with cyano (-CN), oxy (-O-) and hydroxyl (-OH) substituents.

The present study continues our characterization of the solubilizing abilities of ILs in terms of the Abraham solvation parameter model. [22-39] The basic model describes solute transfer to an IL solvent both from the gas phase (Eqns. 1 and 2):

$$\log K = c_k + e_k \cdot \mathbf{E} + s_k \cdot \mathbf{S} + a_k \cdot \mathbf{A} + b_k \cdot \mathbf{B} + l_k \cdot \mathbf{L} \quad (1)$$

$$\begin{aligned} \log K = & (c_{k,\text{cation}} + c_{k,\text{anion}}) + (e_{k,\text{cation}} + e_{k,\text{anion}}) \cdot \mathbf{E} + (s_{k,\text{cation}} + s_{k,\text{anion}}) \cdot \mathbf{S} + (a_{k,\text{cation}} + a_{k,\text{anion}}) \cdot \mathbf{A} \\ & + (b_{k,\text{cation}} + b_{k,\text{anion}}) \cdot \mathbf{B} + (l_{k,\text{cation}} + l_{k,\text{anion}}) \cdot \mathbf{L} \end{aligned} \quad (2)$$

and from water (Eqns. 3 and 4):

$$\log P = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \quad (3)$$

$$\begin{aligned} \log P = & (c_{p,\text{cation}} + c_{p,\text{anion}}) + (e_{p,\text{cation}} + e_{p,\text{anion}}) \cdot \mathbf{E} + (s_{p,\text{cation}} + s_{p,\text{anion}}) \cdot \mathbf{S} + (a_{p,\text{cation}} + a_{p,\text{anion}}) \cdot \mathbf{A} \\ & + (b_{p,\text{cation}} + b_{p,\text{anion}}) \cdot \mathbf{B} + (v_{p,\text{cation}} + v_{p,\text{anion}}) \cdot \mathbf{V} \end{aligned} \quad (4)$$

where K and P denote the gas-to-IL and water-to-IL partition coefficients, respectively. The independent variables in eqns. (1) - (4) are descriptors of the solutes. In brief, E is the solute excess molar refractivity in units of $(\text{cm}^3 \text{mol}^{-1})/10$, S denotes the solute dipolarity/polarizability, A and B represent the overall or summation hydrogen bond acidity and basicity, V refers to the McGowan volume in units of $(\text{cm}^3 \text{mol}^{-1})/100$ and L is defined as the logarithm of the gas-hexadecane partition coefficient measured at 298 K. The lower case quantities in Eqns. 1-4 are called IL-specific (Eqns. 1 and 3) and ion-specific (Eqns. 2 and 4) equation coefficients, and their numerical values are obtained by regression analysis of experimental $\log K$ (or $\log P$) data for a series of solutes in the given IL solvent or set of IL solvents. The ion-specific equation coefficients are calculated as a paired cation-anion sum (*e.g.*, $c_{p,\text{cation}} + c_{p,\text{anion}}$, $e_{p,\text{cation}} + e_{p,\text{anion}}$, *etc.*). In order to calculate equation coefficients for an individual ion, one must know the equation coefficients for the counter-ion in the IL. In other words, to calculate $c_{p,\text{cation}}$ the value of $c_{k,\text{anion}}$ must be known, and *vice versa*. Sprunger *et al.* [14-16] obtained the numerical values of the first sets of ion-specific equation coefficients by setting the six coefficients of the $[\text{Tf}_2\text{N}]^-$ anion equal to zero. In many respects this is analogous to setting a reference point for calculating thermodynamic properties of single ions.

Thus far we have calculated equation coefficients for 38 different cations and 15 different anions (see Table 1 for a list of ions for which equation coefficients have been determined). [24-39] The ion-specific equation coefficients can be combined to allow one to predict solute partition coefficients in 570 (38×15) ionic liquid solvents. While 570 different ILs may seem to be a large number it represents only a small fraction of the known ILs that have been synthesized in recent years. To extend the predictive applicability of the Abraham model to additional IL solvents, we have measured the chromatographic retention factors of a series of 45 different

organic solutes of varying polarity and hydrogen-bonding capability on a 1-butyl-1-methylpyrrolidinium tricyanomethanide ([BMPyr]⁺[C(CN)₃]⁻) stationary phase at 323 K and 353 K. Ion-specific equation coefficients have not been reported previously for the [C(CN)₃]⁻ anion. Results of the chromatographic measurements, combined with published gas-to-IL partition coefficient data for volatile solutes dissolved in ([BMPyr]⁺[C(CN)₃]⁻) [40], were used to derive Abraham model log *K* and log *P* correlations at 298 K and 323 K. As part of the present study we have also updated the cation-specific and anion-specific equation coefficients published in our earlier papers. The last major revision of the numerical values of the coefficients occurred slightly more than three years ago and was based on a total of 1790 log *K* and 1760 log *P* values. [24] More recent publications [28-35] have reported calculated ion-specific equation coefficients by subtracting the known values for the IL counter-ions from the determined IL-specific equation coefficients through $C_{k,\text{cation}} = C_{k,\text{IL}} - C_{k,\text{anion}}$, *etc.* The computational methodology is explained in detail elsewhere. [32]

There has been a considerable amount of experimental partition coefficient data, chromatographic retention factor and solubility data for solutes dissolved in additional IL solvents since the last major update. [25- 73] In fact, our current database of log *K* and log *P* values contains more 3600 measured values. Given the large increase in experimental data points, it is now time to re-determine the equation coefficients so that “better” numerical values are available for future applications. As stated above, the ion-specific equation coefficients are calculated as a paired cation-anion sum. In order to calculate equation coefficients for an individual ion, one must know the equation coefficients for the counter-ion in the IL.

Experimental Chromatographic Method and Construction of ([BMPyr]⁺[C(CN)₃]⁻) Data Set

The sample of 1-butyl-1-methylpyrrolidinium tricyanomethanide, $([\text{BMPyr}^+][\text{C}(\text{CN})_3]^-)$, studied in the present investigation 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) purchased from Supelco (Bellefonte, PA). The IL coating solutions were prepared in dichloromethane using a 0.45% (w/v) concentration of $([\text{BMPyr}^+][\text{C}(\text{CN})_3]^-)$.

Forty-five (45) probe molecules were selected for the characterization of the $([\text{BMPyr}^+][\text{C}(\text{CN})_3]^-)$ stationary phase. The names of the solutes, along with the chemical purities and sources, are provided in Table 2. All solute molecules were used as received from the chemical suppliers. The presence of trace impurities in the samples would in no way affect the experimental results because the main chromatographic peak was clearly distinguished from any minor impurity peak by its much larger intensity.

Chromatographic retention factors, k , were measured on the $([\text{BMPyr}^+][\text{C}(\text{CN})_3]^-)$ stationary phase at both 323 K and 353 K as part of the present investigation. The percent relative standard deviation (% RSD) in the recorded retention times for all solutes included in the present study was less than 1 %. The integrity of the stationary phase was verified periodically during the course of the experimental measurements by monitoring the efficiency and retention factor of the naphthalene separation. The observed $\log k$ values are given in the second and third columns of Table 3. The $\log k$ values at 298 K were calculated from a linear plot of $\log k$ versus $1/T$ based on the measured data at 323 K and 353 K.

The thermodynamic gas-to-ionic liquid partition coefficient, K , can be obtained from isothermal chromatographic measurements through $K = V_N/V_L$, V_L is the volume of the ionic liquid present as the stationary phase and V_N is the volume of the carrier gas needed to elute the solute. [74] The retention factor, is defined as $k = (t_r - t_m)/t_m$ [75], where t_r is the retention time of

the solute under consideration and t_m is the “dead” retention time for an unretained solute, which was methane in the present investigation. The corrected retention time, $t_r - t_m$, is directly proportional to the corrected elution volume V_N , consequently the retention factors and gas-to-ionic liquid stationary phase partition coefficients are related to each other through,

$$K = P^* \cdot k \quad \text{or} \quad \log K = \log P^* + \log k \quad (5)$$

The proportionality constant Eqn. 5 relating the retention factor and gas-to-liquid partition coefficient, P^* , is the phase ratio. This quantity depends only upon the chromatographic conditions, which should remain essentially constant for a given column for the duration of time that it takes to acquire the retention factors.

Thermodynamic gas-to-liquid partition coefficients are required to compute the proportionality constants needed in Eqn. 5 for converting the observed $\log k$ values in Table 2 to $\log K$ data. Domńska and Lukoshko [40] recently published infinite dilution activity coefficients, $\gamma_{\text{solute}}^\infty$, and gas-to-IL partition coefficients, K , of water and 61 organic solutes dissolved in ([BMPyr]⁺[C(CN)₃]⁻) at six temperatures from 318 K to 368 K. Experimental uncertainties in the measured values K and $\gamma_{\text{solute}}^\infty$ were reported to be less than 3 %. The published experimental data were extrapolated to 298 K and 323 K by assuming a linear $\ln K$ versus $1/T$ relationship. There should be very little uncertainty in the extrapolated values because the experimental measurements were performed near both desired temperatures, less than 20 K in most instances. The proportionality constants needed in the Eqn. 5, $\log P^* = 2.339$ for 298 K and $\log P^* = 2.326$ for 323 K, for ([BMPyr]⁺[C(CN)₃]⁻) were the calculated average between the measured $\log k$ and $\log K$ values for 14 common organic compounds (*e.g.*, benzene, toluene, ethylbenzene, *m*-xylene, *o*-xylene, *p*-xylene, 2-propanol, 1-butanol, ethyl acetate, butyraldehyde, 1,4-dioxane, 2-pentanone, 1-nitropropane, and pyridine) in the IL data set

that were studied by both us and Domńska and Lukoshko [40]. The $\log P^*$ values for each individual solute differed from the average values by less than ± 0.03 log units, further suggesting that the proportionality constants did indeed remain constant during the duration of the experimental measurements.

The Abraham model also describes solute transfer between two condensed phases, and in the case of IL solvents it is possible to construct a solute transfer process between water and the anhydrous IL solvent. The transfer process is akin to a partitioning process (or more specifically a hypothetical partitioning process) wherein the ionic liquid and water are not in actual physical contact with each other. In a direct practical partitioning process the two phases would be in physical contact, and the solute would be distributed between an aqueous phase (saturated with the IL solvent) and an IL phase (saturated with water). For some partitioning systems the organic solvent and water are almost completely immiscible with each other, and the presence of trace water in the organic solvent and trace organic solvent dissolved in water has a negligible effect on the solute's partitioning behavior. In other words, the direct practical partition coefficient and indirect hypothetical partition coefficient are nearly identical. There have been insufficient experimental studies on ionic liquid solvents to reach any meaningful conclusions at the present time. Hypothetical indirect partition coefficients are still useful in that predicted $\log P$ values can be converted to $\log K$ and γ_{solute}^{∞} values through standard thermodynamic relationships

$$\log K = \log P + \log K_w \quad (6)$$

and

$$\log P + \log K_w = \log \left(\frac{RT}{\gamma_{solute}^{\infty} P_{solute}^o V_{solvent}} \right) \quad (7)$$

where K_w is the solute's gas-to-water partition coefficients, R is the universal gas constant, $V_{solvent}$ is the molar volume of the IL solvent, and P_{solute}^o is the vapor pressure of the organic solute at the system temperature (T). The solutes' gas phase partition coefficients into water (K_w) needed for these calculations were taken from the published literature. [22, 23, 76]

The calculated $\log K$ and $\log P$ values are compiled in Table 4 for solutes dissolved in ([BMPyrr]⁺[C(CN)₃]⁻). The organic solutes cover a wide range of solvent polarities and hydrogen-bonding capabilities. We note that $\log P$ values are tabulated only for 298 K because $\log K_w$ at 323 K are not currently available for all of the solutes studied. Listed in Table 5 are the numerical solute descriptors for the 82 different organic compounds examined in the present communication. The tabulated solute descriptors were determined from experimental gas-liquid and high-performance liquid chromatographic retention factor data, from measured solubility data and Henry's law constants, and from observed practical partition coefficient measurements for the equilibrium solute distribution between water and an immiscible (or partially miscible) organic solvent.

Development of Abraham Model IL-Specific Correlations for ([BMPyrr]⁺[C(CN)₃]⁻)

There is sufficient experimental partition coefficient data for organic solutes dissolved in ([BMPyrr]⁺[C(CN)₃]⁻) to develop meaningful Abraham model $\log K$ and $\log P$ correlations. A meaningful linear regression analysis generally requires at least 30 experimental data as one needs to determine six curve-fit equation coefficients per correlation. Ideally the data solute should span as wide of a range solute descriptors as possible because the derived correlations applicability is determined the chemical space covered by the solute descriptors. In the present case, the solute descriptors given in Table 5 cover the range: **E** from -0.063 to 0.872; **S** from 0.000 to 1.110; **A** from 0.000 to 0.620; **B** from 0.000 to 0.640; **V** from 0.3082 to 1.4108; and **L**

from 0.970 to 5.143. Many of the volatile organic solutes will have solute descriptors that will fall within the fore-mentioned range of numerical values.

Determination of IL-specific Abraham model correlations requires that one curve-fit the experimental gas-to-IL and water-to-IL partition coefficient data for a series of solutes in the given ionic liquid in accord with Eqns. 1 and 3. Preliminary regression analyses of the tabulated $\log K$ and $\log P$ data in Table 4 showed that the $a_p \cdot \mathbf{A}$ term was negligible in the $\log P$ correlation. The calculated equation coefficient was very small ($a_p = -0.055$) and the standard error in the coefficient was larger than the coefficient itself. The $a_p \cdot \mathbf{A}$ term was removed from the $\log P$ correlation, and the regression analyses were rerun to give the following three mathematical expressions:

$$\begin{aligned} \log K \text{ (at 298 K)} &= -0.461(0.041) + 0.214(0.053) \mathbf{E} + 2.497(0.051) \mathbf{S} + 3.701(0.067) \mathbf{A} \\ &\quad + 0.243(0.061) \mathbf{B} + 0.684(0.012) \mathbf{L} \\ &\quad (\text{SD} = 0.080, \text{N} = 96, R^2 = 0.994, \text{and } F = 2857) \end{aligned} \quad (8)$$

$$\begin{aligned} \log K \text{ (at 323 K)} &= -0.513(0.034) + 0.248(0.044) \mathbf{E} + 2.297(0.043) \mathbf{S} + 3.225(0.056) \mathbf{A} \\ &\quad + 0.201(0.051) \mathbf{B} + 0.579(0.010) \mathbf{L} \\ &\quad (\text{SD} = 0.066, \text{N} = 96, R^2 = 0.995, \text{and } F = 3348) \end{aligned} \quad (9)$$

and

$$\begin{aligned} \log P \text{ (at 298 K)} &= -0.126(0.072) + 0.430(0.074) \mathbf{E} + 0.398(0.077) \mathbf{S} - 4.563(0.085) \mathbf{B} \\ &\quad + 3.333(0.062) \mathbf{V} \\ &\quad (\text{SD} = 0.120, \text{N} = 95, R^2 = 0.993, \text{and } F = 3226) \end{aligned} \quad (10)$$

where SD corresponds to the standard deviation of the derived correlation equation, N refers to the number of experimental data used in developing the correlation equation, R^2 is the squared correlation coefficient and F represents the Fisher F-statistic. As an informational note we remind readers that the number of data points used in each regression analysis is slightly larger than the total number of solutes because the fourteen solutes used in converting the chromatographic retention factors to gas-to-liquid partition coefficients (see Eqn. 5) appear twice in Table 4 – first in the thermodynamic dataset at the top of the table, and then later in the chromatographic retention factor dataset. The standard error in each of the equation coefficients is given in parenthesis immediately following the respective coefficient. The SPSS Statistics (Version 20) software was used in performing all of the regression analyses.

The Abraham model correlations given by Eqns. 8 – 10 are statistically very good with standard deviations of less than 0.120 log units. Figure 1 compares the observed log K (298 K) values against the back-calculated values based on Eqn. 8. The experimental data covers a range of approximately 4.2 log units, from log K = 0.939 for pentane to log K = 5.164 for benzonitrile. A comparison of the back-calculated versus measured log P data is depicted in Figure 2. 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 predictive applicability and limitations of Eqns. 8 – 10 were assessed using training set and test set analyses. The SPSS software randomly sorted each of the three large data sets into two smaller equal sized data sets containing 48 data points each, the first dataset became the training set and the second dataset served as the test set. Analyses of the three training sets gave the following Abraham model equations:

$$\begin{aligned} \log K \text{ (at 298 K)} = & -0.505(0.055) + 0.203(0.067) \mathbf{E} + 2.523(0.072) \mathbf{S} + 3.717(0.103) \mathbf{A} \\ & + 0.178(0.096) \mathbf{B} + 0.696(0.016) \mathbf{L} \end{aligned} \quad (11)$$

(SD = 0.075, N = 48, R² = 0.995, and F = 1591)

$$\begin{aligned} \log K \text{ (at 323 K)} = & -0.543(0.045) + 0.245(0.055) \mathbf{E} + 2.316(0.060) \mathbf{S} + 3.228(0.085) \mathbf{A} \\ & + 0.154(0.099) \mathbf{B} + 0.586(0.013) \mathbf{L} \end{aligned} \quad (12)$$

(SD = 0.062, N = 48, R² = 0.995, and F = 1925)

and

$$\begin{aligned} \log P \text{ (at 298 K)} = & -0.088(0.095) + 0.406(0.096) \mathbf{E} + 0.638(0.106) \mathbf{S} - 4.652(0.131) \mathbf{B} \\ & + 3.290(0.082) \mathbf{V} \end{aligned} \quad (13)$$

(SD = 0.117, N = 48, R² = 0.994, and F = 1670)

Careful examination of Eqns. 8-10 and Eqns. 11-13 reveals 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-IL partition coefficients for the 48 organic solutes in the in the log *K* test sets, and the water-to-IL partition coefficients for the 47 organic solutes in the log *P* test set. For the estimated and experimental values we found SD values of 0.088, 0.069 and 0.125; average absolute error (AAE) values of 0.066, 0.057, and 0.096; and average error (AE) values of 0.031, 0.030 and 0.030 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 ([BMPyrr]⁺[C(CN)₃]⁻). The training and test set analyses were performed three more times with very similar statistical results. Equations 8-10 are expected to predict the log *K* and log *P* values for additional compounds in ([BMPyrr]⁺[C(CN)₃]⁻) to within 0.120 log units or less, provided that the solute

descriptors of the additional compounds are similar to the values of the solutes used in deriving the respective predictive equation.

Revision and Updating of Existing Ion-Specific Abraham Model Equation Coefficients

The Abraham model correlations that have just been derived pertain only to the ([BMPyrr]⁺[C(CN)₃]⁻) ionic liquid. It is possible to use the derived equation coefficients to calculate the anion-specific equation coefficients for [C(CN)₃]⁻ using our previously reported cation-specific equation coefficients for [BMPyrr]⁺ based on only 31 measured log *K* values [24]. We have done this several times in the past [24, 26, 28] as we have added new cations and anions to our large database. Our last major revision and update of the ion-specific equation coefficients occurred slightly more than three years ago and was based on a total of 1790 log *K* and 1760 log *P* values [24]. Our current log *K* and log *P* databases contain more than 3600 experimental values, and is given as Tables S1 – S3 in the supporting materials. Each database has about doubled in size. Several of the more notable changes in the database include replacement of the log *K* and log *P* values for solutes dissolved in 1-(methylethylether)-3-methylimidazolium *bis*(trifluoromethylsulfonyl)imide at 298.15 K [27], addition of several more cations and anions, and the nearly doubling of experimental log *P* and log *K* through recently published activity coefficient, solubility and chromatographic retention data. There was a mathematical error in the computer program used to correct the measured gas-to-liquid partition coefficient for solutes dissolved in 1-(methylethyl-ether)-3-methylimidazolium *bis*(trifluoromethylsulfonyl)imide at 298.15 K back to 298 K. The corrected log *K* and log *P* values are given in Table 6. The Abraham model IL-specific log *K* and log *P* correlations (Eqns. 14 and 15) for 1-(methylethylether)-3-methylimidazolium *bis*(trifluoromethylsulfonyl)imide should be:

$$\begin{aligned} \text{Log } K \text{ (at 298 K)} = & -0.509(0.089) + 0.065(0.111) \mathbf{E} + 2.476(0.112) \mathbf{S} + 2.271(0.153) \mathbf{A} \\ & + 0.671(0.130) \mathbf{B} + 0.603(0.021) \mathbf{L} \end{aligned} \quad (14)$$

$$(\text{SD} = 0.108, \text{N} = 52, \text{R}^2 = 0.981, \text{and } \text{F} = 457)$$

and

$$\begin{aligned} \text{Log } P \text{ (at 298 K)} = & -0.150(0.147) + 0.012(0.138) \mathbf{E} + 0.818(0.145) \mathbf{S} - 1.289(0.192) \mathbf{A} \\ & - 4.263(0.157) \mathbf{B} + 3.116(0.117) \mathbf{V} \end{aligned} \quad (15)$$

$$(\text{SD} = 0.129, \text{N} = 49, \text{R}^2 = 0.993, \text{and } \text{F} = 1224)$$

Equations 14 and 15 provide very reasonable mathematical descriptions for the experimental log K and log P data as documented by standard deviations of 0.13 log units.

Updated numerical values of the cation-specific and anion-specific equation coefficients were determined by regression analysis of the experimental log K and log P values listed in Tables S1 – S3. The experimental data in each of the three tables were analyzed collectively to yield the following Abraham model correlations:

$$\begin{aligned} \log K \text{ (at 298 K)} = & \sum_{\text{cations}} (c_{k,\text{cation}} + e_{k,\text{cation}} \mathbf{E} + s_{k,\text{cation}} \mathbf{S} + a_{k,\text{cation}} \mathbf{A} + b_{k,\text{cation}} \mathbf{B} + l_{k,\text{cation}} \mathbf{L}) + \\ & \sum_{\text{anion}} (c_{k,\text{anion}} + e_{k,\text{anion}} \mathbf{E} + s_{k,\text{anion}} \mathbf{S} + a_{k,\text{anion}} \mathbf{A} + b_{k,\text{anion}} \mathbf{B} + l_{k,\text{anion}} \mathbf{L}) \end{aligned} \quad (16)$$

$$(\text{SD} = 0.123, \text{N} = 3786, \text{R}^2 = 0.998 \text{ and } \text{F} = 7876)$$

$$\begin{aligned} \log K \text{ (at 323 K)} = & \sum_{\text{cations}} (c_{k,\text{cation}} + e_{k,\text{cation}} \mathbf{E} + s_{k,\text{cation}} \mathbf{S} + a_{k,\text{cation}} \mathbf{A} + b_{k,\text{cation}} \mathbf{B} + l_{k,\text{cation}} \mathbf{L}) + \\ & \sum_{\text{anion}} (c_{k,\text{anion}} + e_{k,\text{anion}} \mathbf{E} + s_{k,\text{anion}} \mathbf{S} + a_{k,\text{anion}} \mathbf{A} + b_{k,\text{anion}} \mathbf{B} + l_{k,\text{anion}} \mathbf{L}) \end{aligned} \quad (17)$$

$$(\text{SD} = 0.114, \text{N} = 3660, \text{R}^2 = 0.998 \text{ and } \text{F} = 5859)$$

and

$$\log P(\text{at } 298 \text{ K}) = \sum_{\text{cations}} (c_{p,\text{cation}} + e_{p,\text{cation}} E + s_{p,\text{cation}} S + a_{p,\text{cation}} A + b_{p,\text{cation}} B + v_{p,\text{cation}} V) + \sum_{\text{anion}} (c_{p,\text{anion}} + e_{p,\text{anion}} E + s_{p,\text{anion}} S + a_{p,\text{anion}} A + b_{p,\text{anion}} B + v_{p,\text{anion}} V) \quad (18)$$

$$(\text{SD} = 0.149, N = 3731, R^2 = 0.996 \text{ and } F = 3423)$$

In accordance with the computational methodology recommended by Sprunger et al. [14-16] we have set all equation coefficients for the $[\text{Tf}_2\text{N}]^-$ anion equal to zero. The calculated cation-specific and anion-specific equation coefficients for Eqns. 16 – 18 are listed in Tables 7 – 9, respectively. Reported for the first time are equation coefficients for the tricyanomethanide anion, $[\text{C}(\text{CN})_3]^-$. The standard errors in the ion-specific equation coefficients are listed in parenthesis immediate below the respective coefficients. For the most part, the larger standard errors are noted in the equation coefficients for those ions for which experimental partition coefficient data is limited. The number of data points for the individual ions ranges from a minimum of 27 $\log K$ values for the $[\text{MO}_3\text{Am}]^+$ cation to more than 1700 $\log K$ values for the $[\text{Tf}_2\text{N}]^-$ anion, which is sufficient for the regression analyses. The $\log K$ (at 323 K) database contains a smaller quantity of gas-to-IL partition coefficient data for inorganic gases as researchers often reported the Henry's law constants for hydrogen, oxygen, nitrogen, carbon monoxide, carbon dioxide and sulfur dioxide at only 298 K. Henry's law constants for methane, ethane, propane, butane, ethene and propene tended to be reported at only 298 K as well. Hence, the smaller number of data points in the $\log K$ (at 323 K) data set.

Also included in Tables 7 – 9 are the cation-specific equation coefficients for $[\text{D}_2\text{MIm}]^+$, $[\text{PMPyrr}]^+$, $[\text{PeMPyrr}]^+$, $[\text{HMPyrr}]^+$, $[\text{OMPyrr}]^+$, $[\text{DMPyrr}]^+$, $[\text{MB}_3\text{Am}]^+$, $[\text{OM}_3\text{Am}]^+$, $[\text{OD}_3\text{Am}]^+$, and $[\text{O}_4\text{Am}]^+$ that were taken from our earlier papers [28, 30, 31] which reported IL-specific Abraham model correlations for ionic liquids containing the fore-mentioned cations paired with

the *bis*(trifluoromethylsulfonyl)imide anion. There was nothing to be gained by re-determining the equation coefficients for these ten cations. Each cation appeared only in the single ionic liquid containing the $[\text{Tf}_2\text{N}]^-$ anion, and such cases, the IL-specific and cation-specific equation coefficients are equal. A redetermination would have simply returned our previously published numerical values. Log K equation coefficients for these ions at 323 K were determined in similar fashion by regression the experimental gas-to-partition coefficient data for each ionic liquid as part of the present study.

The three Abraham model linear free energy relationships are statistically very good, and describe the experimental log K and log P data that cover a 12.5 log unit and 8.7 log unit range to within standard deviations of 0.123 log units (Eqn. 16), 0.114 log units (Eqn. 17) and 0.149 log units (Eqn. 18) as shown in Figures 3 – 5, respectively. The figures graphically depict a comparison of the experimental log K and log P data to back-calculated values based on the Abraham model using the ion-specific equation coefficients from Tables 7-9. Based on the limited number of replicate independent activity coefficient measurements that have been performed for solutes dissolved in ILs we believe that 0.05 to 0.15 log units would be a reasonable guesstimate of the uncertainty associated with the experimental log K values. Slightly larger standard deviations are expected for the log P correlation which also includes the experimental uncertainties in the log K_w data used to convert the log K values to log P . In order to assess the robustness of the derived Abraham model correlations (Eqns. 16-18), we divided the data points into a training set and a test set by selecting every other data point in each of the three large databases. This selection method assured that each cation and anion were equally represented in both the training set and test set. Equal representation was important for those ions such as $[\text{NEP}]^+$, $[\text{Et}_3\text{S}]^+$, $[\text{MO}_3\text{Am}]^+$, $[\text{HexomMIm}]^+$, and $[(\text{Hexom})_2\text{Im}]^+$ that

appeared only a few times in the database. We did not want the majority of occurrences for these ions to be in the test set as there would not be sufficient data in the training set to determine the ion-specific equation coefficients. The selected data points became the training sets and the remaining compounds that were left served as the test sets. The experimental data in the log K and log P training sets were analyzed in accordance with the ion-specific version of the Abraham solvation parameter model. The derived training set equations were then used to predict the respective partition coefficients for the compounds in the test sets. To conserve journal space the ion-specific equation coefficients are given in the Supporting Material (see Tables S4 – S6). For the predicted and experimental values, we found SD = 0.171 (Eqn. 16), SD = 0.131 (Eqn. 17) and SD = 0.169 (Eqn. 18), AAE (average absolute error) = 0.113 (Eqn. 16), AAE = 0.097 (Eqn. 17) and AAE = 0.131 (Eqn. 18), and AE (average error) = -0.010 (Eqn. 16), AE = -0.002 (Eqn. 17) and AE = -0.001 (Eqn. 18). There is therefore very little bias in using Eqns. 16-18 with AE equal to -0.010, -0.002 and -0.001 log units. The training and test set analyses were performed two more times with similar results.

The reason for determining the ion-specific equation coefficients is to enable one to predict gas-to-anhydrous IL and water-to-anhydrous IL partition coefficients in those ionic liquids for which an Abraham model IL-specific correlation is not available. As noted above, the ion-specific equation coefficients can be combined through Eqns. 2 and 4 to yield a predictive equation specific to the given cation-anion pair. The new and revised ion-specific equation coefficients that we have now reported for 40 different cations and for 16 different anions can be combined to give predictive equations for 640 ionic liquids. Over the past two years we have been testing our existing ion-specific equation coefficients to predict the newly published partition coefficient data to see how good the predictions might be. We noted in these

calculations that the quality of the predictions depended on the number of experimental data points associated with the given cation/anion at the time the ion-specific equation coefficient was determined, and the number of different ionic liquids in the database that contained the given cation/anion. The first observation was expected based on simple statistical arguments. One can determine the equation of a line based minimally on only two data points, however one is not sure that additional measurements will fall on the straight line determined from the two data points. A more meaningful curve-fit would require several more experimental values distributed over as wide a range of values as possible. The reason for the large standard errors in the ion-specific equation coefficients for ions such as $[\text{F}_3\text{Ac}]^-$ is the limited number of data points that the calculated coefficients are based on. As more data points for $[\text{F}_3\text{Ac}]^-$ -containing ionic liquids become available, a re-determination will result in a change in the numerical values and the standard errors should be reduced. Re-determinations lead to larger changes in the numerical equation coefficients if the values are based on only a few data points. Relatively small numerical changes in equation coefficients are noted in those equation coefficients that are based on a large number of data points.

The second observation concerning the number of different ion liquids in the large database that contain the given ion likely results from the complex way in which the specific ion-coefficients are interrelated. Except for ionic liquids containing the $[\text{Tf}_2\text{N}]^-$ anion, the addition of a new ionic liquid to the $\log K$ and $\log P$ databases will likely affect more than half of the previously calculated equation coefficients. Each anion is tied to several cations in the database, and each cation is tied to several anions in the database. In order to get some idea of the “stability” of the set of equation coefficients for a given cation/anion, we have performed “leave-one-IL-out” method analyses at various stages during the databases expansion. The method

involves removing the given ionic liquid from the log K or log P database just prior to the regression analysis for determining the ion-specific equation coefficients. The calculated coefficients for the cation and anion contained in the given the ionic liquid are then used to calculate the log K values (or log P values), which are then compared to the measured data. Representative results from the “leave-one-IL-out” calculations are given in Table S7 of the Supporting Material. Examination of the statistical information in Table S7 shows that the standard deviations for the log K predictions were generally on the order of SD = 0.080 to SD = 0.165 log units if both the cation and anion appeared in at least three different ionic liquids in the database. We think that this is a realistic estimate of the expected error that would be associated in using the numerical values of the ion-specific equation coefficients given in Tables 6 – 8 to predict the partition coefficients and activity coefficients of volatile organic solutes dissolved in ionic liquid solvents for which Abraham model IL-specific correlations are not available. As noted in several of our earlier publications, IL-specific correlations should provide the better set of predictions, followed by the Abraham model expressions obtained by combining the ion-specific equation coefficients, and then the Abraham model expressions derived from the fragment group contribution values. For many practical design calculations involving chemical separations an error of 0.08 to 0.16 log units will often suffice.

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Table 1. Names and Abbreviations of the Various Cations and Anions Contained in the Different Ionic Liquid Solvents

Ion Abbreviation	Ion Name
Cation	
[MEIm] ⁺	1-methyl-3-ethylimidazolium
[MBIm] ⁺	1-methyl-3-butylimidazolium
[MHIIm] ⁺	1-methyl-3-hexylimidazolium
[MOIm] ⁺	1-methyl-3-octylimidazolium
[MDIm] ⁺	1-methyl-3-decylimidazolium
[M ₂ EIm] ⁺	1,2-dimethyl-3-ethylimidazolium
[PM ₂ Im] ⁺	1-propyl-2,3-dimethylimidazolium
[D ₂ Mim] ⁺	1,3-didecyl-2-methylimidazolium
[HexdMIm] ⁺	1-hexadecyl-3-methylimidazolium
[(Meo) ₂ Im] ⁺	1,3-dimethoxyimidazolium
[MeoeMIm] ⁺	1-methylethylether-3-methylimidazolium
[HexomMIm] ⁺	1-hexyloxymethyl-3-methylimidazolium
[(Hexom) ₂ Im] ⁺	1,3-dihexyloxymethyl-3-methylimidazolium
[EtOHMIm] ⁺	1-ethanol-3-methylimidazolium
[CNPrMIm] ⁺	1-(3-cyanopropyl)-3-methylimidazolium
[3-MBPy] ⁺	3-methyl-N-butylpyridinium
[4-MBPy] ⁺	4-methyl-N-butylpyridinium
[NEP] ⁺	N-ethylpyridinium
[PrOHPy] ⁺	1-(3-hydroxypropyl)pyridinium
[PMPyrr] ⁺	1-propyl-1-methylpyrrolidinium
[BMPyrr] ⁺	1-butyl-1-methylpyrrolidinium
[PeMPyrr] ⁺	1-pentyl-1-methylpyrrolidinium
[HMPyrr] ⁺	1-hexyl-1-methylpyrrolidinium
[OMPyrr] ⁺	1-octyl-1-methylpyrrolidinium
[DMPyrr] ⁺	1-decyl-1-methylpyrrolidinium
[MeoeMPyrr] ⁺	1-(2-methylethyl)-1-methylpyrrolidinium
[PMPip] ⁺	1-propyl-1-methylpiperidinium
[BMPip] ⁺	1-butyl-1-methylpiperidinium
[MeoeMPip] ⁺	1-(2-methoxyethyl)-1-methylpiperidinium
[MeoeMMorp] ⁺	1-(2-methoxyethyl)-1-methylmorpholinium
[M ₃ BAm] ⁺	trimethyl(butyl)ammonium
[MO ₃ Am] ⁺	methyl(trioctyl)ammonium

[MB ₃ Am] ⁺	methyl(tributyl)ammonium
[HexM ₃ Am] ⁺	hexyl(trimethyl)ammonium
[OM ₃ Am] ⁺	octyl(trimethyl)ammonium
[DM ₃ Am] ⁺	decyl(trimethyl)ammonium
[O ₄ Am] ⁺	tetraoctylammonium
[Et ₃ S] ⁺	triethylsulfonium
[MiB ₃ P] ⁺	methyl(triisobutyl)phosphonium
[H ₃ TdP] ⁺	trihexyl(tetradecyl)phosphonium
[OiQu] ⁺ (this study)	N-octylisoquinolinium
Anion	
[Tf ₂ N] ⁻	<i>bis</i> (trifluoromethylsulfonyl)imide
[BF ₄] ⁻	tetrafluoroborate
[PF ₆] ⁻	hexafluorophosphate
[SCN] ⁻	thiocyanate
[EtSO ₄] ⁻	ethylsulfate
[OtSO ₄] ⁻	octylsulfate
[F ₃ Ac] ⁻	trifluoroacetate
[Trif] ⁻	trifluoromethanesulfonate (triflate)
[N(CN) ₂] ⁻	dicyanamide
[E ₂ PO ₄] ⁻	diethylphosphate
[NO ₃] ⁻	nitrate
[FAP] ⁻	<i>tris</i> (pentafluoroethyl)trifluorophosphate
[B(CN) ₄] ⁻	tetracyanoborate
[MeSO ₃] ⁻	methanesulfonate
[BETI] ⁻	<i>bis</i> (pentafluoroethylsulfonyl)imide
[Tos] ⁻	tosylate
[C(CN) ₃] ⁻ (this study)	tricyanomethanide

Table 2. Tabulation of Chemical Solutes, Chemical Sources and Chemical Purities

Solute	Chemical Source ^a	Chemical Purity
Acetic acid	Supelco	99.7%
Benzaldehyde	Sigma-Aldrich	99+%
Benzene	Sigma-Aldrich	99.8%
Benzonitrile	Sigma-Aldrich	99%
Bromoethane	Acros Organics	98%
1-Bromohexane	Sigma-Aldrich	98%
1-Bromooctane	Sigma-Aldrich	99%
Butyraldehyde	Acros Organics	99%
1-Butanol	Fisher Scientific	99.9%
1-Chlorobutane	Sigma-Aldrich	99%
1-Chlorohexane	Sigma-Aldrich	99%
1-Chlorooctane	Sigma-Aldrich	99%
Cyclohexanol	J.T. Baker	99%
Cyclohexanone	Sigma-Aldrich	99.8%
1,2-Dichlorobenzene	Sigma-Aldrich	99%
1,4-Dioxane	Sigma-Aldrich	99.8%
N,N-Dimethylformamide	Fisher Scientific	99.9%
Ethyl acetate	Fisher Scientific	99.9%
Ethylbenzene	Eastman Kodak Co	95+%
1-Iodobutane	Sigma-Aldrich	99%
Methyl caproate	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%
Propionitrile	Sigma-Aldrich	99%
Pyridine	Sigma-Aldrich	99.9%
Pyrrole	Sigma-Aldrich	98%
Toluene	Fisher Scientific	99.80%
<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%
2-Propanol	Fisher Scientific	99.6%

^a 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).

Table 3. Chromatographic Retention Factors for Organic Solutes on a 1-butyl-1-methyl-pyrrolidinium tricyanomethanide, ([BMPyrr]⁺[C(CN)₃]⁻), Stationary Phase at 298 K, 323 K and 353 K

Solute	log <i>k</i> (323 K)	log <i>k</i> (353 K)	log <i>k</i> (298 K)
Acetic acid	1.855	1.168	2.533
Benzaldehyde	2.003	1.339	2.658
Benzene	0.173	-0.279	0.619
Benzonitrile	2.140	1.476	2.795
Bromoethane	-0.576	-0.800	-0.355
1-Bromooctane	1.212	0.555	1.861
1-Butanol	0.935	0.357	1.505
Butyraldehyde	0.148	-0.302	0.592
1-Chlorobutane	-0.299	-0.745	0.140
1-Chlorohexane	0.305	-0.217	0.820
1-Chlorooctane	0.887	0.278	1.489
Cyclohexanol	1.744	1.071	2.408
Cyclohexanone	1.515	0.941	2.082
1,2-Dichlorobenzene	1.488	0.898	2.071
1,4-Dioxane	0.716	0.211	1.214
Ethyl acetate	0.013	-0.399	0.420
Ethylbenzene	0.740	0.217	1.256
1-Iodobutane	0.392	-0.087	0.865
Methyl caproate	0.935	0.325	1.538
1-Nitropropane	1.164	0.614	1.706
1-Octanol	2.127	1.324	2.919
Octylaldehyde	1.344	0.696	1.984
1-Pentanol	1.246	0.626	1.859
2-Pentanone	0.529	0.068	0.983
Phenetole	1.526	0.888	2.156
Propionitrile	0.649	0.198	1.093
Pyridine	0.996	0.480	1.505
Pyrrole	1.971	1.308	2.625
Toluene	0.492	-0.007	0.985
<i>m</i> -Xylene	0.800	0.240	1.353
<i>o</i> -Xylene	0.955	0.384	1.519

<i>p</i> -Xylene	0.796	0.242	1.343
2-Propanol	0.299	-0.205	0.797
1-Bromohexane	0.633	0.094	1.164
Propanoic acid	2.103	1.370	2.826

Table 4. 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 ([BMPyrr]⁺[C(CN)₃]⁻) at 298 K and 323 K

Solute	$\log K$ (298 K)	$\log K$ (323 K)	$\log P$ (298 K)
Based on Thermodynamic Data			
Pentane	0.939	0.673	2.639
Hexane	1.304	0.981	3.124
3-Methylpentane	1.258	0.946	3.098
2,2-Dimethylbutane	1.045	0.759	2.885
Heptane	1.660	1.279	3.620
Octane	2.009	1.569	4.119
2,2,4-Trimethylpentane	1.561	1.197	3.681
Nonane	2.346	1.857	4.496
Decane	2.687	2.141	5.007
Cyclopentane	1.500	1.190	2.380
Cyclohexane	1.828	1.476	2.728
Methylcyclohexane	1.994	1.606	3.244
Cycloheptane	2.379	1.964	2.959
Cyclooctane	2.856	2.379	3.626
1-Pentene	1.223	0.933	2.453
1-Hexene	1.598	1.248	2.758
Cyclohexene	2.226	1.831	2.496
1-Heptene	1.944	1.542	3.164
1-Octene	2.285	1.830	3.697
1-Decene	2.960	2.397	4.600
1-Pentyne	1.985	1.606	1.995
1-Hexyne	2.351	1.918	2.561
1-Heptyne	2.705	2.213	3.145
1-Octyne	3.041	2.498	3.561
Benzene	2.936	2.497	2.306
Toluene	3.314	2.814	2.664
Ethylbenzene	3.611	3.063	3.031
<i>o</i> -Xylene	3.854	3.278	3.194
<i>m</i> -Xylene	3.686	3.123	3.076
<i>p</i> -Xylene	3.673	3.117	3.083

Styrene	4.090	3.497	3.140
α -Methylstyrene	4.312	3.678	3.352
Methanol	2.920	2.491	-0.820
Ethanol	3.092	2.623	-0.578
1-Propanol	3.466	2.937	-0.094
2-Propanol	3.114	2.624	-0.366
1-Butanol	3.841	3.263	0.381
2-Butanol	3.472	2.917	0.082
2-Methyl-1-propanol	3.643	3.081	0.343
<i>tert</i> -Butanol	3.098	2.594	-0.182
Thiophene	3.178	2.718	2.138
Tetrahydrofuran	2.788	2.369	0.238
1,4-Dioxane	3.553	3.043	-0.157
Methyl <i>tert</i> -butyl ether	1.994	1.606	0.375
Ethyl <i>tert</i> -butyl ether	1.867	1.477	0.597
Methyl <i>tert</i> -amyl ether	2.352	1.916	0.882
Diethyl ether	1.669	1.331	0.499
Dipropyl ether	2.169	1.745	1.279
Diisopropyl ether	1.785	1.390	0.735
Dibutyl ether	2.829	2.305	2.139
Acetone	2.778	2.367	-0.012
2-Pentanone	3.360	2.860	0.780
3-Pentanone	3.364	2.863	0.864
Methyl acetate	2.589	2.175	0.289
Ethyl acetate	2.798	2.343	0.638
Methyl propanoate	2.893	2.430	0.743
Methyl butanoate	3.185	2.671	1.105
Butyraldehyde	2.920	2.480	0.590
Acetonitrile	3.216	2.799	0.366
Pyridine	3.848	3.323	0.408
1-Nitropropane	4.033	3.491	1.583
Based on Chromatographic Retention Factor Data			
Acetic Acid	4.872	4.184	-0.038
Benzaldehyde	4.997	4.329	2.047
Benzene	2.958	2.499	2.328
Benzonitrile	5.134	4.466	2.044
Bromoethane	1.984	1.750	1.444

1-Bromooctane	4.200	3.538	4.580
Butyraldehyde	2.931	2.474	0.601
1-Butanol	3.844	3.261	0.384
1-Chlorobutane	2.479	2.027	2.359
1-Chlorohexane	3.159	2.631	3.159
1-Chlorooctane	3.828	3.213	4.085
Cyclohexanol	4.747	4.070	0.737
Cyclohexanone	4.421	3.841	0.821
1,2-Dichlorobenzene	4.410	3.814	3.510
1,4-Dioxane	3.553	3.042	-0.157
Ethyl acetate	2.759	2.339	0.599
Ethylbenzene	3.595	3.066	3.015
1-Iodobutane	3.204	2.718	3.024
Methyl caproate	3.877	3.261	2.047
1-Nitropropane	4.045	3.490	1.595
1-Octanol	5.258	4.453	2.258
Octylaldehyde	4.323	3.670	2.643
1-Pentanol	4.198	3.572	0.848
2-Pentanone	3.322	2.855	0.742
Phenetole	4.495	3.852	2.865
2-Propanol	3.136	2.625	-0.344
Propionitrile	3.432	2.975	0.612
Pyridine	3.844	3.322	0.404
Pyrrole	4.964	4.297	
Toluene	3.324	2.818	2.674
<i>m</i> -Xylene	3.692	3.126	3.082
<i>o</i> -Xylene	3.858	3.281	3.198
<i>p</i> -Xylene	3.682	3.122	3.092
1-Bromohexane	3.503	2.959	3.633
Propanoic acid	5.165	4.429	0.425

Table 5. Abraham model solute descriptors of the organic compounds considered in the present study

Solute	E	S	A	B	L	V
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
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
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
α -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
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	0.7466
Methyl butanoate	0.106	0.600	0.000	0.450	2.943	0.8880
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
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
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
Bromoethane	0.370	0.400	0.000	0.120	2.120	0.5654
1-Bromooctane	0.339	0.400	0.000	0.120	5.143	1.4108
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
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
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
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.5450
Pyrrole	0.613	0.910	0.220	0.250	2.792	0.5774
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

Table 6. Corrected Logarithm of Partition Coefficients, $\log K$ and $\log P$, for Organic Solutes in 1-(Methylethylether)-3-methylimidazolium *bis*(Trifluoromethylsulfonyl)imide at 298.15 K

Solute	Log K	Log P		Solute	Log K	Log P
Hexane	1.108	2.928		3-Pentanone	3.220	0.720
3-Methylpentane	1.082	2.922		1,4-Dioxane	3.398	-0.312
Heptane	1.399	3.359		Methanol	2.386	-1.354
2,2,4-Trimethylpentane	1.415	3.535		Ethanol	2.635	-1.035
Octane	1.703	3.813		1-Propanol	2.955	-0.605
Nonane	2.006	4.156		2-Propanol	2.678	-0.802
Decane	2.309	4.569		2-Methyl-1-propanol	3.098	-0.202
Undecane	2.604	4.984		1-Butanol	3.293	-0.167
Dodecane	2.905	5.405		Trifluoroethanol	3.183	0.023
Tridecane	3.182			Diethyl ether	1.580	0.410
Tetradecane	3.504			Diisopropyl ether	1.705	0.655
Methylcyclopentane	1.404	2.574		Chloroform	2.446	1.656
Cyclohexane	1.528	2.428		Dichloromethane	2.125	1.165
Methylcyclohexane	1.679	2.929		Tetrachloromethane	2.128	2.318
Cycloheptane	2.011	2.601		Acetonitrile	3.103	0.253
Benzene	2.633	2.003		Nitromethane	3.434	0.484
Toluene	2.986	2.336		1-Nitropropane	3.802	1.352
Ethylbenzene	3.243	2.663		Triethylamine	1.653	-0.707
<i>m</i> -Xylene	3.313	2.703		Pyridine	3.621	0.181
<i>p</i> -Xylene	3.298	2.708		Thiophene	2.791	1.751
<i>o</i> -Xylene	3.470	2.730		Formaldehyde	2.455	
1-Hexene	1.349	2.509		Propionaldehyde	2.639	0.119
1-Hexyne	2.025	2.235		Butyraldehyde	3.395	1.065
1-Heptyne	2.324	2.764		Ethyl acetate	2.787	0.627
2-Butanone	2.999	0.279		Butyl acetate	3.382	1.442
2-Pentanone	3.246	0.666		Tetrahydrofuran	2.608	0.048

Table 7. Cation-specific and Anion-specific Equation Coefficients for the Abraham Model Gas-to-Anhydrous Ionic Liquid Partition Coefficient Correlations, $\log K$, at 298 K.

Ion	c_k	e_k	s_k	a_k	b_k	l_k
Cations						
[MEIm] ⁺	-0.505	0.088	2.305	2.381	0.683	0.654
(N = 561) ^a	(0.024)	(0.058)	(0.065)	(0.079)	(0.074)	(0.008)
[MBIm] ⁺	-0.421	0.033	2.134	2.281	0.603	0.712
(N = 485) ^a	(0.022)	(0.051)	(0.057)	(0.071)	(0.071)	(0.007)
[MHIm] ⁺	-0.379	-0.103	2.081	2.298	0.533	0.751
(N = 335) ^a	(0.025)	(0.058)	(0.063)	(0.071)	(0.069)	(0.008)
[MOIm] ⁺	-0.197	-0.216	1.301	2.021	0.994	0.837
(N = 160) ^a	(0.033)	(0.082)	(0.095)	(0.102)	(0.108)	(0.010)
[MDIm] ⁺	-0.391	-0.162	2.036	2.054	0.524	0.786
(N = 43) ^a	(0.091)	(0.178)	(0.211)	(0.173)	(0.191)	(0.028)
[HexdMIm] ⁺	0.008	-0.461	0.848	1.925	0.402	1.004
(N = 31) ^a	(0.154)	(0.169)	(0.176)	(0.269)	(0.199)	(0.047)
[M ₂ EIm] ⁺	-0.611	0.188	2.380	2.101	0.899	0.667
(N = 39) ^a	(0.078)	(0.146)	(0.154)	(0.190)	(0.149)	(0.023)
[PM ₂ Im] ⁺	-0.833	0.771	2.385	3.547	0.805	0.533
(N = 34) ^a	(0.129)	(0.181)	(0.210)	(0.243)	(0.220)	(0.038)
[D ₂ MIm] ⁺	-0.252	-0.269	1.603	1.946	0.354	0.856
(N = 40) ^a	(0.089)	(0.088)	(0.082)	(0.125)	(0.093)	(0.027)
[(Meo) ₂ Im] ⁺	-0.762	-0.013	2.557	2.427	1.154	0.584
(N = 48) ^a	(0.090)	(0.112)	(0.104)	(0.152)	(0.110)	(0.021)
[MeoeMIm] ⁺	-0.509	0.065	2.476	2.271	0.671	0.603
(N = 52) ^a	(0.089)	(0.111)	(0.112)	(0.153)	(0.130)	(0.021)
[HexomMIm] ⁺	-0.463	-0.394	2.478	2.428	0.337	0.786
(N = 34) ^a	(0.118)	(0.230)	(0.295)	(0.222)	(0.235)	(0.035)
[(Hexom) ₂ Im] ⁺	-0.314	-0.479	2.076	2.376	0.287	0.835
(N = 34) ^a	(0.118)	(0.230)	(0.295)	(0.222)	(0.235)	(0.035)
[EtOHMIm] ⁺	-0.843	0.095	2.462	2.694	1.331	0.580
(N = 151) ^a	(0.042)	(0.064)	(0.066)	(0.079)	(0.078)	(0.011)
[CNPrMIm] ⁺	-1.119	0.073	2.617	2.543	0.816	0.699
(N = 45) ^a	(0.110)	(0.150)	(0.147)	(0.204)	(0.166)	(0.029)
[3-MBPY] ⁺	-0.338	0.035	2.325	2.289	0.189	0.714
(N = 37) ^a	(0.098)	(0.203)	(0.249)	(0.246)	(0.232)	(0.030)
[4-MBPY] ⁺	-0.449	0.157	2.270	2.416	0.566	0.714
(N = 109) ^a	(0.054)	(0.106)	(0.124)	(0.131)	(0.114)	(0.016)
[NEP] ⁺	-0.668	0.246	2.399	2.403	0.936	0.672
(N = 31) ^a	(0.083)	(0.208)	(0.195)	(0.226)	(0.163)	(0.031)

[PrOHPy] ⁺	-0.713	0.151	2.663	2.874	1.311	0.611
(N = 122) ^a	(0.055)	(0.088)	(0.098)	(0.095)	(0.106)	(0.016)
[PMPyrr] ^{+,b}	-0.466	0.000	2.562	2.505	0.271	0.682
(N = 39) ^a	(0.115)		(0.087)	(0.184)	(0.107)	(0.032)
[BMPyrr] ⁺	-0.363	0.119	2.207	2.363	0.388	0.679
(N = 474) ^a	(0.033)	(0.058)	(0.061)	(0.076)	(0.067)	(0.010)
[PeMPyrr] ^{+,b}	-0.549	0.000	2.317	2.425	0.385	0.747
(N = 42) ^a	(0.087)		(0.092)	(0.155)	(0.096)	(0.023)
[HMPyrr] ^{+,b}	-0.533	-0.110	2.146	2.278	0.650	0.767
(N = 36) ^a	(0.093)	(0.099)	(0.095)	(0.196)	(0.114)	(0.026)
[OMPyrr] ^{+,b}	-0.587	-0.064	2.080	2.176	0.486	0.822
(N = 37) ^a	(0.082)	(0.090)	(0.086)	(0.160)	(0.103)	(0.023)
[DMPyrr] ^{+,b}	-0.395	-0.241	1.991	2.112	0.268	0.822
(N = 40) ^a	(0.062)	(0.070)	(0.069)	(0.110)	(0.076)	(0.018)
[MeoeMPyrr] ⁺	-0.380	0.018	2.497	2.534	0.162	0.671
(N = 104) ^a	(0.064)	(0.092)	(0.095)	(0.107)	(0.113)	(0.019)
[PMPip] ⁺	-0.435	0.149	2.281	2.476	0.410	0.675
(N = 79) ^a	(0.068)	(0.086)	(0.098)	(0.097)	(0.124)	(0.018)
[BMPip] ⁺	-0.364	0.134	2.271	2.467	0.327	0.679
(N = 111) ^a	(0.054)	(0.081)	(0.092)	(0.095)	(0.111)	(0.016)
[PeMPip] ^{+,c}	-0.477	-0.186	2.639	2.450	0.103	0.761
(N = 41) ^a	(0.065)	(0.099)	(0.123)	(0.119)	(0.112)	(0.018)
[HMPip] ^{+,d}	-0.404	-0.245	2.469	2.348	0.075	0.775
(N = 42) ^a	(0.057)	(0.088)	(0.109)	(0.105)	(0.099)	(0.016)
[MeoeMPip] ⁺	-0.440	0.065	2.484	2.537	0.241	0.688
(N = 162) ^a	(0.051)	(0.073)	(0.074)	(0.091)	(0.085)	(0.015)
[MeoeMMorp] ⁺	-0.675	0.021	2.823	2.588	0.542	0.644
(N = 160) ^a	(0.051)	(0.021)	(0.073)	(0.080)	(0.081)	(0.015)
[M ₃ BAm] ⁺	-0.458	-0.005	2.188	2.374	0.664	0.668
(N = 58) ^a	(0.049)	(0.133)	(0.153)	(0.202)	(0.201)	(0.013)
[MO ₃ Am] ⁺	-0.387	-0.130	1.460	2.327	0.501	0.927
(N = 32) ^a	(0.070)	(0.241)	(0.382)	(0.364)	(0.502)	(0.022)
[MB ₃ Am] ^{+,b}	-0.506	-0.169	2.103	2.298	0.412	0.777
(N = 44) ^a	(0.079)	(0.083)	(0.080)	(0.115)	(0.092)	(0.022)
[HexM ₃ Am] ⁺	-0.469	-0.056	2.083	2.176	0.620	0.689
(N = 93) ^a	(0.056)	(0.071)	(0.075)	(0.085)	(0.090)	(0.014)
[OM ₃ Am] ^{+,b}	-0.426	-0.338	2.242	2.195	0.684	0.779
(N = 44) ^a	(0.082)	(0.089)	(0.082)	(0.123)	(0.021)	(0.022)
[DM ₃ Am] ^{+,b}	-0.363	-0.339	1.986	2.144	0.422	0.809
(N = 46) ^a	(0.089)	(0.098)	(0.090)	(0.135)	(0.094)	(0.024)
[O ₄ Am] ^{+,b}	0.000	-0.287	1.478	1.845	0.189	0.816
(N = 42) ^a		(0.134)	(0.110)	(0.158)	(0.121)	(0.013)

[Et ₃ S] ⁺	-0.606	-0.196	2.992	2.444	0.355	0.690
(N = 31) ^a	(0.121)	(0.302)	(0.399)	(0.261)	(0.276)	(0.036)
[H ₃ TdP] ⁺	-0.358	-0.466	1.498	2.283	0.281	0.904
(N = 98) ^a	(0.057)	(0.104)	(0.105)	(0.145)	(0.125)	(0.018)
[OiQu] ⁺	-0.338	-0.417	2.502	2.364	-0.229	0.811
(N = 36) ^a	(0.117)	(0.197)	(0.250)	(0.204)	(0.241)	(0.033)
Anions						
[Tf ₂ N] ⁻	0.000	0.000	0.000	0.000	0.000	0.000
(N = 1718) ^a						
[BF ₄] ⁻	-0.192	0.227	0.343	0.978	-0.287	-0.075
(N = 310) ^a	(0.028)	(0.067)	(0.072)	(0.090)	(0.083)	(0.009)
[PF ₆] ⁻	-0.016	-0.158	0.529	0.035	-0.149	-0.096
(N = 206) ^a	(0.029)	(0.066)	(0.071)	(0.083)	(0.085)	(0.010)
[SCN] ⁻	-0.566	0.431	0.534	2.806	-0.272	-0.040
(N = 223) ^a	(0.044)	(0.077)	(0.089)	(0.104)	(0.095)	(0.013)
[EtSO ₄] ⁻	-0.173	-0.072	0.239	2.931	-0.668	-0.066
(N = 53) ^a	(0.066)	(0.145)	(0.161)	(0.202)	(0.189)	(0.017)
[OtSO ₄] ⁻	0.057	-0.126	-0.077	2.575	-0.587	0.108
(N = 97) ^a	(0.063)	(0.091)	(0.099)	(0.152)	(0.126)	(0.017)
[F ₃ Ac] ⁻	-0.295	-0.186	0.545	3.113	-0.078	0.014
(N = 32) ^a	(0.059)	(0.249)	(0.368)	(0.735)	(0.783)	(0.020)
[Trif] ⁻	-0.275	0.035	0.323	1.709	-0.175	-0.002
(N = 199) ^a	(0.039)	(0.083)	(0.093)	(0.109)	(0.102)	(0.012)
[N(CN) ₂] ⁻	-0.372	0.345	0.476	2.270	-0.198	-0.055
(N = 150) ^a	(0.051)	(0.095)	(0.092)	(0.124)	(0.097)	(0.015)
[E ₂ PO ₄] ⁻	0.093	0.107	-0.068	5.071	-0.774	0.061
(N = 38) ^a	(0.113)	(0.181)	(0.184)	(0.240)	(0.184)	(0.037)
[NO ₃] ⁻	-0.220	0.398	0.580	2.881	-0.699	-0.108
(N = 97) ^a	(0.102)	(0.115)	(0.118)	(0.172)	(0.119)	(0.032)
[FAP] ⁻	0.229	-0.049	-0.114	-1.277	0.341	-0.039
(N = 630) ^a	(0.030)	(0.053)	(0.057)	(0.064)	(0.063)	(0.009)
[B(CN) ₄] ⁻	0.048	-0.009	0.345	0.371	-0.143	-0.012
(N = 245) ^a	(0.044)	(0.079)	(0.088)	(0.099)	(0.093)	(0.013)
[MeSO ₃] ⁻	-0.827	0.463	0.417	4.083	-0.280	-0.023
(N = 51) ^a	(0.094)	(0.135)	(0.133)	(0.216)	(0.152)	(0.023)
[BETI] ⁻	-0.039	0.107	0.072	-0.301	0.093	-0.099
(N = 53) ^a	(0.064)	(0.121)	(0.115)	(0.158)	(0.129)	(0.017)
[C(CN) ₃] ⁻	-0.098	0.094	0.290	1.338	-0.145	0.005
(N = 96) ^a	(0.072)	(0.101)	(0.101)	(0.129)	(0.117)	(0.021)

^a N is the number of experimental data points associated with the given ion.

^b The numerical values of the cation-specific equation coefficients were taken from a previously published paper [28, 30, 31] that reported the Abraham model log K correlation equation for solutes dissolved in the ([Cation]⁺[Tf₂N]⁻) ionic liquid. In this case the cation-specific and IL-specific equation coefficients are equal because the coefficients for the [Tf₂N]⁻ anion are equal to zero.

^c The cation is 1-pentyl-1-methylpiperidinium, [PeMPip]⁺. Numerical values for the equation coefficients were determined by Paduszynski and Domńska [60].

^d The cation is 1-hexyl-1-methylpiperidinium, [HMPip]⁺. Numerical values for the equation coefficients were determined by Paduszynski and Domńska [60].

Table 8. Cation-specific and Anion-specific Equation Coefficients for the Abraham Model Gas-to-Anhydrous Ionic Liquid Partition Coefficient Correlations, $\log K$, at 323 K.

Ion	c_k	e_k	s_k	a_k	b_k	l_k
Cations						
[MEIm] ⁺	-0.422	0.266	1.884	1.905	0.719	0.525
(N = 552) ^a	(0.029)	(0.059)	(0.064)	(0.078)	(0.072)	(0.009)
[MBIm] ⁺	-0.454	0.130	1.922	2.039	0.552	0.604
(N = 476) ^a	(0.025)	(0.051)	(0.056)	(0.071)	(0.069)	(0.008)
[MHIm] ⁺	-0.345	0.016	1.855	1.944	0.423	0.625
(N = 298) ^a	(0.028)	(0.058)	(0.066)	(0.075)	(0.072)	(0.008)
[MOIm] ⁺	-0.353	-0.083	1.479	1.826	0.698	0.720
(N = 107) ^a	(0.048)	(0.109)	(0.145)	(0.173)	(0.178)	(0.015)
[MDIm] ⁺	-0.623	-0.144	2.061	1.966	0.439	0.739
(N = 42) ^a	(0.111)	(0.172)	(0.205)	(0.167)	(0.193)	(0.033)
[HexdMIm] ⁺	-0.186	-0.416	0.821	1.351	0.358	0.861
(N = 31) ^a	(0.144)	(0.159)	(0.165)	(0.247)	(0.186)	(0.044)
[M ₂ EIm] ⁺	-0.644	0.175	2.209	1.810	0.789	0.564
(N = 36) ^a	(0.109)	(0.148)	(0.157)	(0.182)	(0.140)	(0.031)
[PM ₂ Im] ⁺	-1.006	0.618	1.938	2.913	0.792	0.574
(N = 33) ^a	(0.128)	(0.180)	(0.199)	(0.232)	(0.208)	(0.040)
[D ₂ MIm] ^{+,b}	-0.328	-0.300	1.681	1.852	-0.064	0.751
(N = 41) ^a	(0.115)	(0.113)	(0.098)	(0.158)	(0.100)	(0.034)
[(Meo) ₂ Im] ⁺	-0.734	0.115	2.358	1.993	0.999	0.476
(N = 48) ^a	(0.083)	(0.104)	(0.096)	(0.141)	(0.102)	(0.020)
[MeoeMIm] ⁺	-0.397	-0.053	2.426	1.846	0.367	0.482
(N = 52) ^a	(0.079)	(0.101)	(0.094)	(0.135)	(0.101)	(0.019)
[HexomMIm] ⁺	-0.482	-0.210	2.129	2.050	0.342	0.664
(N = 34) ^a	(0.109)	(0.214)	(0.274)	(0.206)	(0.219)	(0.033)
[(Hexom) ₂ Im] ⁺	-0.382	-0.305	1.800	1.988	0.289	0.717
(N = 34) ^a	(0.109)	(0.214)	(0.274)	(0.206)	(0.219)	(0.033)
[EtOHMIm] ⁺	-0.770	0.121	2.290	2.231	1.116	0.473
(N = 137) ^a	(0.047)	(0.060)	(0.063)	(0.073)	(0.075)	(0.011)
[CNPrMIm] ⁺	-0.840	0.216	2.238	1.943	0.730	0.520
(N = 45) ^a	(0.116)	(0.143)	(0.143)	(0.196)	(0.159)	(0.030)
[3-MBPy] ⁺	-0.502	-0.080	2.494	2.268	0.005	0.664
(N = 37) ^a	(0.093)	(0.189)	(0.232)	(0.230)	(0.218)	(0.028)
[4-MBPy] ⁺	-0.484	0.165	2.002	1.846	0.547	0.611
(N = 125) ^a	(0.060)	(0.099)	(0.117)	(0.122)	(0.107)	(0.018)
[NEP] ⁺	-0.693	0.265	2.135	2.170	0.843	0.575
(N = 37) ^a	(0.111)	(0.180)	(0.180)	(0.218)	(0.143)	(0.036)
[PrOHPy] ⁺	-0.752	0.260	2.371	2.451	1.123	0.505

(N = 120) ^a	(0.053)	(0.083)	(0.093)	(0.096)	(0.101)	(0.016)
[PMPyrr] ^{+,b}	-0.559	0.067	2.269	2.199	0.268	0.587
(N = 39) ^a	(0.093)	(0.110)	(0.107)	(0.153)	(0.099)	(0.027)
[BMPyrr] ⁺	-0.663	0.094	2.285	2.282	0.425	0.663
(N = 466) ^a	(0.039)	(0.058)	(0.060)	(0.075)	(0.065)	(0.011)
[PeMPyrr] ^{+,b}	-0.585	0.016	2.138	2.109	0.323	0.641
(N = 42) ^a	(0.075)	(0.088)	(0.080)	(0.135)	(0.084)	(0.020)
[HMPyrr] ^{+,b}	-0.539	-0.062	2.005	2.027	0.367	0.647
(N = 37) ^a	(0.082)	(0.087)	(0.085)	(0.173)	(0.098)	(0.023)
[OMPyrr] ^{+,b}	-0.457	-0.108	1.915	1.965	0.330	0.688
(N = 39) ^a	(0.062)	(0.068)	(0.066)	(0.116)	(0.077)	(0.018)
[DMPyrr] ^{+,b}	-0.439	-0.204	1.840	1.824	0.214	0.715
(N = 40) ^a	(0.051)	(0.057)	(0.056)	(0.090)	(0.065)	(0.014)
[MeoeMPyrr] ⁺	-0.523	0.131	2.227	2.201	0.173	0.561
(N = 106) ^a	(0.062)	(0.086)	(0.089)	(0.102)	(0.105)	(0.018)
[PMPip] ⁺	-0.465	0.178	2.074	2.174	0.336	0.569
(N = 81) ^a	(0.061)	(0.080)	(0.091)	(0.090)	(0.115)	(0.017)
[BMPip] ⁺	-0.384	0.105	2.111	2.132	0.196	0.581
(N = 116) ^a	(0.051)	(0.073)	(0.084)	(0.085)	(0.102)	(0.015)
[MeoeMPip] ⁺	-0.496	0.172	2.166	2.157	0.244	0.568
(N = 166) ^a	(0.049)	(0.068)	(0.069)	(0.087)	(0.078)	(0.015)
[MeoeMMorp] ⁺	-0.657	0.103	2.534	2.292	0.415	0.518
(N = 162) ^a	(0.050)	(0.069)	(0.069)	(0.082)	(0.078)	(0.015)
[M ₃ BAm] ⁺	-0.396	0.248	1.897	1.851	0.636	0.546
(N = 51) ^a	(0.075)	(0.131)	(0.157)	(0.198)	(0.194)	(0.018)
[MO ₃ Am] ⁺	-0.072	0.167	0.731	1.315	0.789	0.713
(N = 27) ^a	(0.119)	(0.266)	(0.442)	(0.393)	(0.566)	(0.034)
[MB ₃ Am] ^{+,b}	-0.490	-0.111	1.909	1.965	0.345	0.659
(N = 44) ^a	(0.074)	(0.078)	(0.075)	(0.107)	(0.086)	(0.021)
[HexM ₃ Am] ⁺	-0.513	-0.038	1.999	1.956	0.477	0.601
(N = 50) ^a	(0.083)	(0.103)	(0.096)	(0.139)	(0.101)	(0.020)
[OM ₃ Am] ^{+,b}	-0.471	-0.214	1.993	1.966	0.294	0.649
(N = 44) ^a	(0.071)	(0.078)	(0.072)	(0.107)	(0.076)	(0.019)
[DM ₃ Am] ^{+,b}	-0.443	-0.278	1.838	1.908	0.316	0.700
(N = 46) ^a	(0.081)	(0.089)	(0.082)	(0.123)	(0.085)	(0.022)
[O ₄ Am] ^{+,b}	-0.114	-0.304	1.408	1.452	0.061	0.721
(N = 40) ^a	(0.126)	(0.125)	(0.104)	(0.164)	(0.105)	(0.038)
[Et ₃ S] ⁺	-0.657	0.039	2.486	2.119	0.424	0.586
(N = 31) ^a	(0.113)	(0.280)	(0.370)	(0.243)	(0.256)	(0.034)
[H ₃ TdP] ⁺	-0.354	-0.344	1.421	1.724	0.231	0.773
(N = 92) ^a	(0.062)	(0.100)	(0.102)	(0.141)	(0.118)	(0.020)
[MiB ₃ P] ⁺	-0.817	0.253	1.069	2.631	0.904	0.830

(N = 32) ^a	(0.134)	(0.305)	(0.398)	(0.279)	(0.294)	(0.040)
[OiQu] ⁺	-0.435	-0.316	2.277	2.117	-0.208	0.705
(N = 35) ^a	(0.111)	(0.183)	(0.232)	(0.203)	(0.224)	(0.031)
Anions						
[Tf ₂ N] ⁻	0.000	0.000	0.000	0.000	0.000	0.000
(N = 1633) ^a						
[BF ₄] ⁻	-0.223	0.144	0.459	1.150	-0.390	-0.060
(N = 296) ^a	(0.031)	(0.067)	(0.070)	(0.092)	(0.081)	(0.010)
[PF ₆] ⁻	-0.022	-0.176	0.352	-0.011	-0.184	-0.077
(N = 149) ^a	(0.035)	(0.071)	(0.078)	(0.102)	(0.103)	(0.011)
[SCN] ⁻	-0.541	0.513	0.423	2.503	-0.189	-0.053
(N = 188) ^a	(0.053)	(0.091)	(0.116)	(0.106)	(0.107)	(0.015)
[EtSO ₄] ⁻	-0.453	-0.050	0.521	2.951	-0.719	-0.003
(N = 50) ^a	(0.078)	(0.143)	(0.167)	(0.212)	(0.202)	(0.019)
[OtSO ₄] ⁻	-0.085	-0.140	-0.099	2.429	-0.493	0.130
(N = 93) ^a	(0.068)	(0.090)	(0.094)	(0.147)	(0.119)	(0.021)
[F ₃ Ac] ⁻	-0.301	-0.151	0.587	2.797	-0.171	-0.002
(N = 29) ^a	(0.100)	(0.274)	(0.420)	(0.725)	(0.780)	(0.031)
[Trif] ⁻	-0.050	0.202	-0.094	1.175	-0.028	-0.083
(N = 233) ^a	(0.044)	(0.077)	(0.088)	(0.105)	(0.101)	(0.013)
[N(CN) ₂] ⁻	-0.370	0.221	0.488	2.097	-0.243	-0.036
(N = 139) ^a	(0.073)	(0.094)	(0.095)	(0.126)	(0.100)	(0.019)
[E ₂ PO ₄] ⁻	0.193	-0.101	0.258	4.830	-0.875	0.013
(N = 41) ^a	(0.128)	(0.147)	(0.139)	(0.213)	(0.155)	(0.041)
[NO ₃] ⁻	-0.326	0.392	0.802	2.641	-0.739	-0.120
(N = 47) ^a	(0.150)	(0.146)	(0.150)	(0.237)	(0.150)	(0.045)
[FAP] ⁻	0.262	-0.126	-0.073	-1.148	0.272	-0.019
(N = 625) ^a	(0.035)	(0.052)	(0.055)	(0.064)	(0.061)	(0.010)
[B(CN) ₄] ⁻	0.251	0.044	0.086	0.148	-0.124	0.075
(N = 238) ^a	(0.050)	(0.076)	(0.085)	(0.096)	(0.090)	(0.015)
[MeSO ₃] ⁻	-0.788	0.177	0.838	3.896	-0.597	-0.035
(N = 51) ^a	(0.090)	(0.125)	(0.125)	(0.204)	(0.144)	(0.022)
[BETI] ⁻	-0.010	0.022	0.069	-0.365	0.015	-0.89
(N = 49) ^a	(0.086)	(0.116)	(0.112)	(0.156)	(0.124)	(0.021)
[Tos] ⁻	-0.514	0.062	0.601	2.955	-0.595	-0.004
(N = 114) ^a	(0.080)	(0.115)	(0.134)	(0.156)	(0.139)	(0.024)
[C(CN) ₃] ⁻	0.150	0.154	0.012	0.943	-0.225	-0.084
(N = 96) ^a	(0.071)	(0.096)	(0.096)	(0.123)	(0.110)	(0.020)

^a N is the number of experimental data points associated with the given ion.

^b Determined as part of the present study by regressing the log K values for solutes dissolved in each of the individual ([Cation]⁺[Tf₂N]⁻) ionic liquids at 323 K. In this case the cation-specific and IL-specific equation coefficients are equal because the coefficients for the [Tf₂N]⁻ anion are equal to zero.

Table 9. Cation-specific and Anion-specific Equation Coefficients for the Abraham Model

Water-to-Anhydrous Ionic Liquid Partition Coefficient Correlations, $\log P$, at 298 K.

Ion	c_p	e_p	s_p	a_p	b_p	v_p
Cations						
[MEIm] ⁺	-0.049	0.215	0.428	-1.294	-4.209	3.163
(N =) ^a	(0.039)	(0.067)	(0.081)	(0.098)	(0.091)	(0.039)
[MBIm] ⁺	-0.048	0.328	0.296	-1.382	-4.337	3.390
(N = 509) ^a	(0.035)	(0.059)	(0.071)	(0.089)	(0.087)	(0.033)
[MHIm] ⁺	-0.083	0.098	0.348	-1.275	-4.426	3.585
(N = 335) ^a	(0.036)	(0.068)	(0.077)	(0.087)	(0.084)	(0.033)
[MOIm] ⁺	0.018	0.050	-0.201	-1.453	-4.106	3.878
(N = 156) ^a	(0.054)	(0.097)	(0.117)	(0.126)	(0.132)	(0.051)
[MDIm] ⁺	0.036	-0.064	0.395	-1.611	-4.546	3.587
(N = 42) ^a	(0.171)	(0.227)	(0.269)	(0.219)	(0.253)	(0.146)
[HexdMIm] ⁺	0.158	-0.245	-0.415	-1.759	-4.732	4.482
(N = 31) ^a	(0.223)	(0.188)	(0.235)	(0.323)	(0.241)	(0.199)
[M ₂ EIm] ⁺	-0.103	0.277	0.452	-1.670	-4.035	3.190
(N = 39) ^a	(0.122)	(0.165)	(0.198)	(0.237)	(0.182)	(0.109)
[PM ₂ Im] ⁺	-0.528	0.644	0.618	-0.100	-4.151	2.952
(N = 34) ^a	(0.182)	(0.200)	(0.267)	(0.294)	(0.266)	(0.159)
[D ₂ MIm] ^{+,b}	-0.093	-0.052	0.040	-1.620	-4.667	4.034
(N = 40) ^a	(0.147)	(0.118)	(0.128)	(0.176)	(0.132)	(0.132)
[(Meo) ₂ Im] ⁺	-0.414	-0.103	0.764	-1.120	-3.781	3.056
(N = 46) ^a	(0.150)	(0.138)	(0.139)	(0.192)	(0.132)	(0.119)
[MeoeMIm] ⁺	-0.150	0.012	0.653	-1.289	-4.263	3.116
(N = 47) ^a	(0.147)	(0.138)	(0.145)	(0.192)	(0.157)	(0.117)
[HexomMIm] ⁺	-0.071	-0.558	1.080	-1.351	-4.718	3.646
(N = 34) ^a	(0.172)	(0.269)	(0.353)	(0.269)	(0.290)	(0.150)
[(Hexom) ₂ Im] ⁺	0.074	-0.541	0.642	-1.419	-4.748	3.787
(N = 34) ^a	(0.172)	(0.269)	(0.353)	(0.269)	(0.290)	(0.150)
[EtOHMIm] ⁺	-0.410	0.208	0.549	-1.009	-3.572	2.951
(N = 148) ^a	(0.065)	(0.074)	(0.084)	(0.097)	(0.095)	(0.055)
[CNPrMIm] ⁺	-0.680	0.206	0.782	-1.167	-4.055	3.301
(N = 44) ^a	(0.175)	(0.180)	(0.191)	(0.255)	(0.201)	(0.145)
[3-MBPy] ⁺	0.040	0.087	0.657	-1.197	-4.970	3.435
(N = 36) ^a	(0.146)	(0.226)	(0.300)	(0.300)	(0.279)	(0.132)
[4-MBPy] ⁺	-0.090	0.238	0.549	-1.246	-4.417	3.433
(N = 71) ^a	(0.082)	(0.119)	(0.153)	(0.161)	(0.138)	(0.073)
[NEP] ⁺	-0.322	0.323	0.552	-1.234	-3.951	3.370
(N = 31) ^a	(0.138)	(0.233)	(0.244)	(0.287)	(0.199)	(0.147)

[PrOHPy] ⁺	-0.309	0.176	0.790	-0.759	-3.570	3.077
(N = 121) ^a	(0.082)	(0.103)	(0.122)	(0.117)	(0.131)	(0.072)
[PMPyrr] ^{+,b}	-0.236	0.000	0.908	-1.015	-4.691	3.446
(N = 39) ^a	(0.170)		(0.172)	(0.239)	(0.149)	(0.143)
[BMPyrr] ⁺	-0.034	0.380	0.308	-1.276	-4.474	3.330
(N = 466) ^a	(0.053)	(0.068)	(0.077)	(0.094)	(0.081)	(0.046)
[PeMPyrr] ^{+,b}	-0.303	0.000	0.727	-1.107	-4.622	3.630
(N = 42) ^a	(0.134)		(0.113)	(0.212)	(0.116)	(0.109)
[HMPyrr] ^{+,b}	-0.226	-0.083	0.560	-1.301	-4.501	3.673
(N = 36) ^a	(0.152)	(0.132)	(0.144)	(0.275)	(0.159)	(0.128)
[OMPyrr] ^{+,b}	-0.253	0.000	0.520	-1.460	-4.696	3.815
(N = 37) ^a	(0.121)		(0.096)	(0.203)	(0.116)	(0.103)
[DMPyrr] ^{+,b}	-0.083	-0.142	0.419	-1.467	-4.859	3.824
(N = 40) ^a	(0.128)	(0.114)	(0.124)	(0.197)	(0.129)	(0.108)
[MeoeMPyrr] ⁺	-0.068	0.119	0.691	-1.140	-4.694	3.324
(N = 102) ^a	(0.098)	(0.105)	(0.122)	(0.132)	(0.138)	(0.086)
[PMPip] ⁺	-0.230	0.458	0.342	-1.259	-4.296	3.409
(N = 78) ^a	(0.100)	(0.101)	(0.120)	(0.122)	(0.152)	(0.082)
[BMPip] ⁺	-0.115	0.448	0.322	-1.108	-4.452	3.390
(N = 110) ^a	(0.081)	(0.096)	(0.115)	(0.117)	(0.138)	(0.070)
[MeoeMPip] ⁺	-0.102	0.191	0.660	-1.094	-4.665	3.360
(N = 162) ^a	(0.077)	(0.082)	(0.093)	(0.112)	(0.103)	(0.068)
[MeoeMMorp] ⁺	-0.264	0.067	0.995	-1.058	-4.381	3.168
(N = 161) ^a	(0.077)	(0.081)	(0.092)	(0.099)	(0.097)	(0.067)
[M ₃ BAm] ⁺	0.046	-0.063	0.362	-1.253	-4.411	3.213
(N = 57) ^a	(0.074)	(0.163)	(0.189)	(0.249)	(0.244)	(0.061)
[MO ₃ Am] ⁺	-0.108	0.092	-0.231	-1.166	-4.529	4.133
(N = 32) ^a	(0.109)	(0.278)	(0.458)	(0.438)	(0.604)	(0.100)
[MB ₃ Am] ^{+,b}	-0.233	0.000	0.404	-1.313	-4.542	3.687
(N = 44) ^a	(0.123)		(0.101)	(0.154)	(0.113)	(0.104)
[HexM ₃ Am] ⁺	-0.324	0.238	0.288	-1.379	-4.269	3.518
(N = 90) ^a	(0.085)	(0.082)	(0.095)	(0.107)	(0.109)	(0.070)
[OM ₃ Am] ^{+,b}	-0.165	-0.181	0.569	-1.419	-4.677	3.711
(N =) ^a	(0.129)	(0.118)	(0.118)	(0.164)	(0.115)	(0.103)
[DM ₃ Am] ^{+,b}	-0.128	-0.131	0.329	-1.458	-4.550	3.818
(N = 46) ^a	(0.135)	(0.125)	(0.126)	(0.175)	(0.120)	(0.108)
[O ₄ Am] ^{+,b}	0.226	0.000	-0.212	-1.756	-4.739	3.825
(N = 42) ^a	(0.198)		(0.144)	(0.240)	(0.139)	(0.174)
[Et ₃ S] ⁺	-0.111	-1.162	2.484	-1.481	-5.165	3.291
(N = 31) ^a	(0.179)	(0.367)	(0.482)	(0.318)	(0.343)	(0.156)
[H ₃ TdP] ⁺	-0.049	-0.166	-0.134	-1.356	-4.775	4.045
(N = 97) ^a	(0.089)	(0.122)	(0.130)	(0.177)	(0.146)	(0.082)

[OiQu] ⁺	0.065	-0.422	0.969	-1.247	-5.404	3.701
(N = 36) ^a	(0.170)	(0.240)	(0.302)	(0.248)	(0.295)	(0.142)
Anions						
[Tf ₂ N] ⁻	0.000	0.000	0.000	0.000	0.000	0.000
(N = 1746) ^a						
[BF ₄] ⁻	-0.075	0.156	0.207	0.983	-0.266	-0.317
(N = 306) ^a	(0.045)	(0.077)	(0.090)	(0.111)	(0.101)	(0.044)
[PF ₆] ⁻	0.007	-0.230	0.417	0.131	-0.120	-0.297
(N = 201) ^a	(0.047)	(0.077)	(0.088)	(0.102)	(0.104)	(0.047)
[SCN] ⁻	-0.534	0.187	0.644	2.801	-0.315	-0.130
(N = 220) ^a	(0.091)	(0.093)	(0.112)	(0.128)	(0.121)	(0.061)
[EtSO ₄] ⁻	-0.029	-0.245	0.129	2.792	-0.745	-0.264
(N = 53) ^a	(0.099)	(0.171)	(0.199)	(0.248)	(0.230)	(0.078)
[OtSO ₄] ⁻	-0.040	-0.043	0.002	2.583	-0.577	0.424
(N = 95) ^a	(0.106)	(0.107)	(0.127)	(0.204)	(0.153)	(0.095)
[F ₃ Ac] ⁻	-0.286	-0.697	0.859	2.284	0.475	0.056
(N = 32) ^a	(0.098)	(0.278)	(0.443)	(0.893)	(0.948)	(0.099)
[Trif] ⁻	-0.228	-0.088	0.367	1.560	-0.091	-0.047
(N = 161) ^a	(0.061)	(0.096)	(0.114)	(0.136)	(0.125)	(0.057)
[N(CN) ₂] ⁻	-0.257	0.164	0.446	2.217	-0.256	-0.243
(N = 136) ^a	(0.087)	(0.111)	(0.120)	(0.157)	(0.120)	(0.079)
[E ₂ PO ₄] ⁻	0.071	0.073	0.006	5.089	-0.832	0.184
(N = 38) ^a	(0.171)	(0.192)	(0.239)	(0.297)	(0.224)	(0.162)
[NO ₃] ⁻	-0.068	0.203	0.425	2.793	-0.681	-0.411
(N = 97) ^a	(0.139)	(0.116)	(0.157)	(0.208)	(0.146)	(0.126)
[FAP] ⁻	0.198	0.049	-0.214	-1.344	0.449	-0.109
(N = 620) ^a	(0.049)	(0.061)	(0.071)	(0.079)	(0.078)	(0.043)
[B(CN) ₄] ⁻	0.072	-0.075	0.347	0.312	-0.121	-0.061
(N = 244) ^a	(0.069)	(0.092)	(0.109)	(0.123)	(0.115)	(0.061)
[MeSO ₃] ⁻	-0.646	0.347	0.315	3.997	-0.336	-0.242
(N = 49) ^a	(0.158)	(0.164)	(0.173)	(0.275)	(0.183)	(0.128)
[BETI]	0.071	-0.245	0.038	-0.318	0.101	-0.349
(N = 51) ^a	(0.103)	(0.146)	(0.146)	(0.196)	(0.157)	(0.089)
[C(CN) ₃] ⁻	-0.079	0.056	0.276	1.223	-0.070	-0.008
(N = 95) ^a	(0.109)	(0.116)	(0.128)	(0.161)	(0.143)	(0.094)

^a N is the number of experimental data points associated with the given ion.

^b The numerical values of the cation-specific equation coefficients were taken from a previously published paper [28, 30, 31] that reported the Abraham model log K correlation equation for solutes dissolved in the ([Cation]⁺[Tf₂N]⁻) ionic liquid. In this case the cation-specific and IL-

specific equation coefficients are equal because the coefficients for the $[\text{Tf}_2\text{N}]^-$ anion are equal to zero.

Figure 1

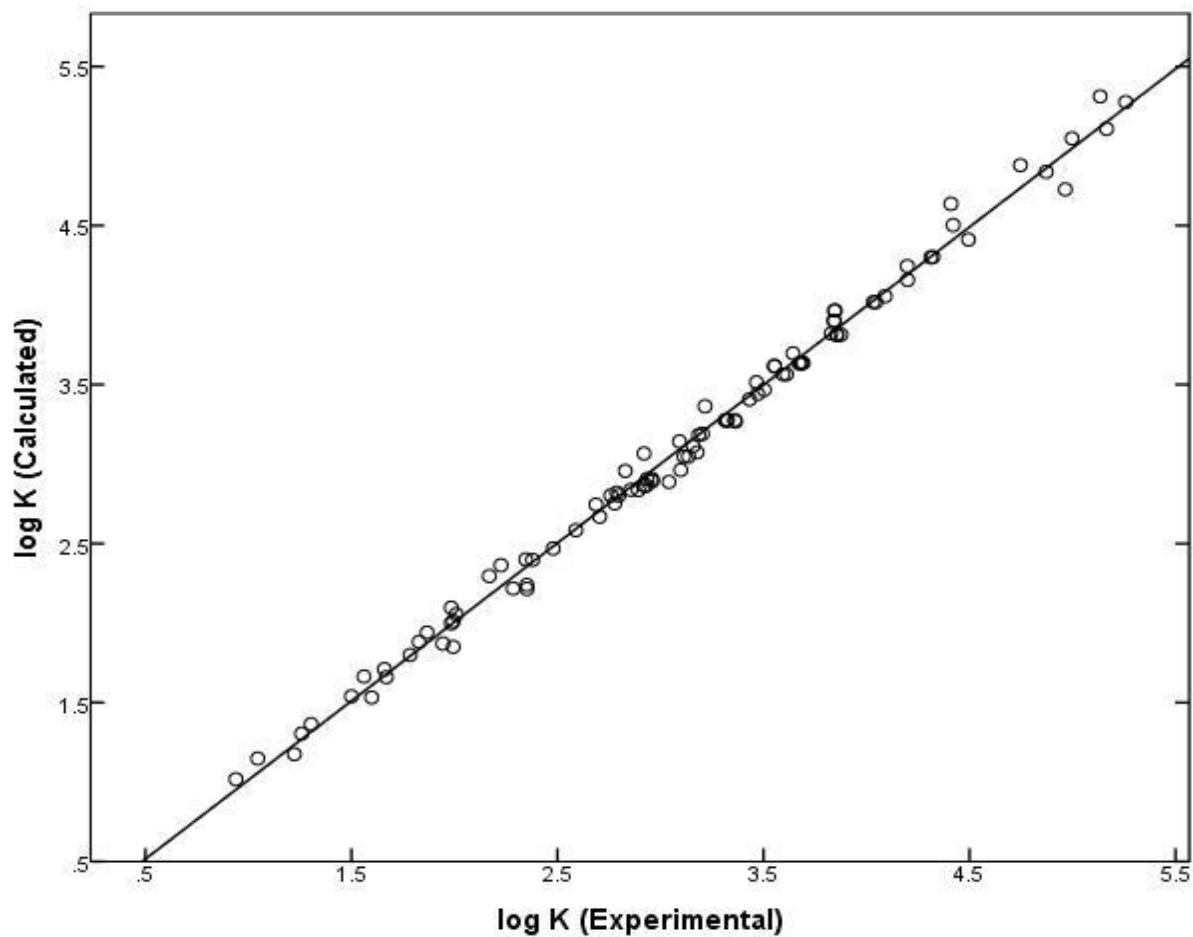


Figure 1: Comparison between observed $\log K$ data and calculated $\log K$ values based on Eqn. 8 for solutes dissolved in $([\text{BMPyr}^+][\text{C}(\text{CN})_3]^-)$ at 298 K.

Figure 2

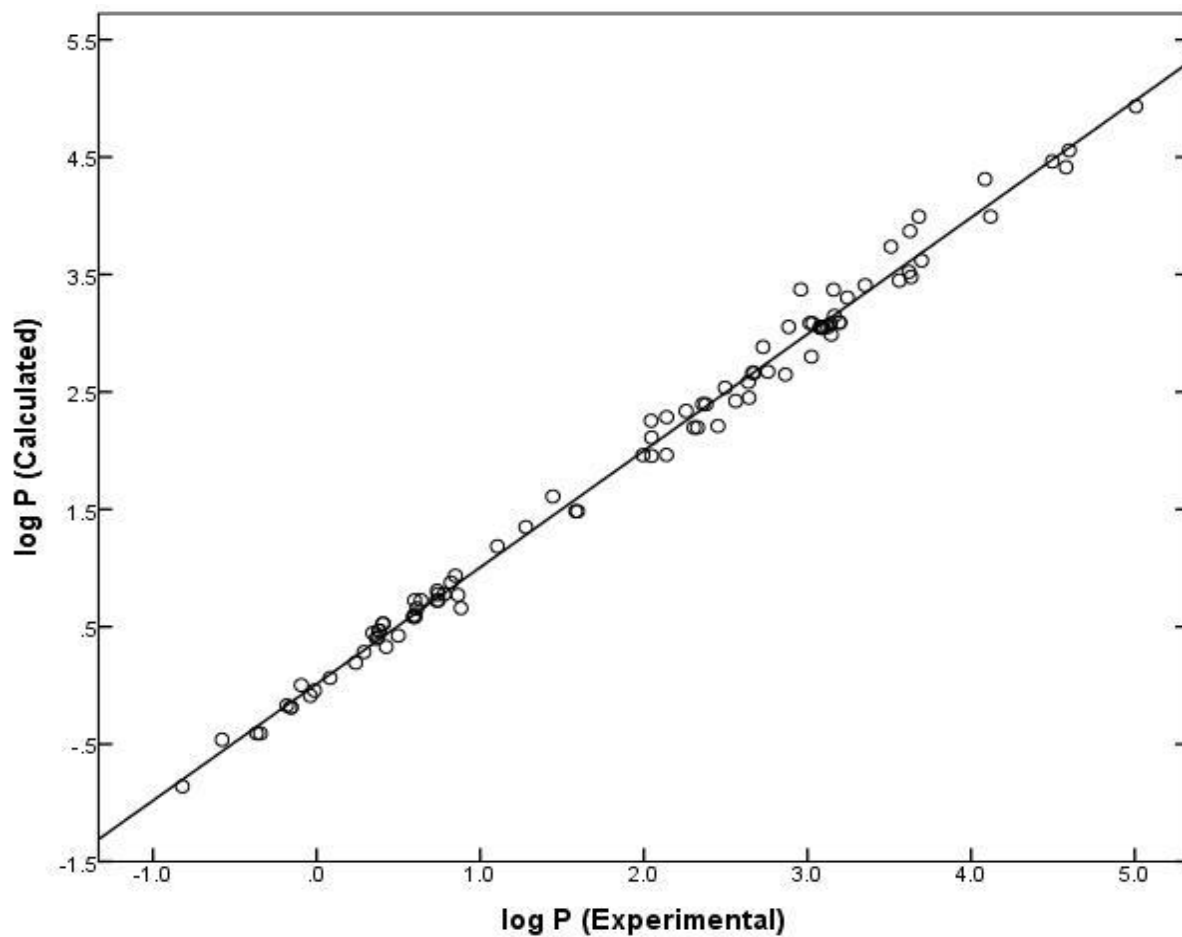


Figure 2: Comparison between observed log *P* data and calculated log *P* values based on Eqn. 10 for solutes dissolved in ([BMPyrr]⁺[C(CN)₃]⁻) at 298 K.

Figure 3

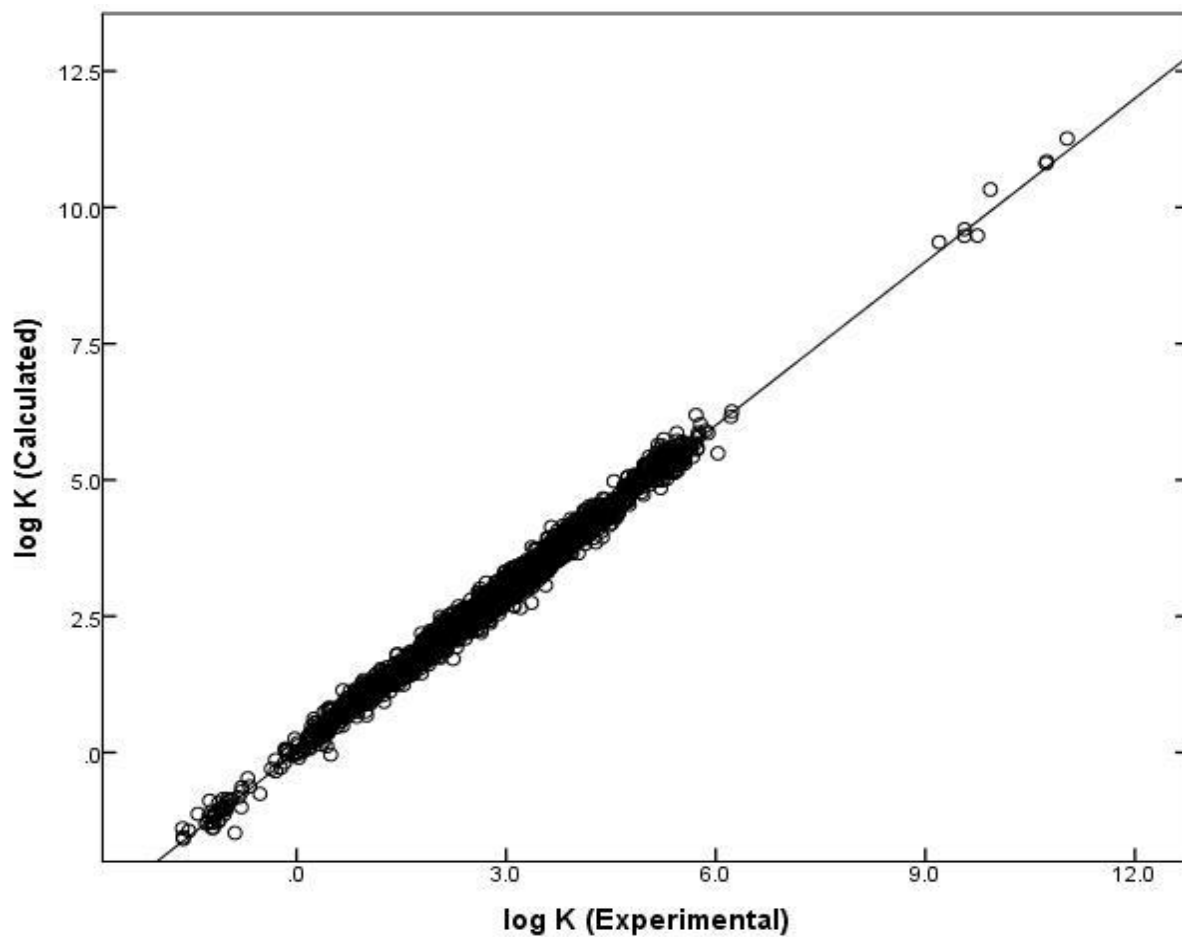


Figure 3: Comparison of experimental log K (at 298 K) data to back-calculated values based on Eqn. 16 with the ion-specific equation coefficients given in Table 7.

Figure 4

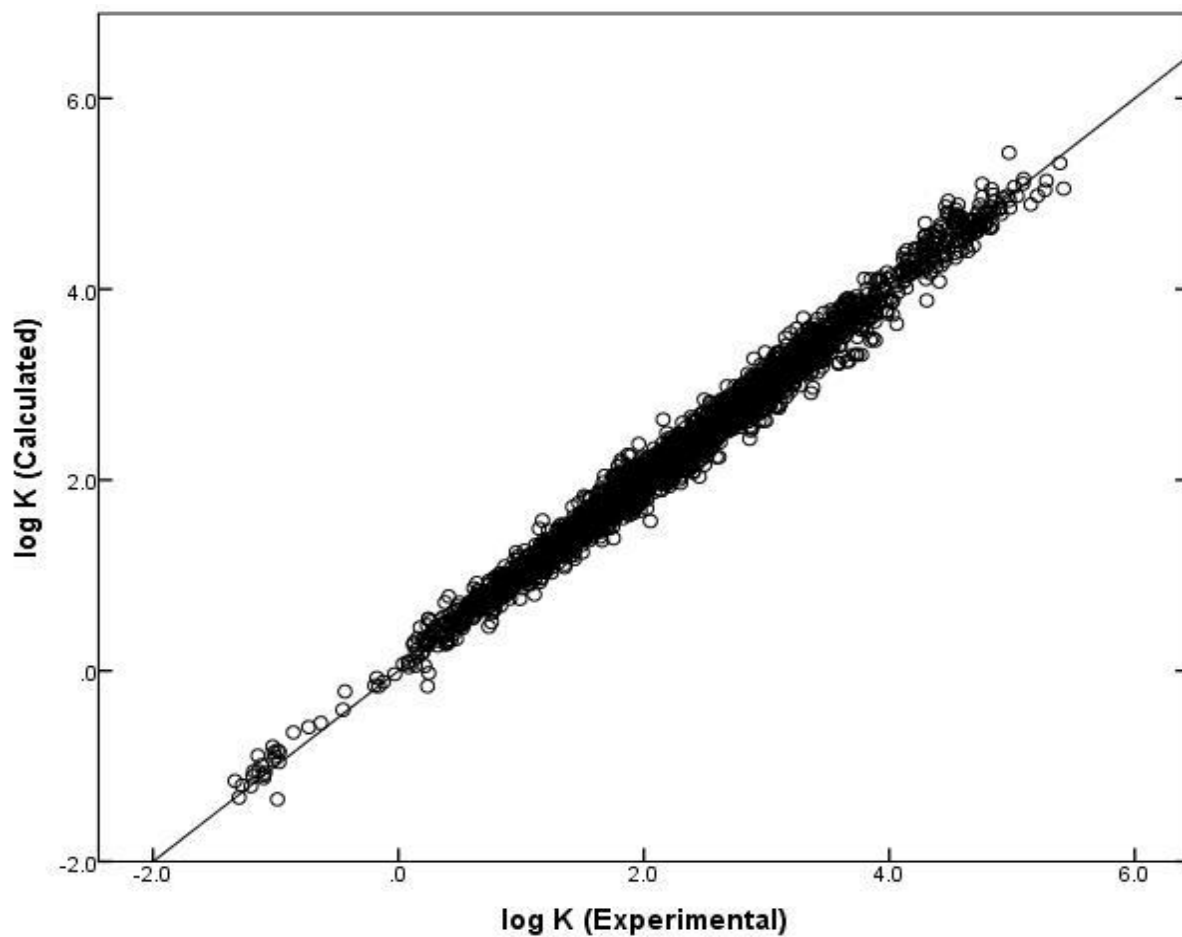


Figure 4: Comparison of experimental $\log K$ (at 323 K) data to calculated values based on Eqn. 17 with the ion-specific equation coefficients given in Table 8.

Figure 5

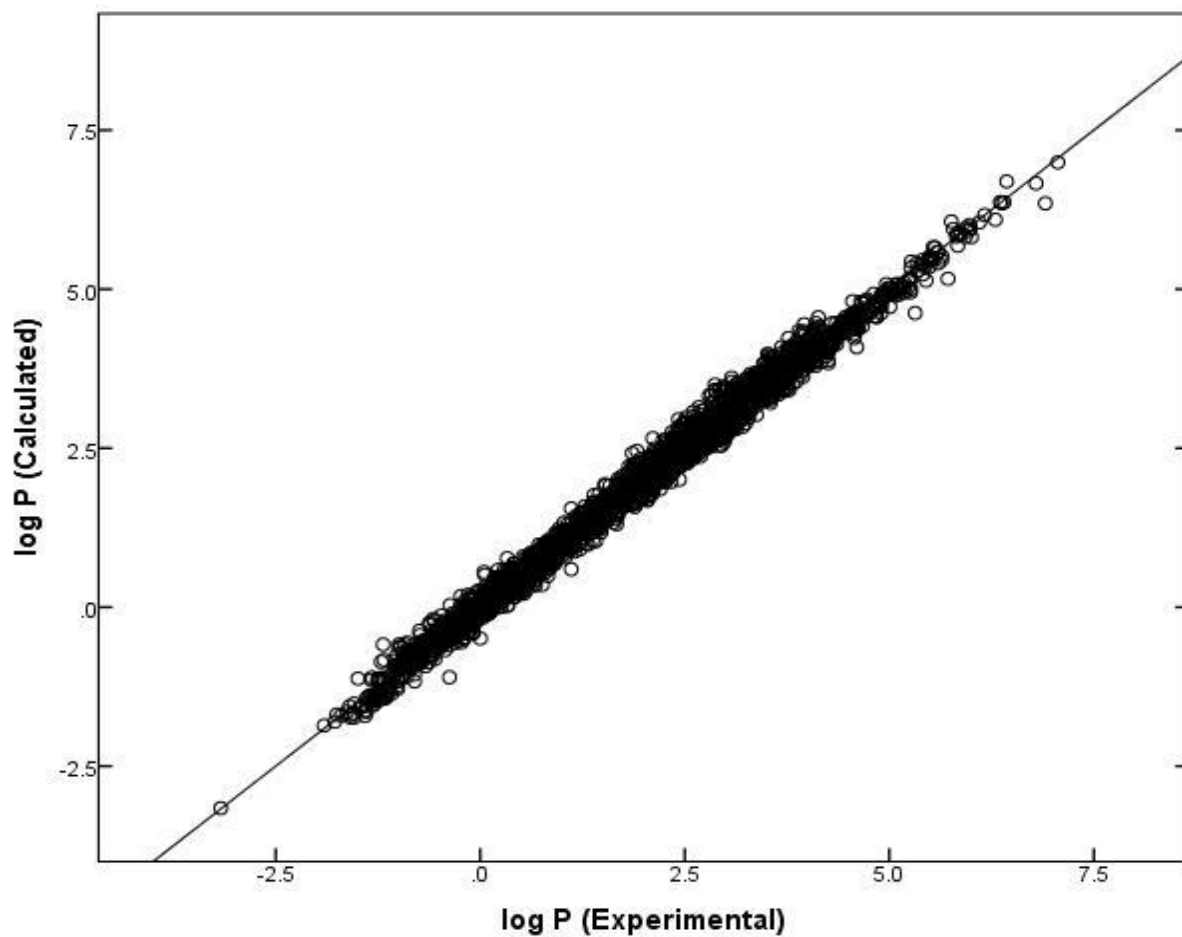


Figure 5: Comparison of experimental $\log P$ (at 298 K) data to calculated values based on Eqn. 18 with the ion-specific equation coefficients given in Table 9.