THE ABRAHAM SOLVATION MODEL USED FOR PREDICTION OF SOLVENT-SOLUTE INTERACTIONS AND NEW METHODS FOR UPDATING PARAMETERS

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Dissertation Prepared for the Degree of

DOCTOR OF PHILOSOPHY

UNIVERSITY OF NORTH TEXAS

May 2021

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Churchill, Brittani N. *The Abraham Solvation Model Used for Prediction of Solvent-Solute Interactions and New Methods for Updating Parameters*. Doctor of Philosophy (Chemistry), May 2021, 313 pp., 27 tables, 36 figures, 4 appendices, 178 numbered references.

The Abraham solvation model (ABSM) is an experimentally derived predictive model used to help predict various solute properties. This work covers various uses for the ABSM including predicting molar enthalpies of vaporization, predicting solvent coefficients for two new solvents (2,2,5,5-tetramethyloxolane and diethyl carbonate), predicting values for multiple new ionic liquids (ILs). This work also introduces a novel method for updating IL ABSM parameters by updating cation- and anion-specific values using linear algebra and binary matrices.

ACKNOWLEDGEMENTS

Throughout the writing of this dissertation I have received a great deal of support and assistance.

I would first like to thank my supervisor, Dr. William E. Acree Jr., who has guided me since before graduate school and showed me a field which I love. Your feedback was always insightful and helped me bring my work to a higher level while sharpening my thinking and your humor always made things fun. I am very glad that I've gotten to know you through the years.

I also want to thank all of the professors who have taught me chemistry over the years. Without their teachings and guidance I may not have chosen this field to pursue. I would especially like to thank Dr. Diana Mason for showing my class a chemistry demonstration which began my interest in chemisty. I would also like to thank Dr. Sushama Dandekar whose passion and energy made organic chemisty fun both to learn and to teach. You also taught me that how you say things matters as much as what you are saying, a lesson which has been applicable outside of academia as much as it has within it.

In addition, I would like to thank my parents for always believing in me and giving me their utmost support. I would also like to thank my friends, all of which made my time learning chemistry a fun social experience.

Finally, I would like to thank my husband, Chris, who has been with me every step of the way through my journey back to school. Without him I would not be the person I am and I would not be where I am today. He is my rock, my best friend, and my world.

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CHAPTER 1

THE ABRAHAM SOLVATION MODEL

1.1 Introduction

The Abraham solvation model (ABSM) is a quantitative linear free energy relationship (LSER) model which is used to determine various solute properties of system for neutral molecules.[1] The theory behind the ABSM is the cavity theory of solvation.[1–3] This theory has the following steps:[4]

1. A cavity to accommodate the solute is created in the solvent. Endergonic breaking of solvent-solvent interactions occurs during this step. The energy for this step is proportional to the size of the cavity which is appropriately sized for the solute.
2. The solvent molecules at the perimeter of the cavity reorganize into their equilibrium position for interaction with the solute.
3. The solute enters into the reorganized cavity, and solute-solvent interactions begin. These interactions are exoergic and are key to the process of solution.

Step 3 is the most exergonic step -- that is it is the driving force -- of the solvation process. It is the interactions in this step which must be defined and characterized.[3] Characterization of the solute-solvent interactions can be performed by the ABSM. The equations for these properties are shown in Equations 1.1 and 1.2.[5–19]

$$log\ SP = c + eE + sS + aA + bB + lL \quad \textbf{(Eq. 1.1)}$$

$$log\ SP = c + eE + sS + aA + bB + vV \quad \textbf{(Eq. 1.2)}$$

The terms on the right-hand side of Equations 1.1 and 1.2 describe the various types of solute-solvent molecular interactions that are believed to be present in solution. Each type of molecular interaction is quantified by the product of a solute property (solute descriptors) and the complimentary solvent property (solvent descriptors).[20] The lowercase letters denote

descriptors for a chosen solvent and the uppercase letters denote descriptors for a chosen solute. [5,9] These descriptors include the constant derived from linear regression (cC), the excess molar refraction (eE), dipolarity/polarizability (sS), the hydrogen-bond acidity (aA), the hydrogen-bond basicity (bB), the McGowan's characteristic volume (vV), the gas-liquid partition of n-hexadecane at 25 °C (lL). All of these terms are explained in more detail later in the chapter.

On the left side of Equations 1.1 and 1.2 the term SP is the solute property. SP is most commonly the water-to-organic solvent partition/ transfer coefficients, log *P*, and logarithms of experimental gas-to-organic solvent partition/transfer coefficients, log *K*.[1,20] Other solute parameters such as $\Delta_{\mathrm{solv}}\mathrm{H}_{\mathrm{m}}^{0}$,[8] and $\Delta\mathrm{S}_{\mathrm{solv}}$[3] can also be on the left side of the equation.

Solute and solvent coefficients, most commonly the solvent values, are determined by regression analysis of experimental SP values for a series of organic solutes and inorganic gases dissolved in the given solvent.[8,9,18,20,21] The numerical values of the respective properties are specific to the given solvent or solute and can be used to estimate solute properties.[9] By keeping the solvent phase constant, only the solute parameters will need to be determined. The properties of solvation can then be put into an equation to determine solvation parameters.[4] The complementary solvent properties (lowercase letters) in Equations 1.1 and 1.2 are obtained by curve-fitting logarithms of experimental solute parameters.[8,9,20–24] One must be careful to acquire ABSM parameters through a healthy/wide variety of compounds in order to obtain a more accurate Abraham correlation coefficient value.[4]

1.2 Solute Descriptors and Solvent Descriptors

1.2.1 E: Excess Molar Refraction

The excess molar refraction, E, can be calculated from the characteristic volume, or, more commonly, by the experimental refractive index at 20 °C for the sodium D-line.[1] Since E is derived from molar refraction, it gives a measure of the polarizable electrons in a molecule.[4] E also corresponds to the molar refraction of the given solute in excess of that of a linear alkane having a comparable molecular size.[20] The E parameter can be used as an indication of the solute-solvent interaction that arises through the presence of polarizable electrons in the solute.[4] The units for E are (cm^3 mol^{-1}) / 10.[18]

1.2.2 S: Dipolarity/Polarizability

S is a combination of the electrostatic polarity and polarizability of the dissolved solute and must be determined experimentally.[1,20] Originally, this term was determined by normal phase gas chromatography, but it is now more commonly determined by liquid-liquid partition constants for aqueous or organic biphasic systems combined with gas chromatography retention data.[1]

1.2.3 A and B: Hydrogen-Bond Acidity and Basicity

A and its partner parameter B represent the total hydrogen-bond capability between a solute and solvent in a given system. The A parameter represents the ability of a solute to donate a hydrogen bond and not necessarily the ability to donate a proton.[3]

The A and B parameters must be determined experimentally. The A parameter is generally determined by gas chromatography. Some phases in gas chromatography, notably the poly(siloxane) and poly(ethylene glycol) stationary phases, are hydrogen-bond bases and can be used A parameter.[1] In order to obtain A values for a compound, the stationary phase must be

calibrated and the values of SP, E, S, and L must be known.[4]

The B descriptor can be determined in several ways for water soluble compounds: biphasic systems in which one phase is aqueous (e.g. reversed-phased liquid chromatography), micellar electrokinetic chromatography, and water-organic solvent liquid-liquid partition. Liquid-liquid partition in totally organic biphasic systems can be used for compounds with low water solubility or those which are unstable in water.[1]

1.2.4 V: McGowan's Characteristic Volume

The McGowan characteristic volume is the only parameter from the Abraham solvation model which can be calculated from a known structure.[1] It can be calculated by assigning atomic fragments values and by the number of bonds in a molecule, all bonds being counted as one, no matter whether single, double, or triple. For complicated molecules, an algorithm made by Abraham can be used to count the number of bonds. This parameter was originally set up to be a measure of the cavity effect, that is the endoergic effect of disrupting solvent-solvent bonds.[4] However, solute volume is always well correlated with molar refraction and with polarizability, and so will include not only the endoergic cavity effect but also exoergic solute-solvent affects that arise due to solute polarizability.[4] V refers to the solute's McGowan molecular volume (calculated from atomic sizes and chemical bond numbers).[20,25] The solute's McGowan volume is in units of$(cm^3\ mol^{-1})/100$.[18]

1.2.5 L: Gas-Liquid Partition of the Solute in Hexadecane at 25°C

The gas-liquid partition of the solute in hexadecane at 25 °C, L, must be determined experimentally.[1] L is defined as the logarithm of the equilibrium constant where the solvent is

in hexadecane at 25 °C, L = log *K* (gas to hexadecane). L also includes exoergic solute-solvent effects, just as the V descriptor does.[4] It has been shown that L values can be obtained from GLC retention data on rather non-polar columns at temperatures between 60 and 102 °C with an equation (SP = c + eE + lL) to extrapolate down to 25 °C.[4] L denotes the logarithm of the solute's measured gas-to-hexadecane partition coefficient at 298.15 K.[20]

1.3 Ion Specific Parameters

Equations 1.1 and 1.2 describe the general Abraham solvation model. However, there are more specific variations of the model. One such variation is the ion specific Abraham solvation model.[26–30]

$$log\ SP = c_{cation} + c_{anion} + (e_{cation} + e_{anion})E + (s_{cation} + s_{anion})S + (a_{cation} + a_{anion})A + (b_{cation} + b_{anion})B + (l_{cation} + l_{anion})L \quad \textbf{(Eq. 1.3)}$$

$$log\ SP = c_{cation} + c_{anion} + (e_{cation} + e_{anion})E + (s_{cation} + s_{anion})S + (a_{cation} + a_{anion})A + (b_{cation} + b_{anion})B + (v_{cation} + v_{anion})V \quad \textbf{(Eq. 1.4)}$$

This equation allows for specific cations and anions to be substituted without having to determine the parameters for each combination of ions individually. This allows for more flexibility and customization in using the model.[4] Equations 1.3 and 1.4 are most commonly used with ionic liquids, therefore each unique cation-anion pair represents a different ionic liquid.[9] Ionic liquids are described in more detail later in the chapter.

1.4 Applications

The ABSM has three major applications: determining solubility of one compound in another, determining the change in enthalpy of various solute systems, and using known solute

parameters to determine solvent parameters for ionic liquids, which can then be used as solvents for a multitude of processes.

1.4.1 Solute Partitioning

Solute partitioning is the most common use of the ABSM. The partitioning can be between a gas phase and a condensed phase using the parameter K, and can also be between two condensed phases using the parameter P. The chemical and mathematical expressions for these terms can be seen below in Equations 1.5 – 1.7.

Chemical Equation	Mathematical Equation	Eq. #
Solute (gas phase) ⇋ Solute (condensed phase)	$\mathrm{K} = \frac{[\mathrm{solute}]_{\mathrm{organic\ solvent}}}{[\mathrm{solute}]_{\mathrm{gas}}}$	**1.1**
Solute (water) ⇋ Solute (condensed phase)	$\mathrm{P} = \frac{[\mathrm{solute}]_{\mathrm{organic\ solvent}}}{[\mathrm{solute}]_{\mathrm{water}}}$	**1.2**
Solute (gas phase) ⇋ Solute (water)	$\mathrm{K_w} = \frac{[\mathrm{solute}]_{\mathrm{water}}}{[\mathrm{solute}]_{\mathrm{gas}}}$	**1.3**

log *P* and log *K* are related by the following equation[20]:

$$log\ P = (log\ K - log\ K_{water}) \qquad \textbf{(Eq. 1.8)}$$

where $\mathrm{K_{water}}$ (also written as $\mathrm{K_w}$) is the solute's gas-to-water partition coefficient.[9] It should also be noted that water-to-IL partition coefficients calculated through Equation 1.8 pertain to a hypothetical partitioning process involving solute transfer from water to the anhydrous IL.

It is important to note that all of the parameters in Equations 1.1 and 1.2 must linearly correlate with the K and P terms. This is done by taking the log of both sides of the equation. This means all reported parameters for K and P are in log units. Also notice that Equations 1.1

and 1.2 have different parameters; Equation 1.1 has the lL term and Equation 1.2 has the vV term. log *K* uses Equation 1.1 and log *P* uses Equation 1.2.

The solvents and solutes plus their respective parameters used for correlations in this dissertation are listed in Appendix A. Equations 1.1 and 1.2 can be used to predict molar solute solubilities and infinite dilution activity coefficients in additional organic solvents. The advantage that the Abraham model offers over other solution models used by other researchers is that once an Abraham model equation coefficients have been determined for a given solvent, one can then predict the solubility and/or infinite dilution activity coefficients of more than 8,000 different compounds in the given solvent.[20,22]

1.4.2 $\Delta_{\mathrm{solv}}\mathrm{H}^0_{\mathrm{m}}$ and $\Delta_{\mathrm{vap}}\mathrm{H}^0_{\mathrm{m}}$

Another commonly used application of the ABSM is the prediction of the enthalpy of solvation. The enthalpy of solvation allows one to extrapolate log *K* values predicted at 298.15 K to other temperatures. This, in turn, allows one to calculate the enthalpy of vaporization. In this dissertation, the experimental values for comparing the predicted enthalpies of vaporization were determined by standard calorimetric methods and to the variation of the compound's vapor pressure with temperature. Chapter 4 covers this topic and the results in more detail.

1.4.3 Ionic Liquids

Ionic liquids (ILs) have received considerable attention in recent years for a variety of reasons. They have extremely small vapor pressures, which fulfills an important requirement for being classified as environmentally friendly solvents.[9] This leads them to being potential replacement solvents for organic solvents.

ILs have shown enormous promise as solvents in chemical separation processes.[9] The non-volatile nature and high thermal and chemical stability of a great many ILs facilitates their use as solvent media for high-temperature chemical reactions.[22] Moreover, their selectivity can be fine-tuned by judicious selection of cation-anion pair.[9] ILs have been effectively used as stationary phases in gas-liquid chromatography[31–34], adsorbents in gas separation membranes[35–37], entrainers in extractive azeotropic distillations[38–41], and solvents in micro-extraction devices[42–45]. Their unique properties also have potential applicability in many industrial chemical processes.[18] Modern ILs are popular solvent choices in manufacturing processes for nanomaterials and composite materials[46–49], and as possible pharmaceutical drug candidates and drug delivery systems[50,51]. ILs have also been used extensively as reservoirs for the time-controlled release of active pharmaceutical ingredients from drug formulations[52], and as the organic component of a biphasic extraction system for removal of hazardous compounds from industrial waste effluents[53,54]. In synthetic processes, ILs serve as a liquid media for mass and heat transfer and, in select applications, they have been linked to increased product yields and reduced reaction times.[55]

The enhanced solvation ability and chemical specificity for a particular class of polar and/or hydrogen-bonding organic compounds results from the IL's ionic character, which can be judiciously modified through the selection of different cation-anion pairs, and by modification of the functionality on the alkyl chain attached to the cationic (or anionic) moiety.[18]

Ionic liquids (ILs) are conventionally defined as liquid salts or a “liquid comprised entirely of ions”.[56] The most common type of ionic liquid is room temperature ionic liquids (RTILs),

which are salts with melting points below room temperature.[57] The first RTIL, ethyl ammonium nitrate, was worked on as early as 1928 with a melting point of 12 °C.[58] ILs were used mostly for electroplating and electrochemistry until the 1967 when tetra-n-hexylammonium benzoate was used as a solvent for kinetic and electrochemical investigations. It was not until the late 1980s that ILs were used for catalysts in organic synthesis.[59]

IL physical properties, including but not limited to the solubilizing character, miscibility in water, and achieving the desired chemical separation can be fine-tuned through judicious selection of cation-anion combination[9,22], or by the introduction of functional groups on the alkyl chains of the respective ions that comprise the IL solvent.[9]

In this dissertation Chapter 3, Chapter 6, Chapter 7, Chapter 8, and Chapter 9 cover the determination of IL solvent descriptors for new ILs. Chapter 10 covers a novel method for updating IL solvent descriptors. All the IL cations and anions used in this dissertation, their abbreviations, their chemical names, and their structures are listed in Appendix A.

1.4.4 Other Applications of the ABSM

The ABSM can also be used to determine and elucidate the retention properties of molecules in chromatography.[60] For example, in gas chromatography, if the stationary phase and the solute in question are characterized, one can predict how the solute and stationary phase interact with each other and, by proxy, their approximate retention order. This can be useful in fields where multichemical separation is performed on a continuous basis such as the pharmaceutical industry or in environmental studies.

CHAPTER 2

COMPUTATIONAL ANALYSIS OF DATA

2.1 Introduction

The coefficients listed throughout Chapter 1 for all Abraham model correlations are determined through linear regression analysis. This analysis is performed by using Microsoft® Excel® and IBM® SPSS® Statistics software. Other values were also determined including the Fisher F-statistic value (F), the standard deviation of the correlation (SD), and the coefficient of determination value (R^2). This chapter covers the calculations and methods used to determine these values.

2.2 Data Collection and Transformation into Linear Formulas

Before data can be correlated and processed for linear regression, all data must be in a format suitable for analysis. The most common solvation parameters used to determine ABSM coefficients is the logarithm of the gas-to-solvent partition coefficient (log *K*) and the logarithm of the water-to-solvent partition coefficient (log *P*). To convert gas chromatographically determined most activity coefficients at infinite dilution (γ^{∞}) into log *K* (Eq. 2.1):

$$log\, K = log(\frac{RT}{\gamma^{\infty}_{solute} p^{0}_{solute} V_{solvent}}) \quad \textbf{(Eq. 2.1)}$$

where R is the universal gas constant in units of $\frac{\mathrm{L \cdot kPa}}{\mathrm{mol \cdot K}}$, T is the system temperature in units of Kelvin, $\gamma^{\infty}_{\mathrm{solute}}$ is the unitless activity coefficient at infinite dilution, $\mathrm{p^{\circ}_{solute}}$ is the saturated vapor pressure of solute in its standard state at temperature T in units kPa, and $\mathrm{V_{solvent}}$ is the molar volume of the organic solvent which is in units of $\frac{\mathrm{L}}{\mathrm{mol}}$. $\mathrm{V_{solvent}}$ can be calculated by known the molecular weight of the solvent and the density of the solvent.

However, many of these values are recorded at temperatures above 298 K. Gibbs solvation energies at 298.15K can be calculated computationally.[61–63] To extrapolate log *K* to 298 K, one only needs to correlate log $K = T^{-1}$, which is a linear relationship. From there, Equation 1.8 can be used to determine log *P* values. Having ABSM parameters at 298 K allows for calculation of log *P* parameters and also represents room temperature solvation more accurately. Then the log *K* and log *P* values are collated with the corresponding ABSM descriptors and a linear regression is performed in SPSS®.

2.3 Performing Multiple Linear Regression

Multiple linear regression is performed by using IBM SPSS® Statistics Version 25.This program has a built in function which allows the user to perform multiple linear regressions at the same time with a short wait. Before one can perform the regression, one must define the parameters which will be dependent (aka held constant) and which paramaters will be independent (aka variable). This can be seen in Figure 2.1. Figures 2.2 to 2.5 show the other parameters needed for analysis.

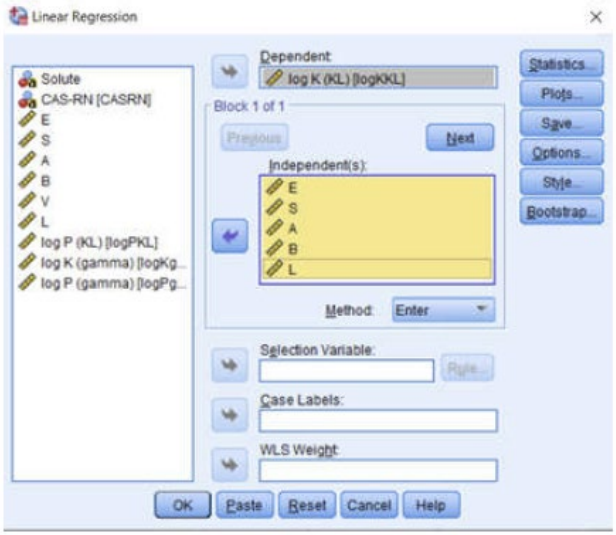


Figure 2.1: Parameters in the Linear Regression menu. For log P, L is replaced with V.

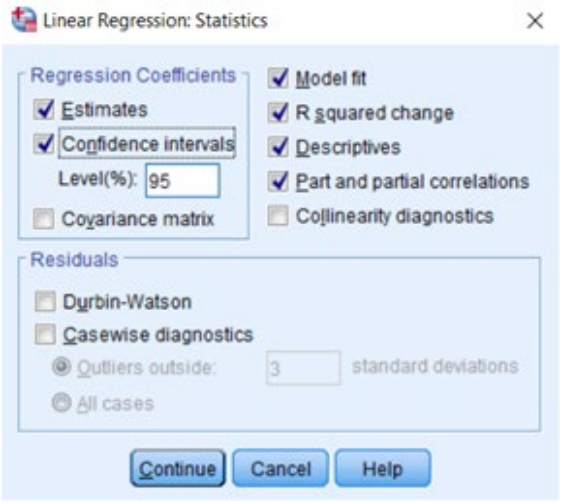


Figure 2.2: Settings of the "Statistics" submenu.

Figure 2.3: Settings for the "Plots" submenu.

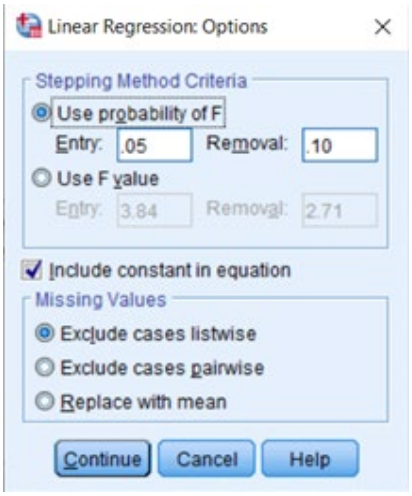


Figure 2.4: Settings for the "Options" submenu.

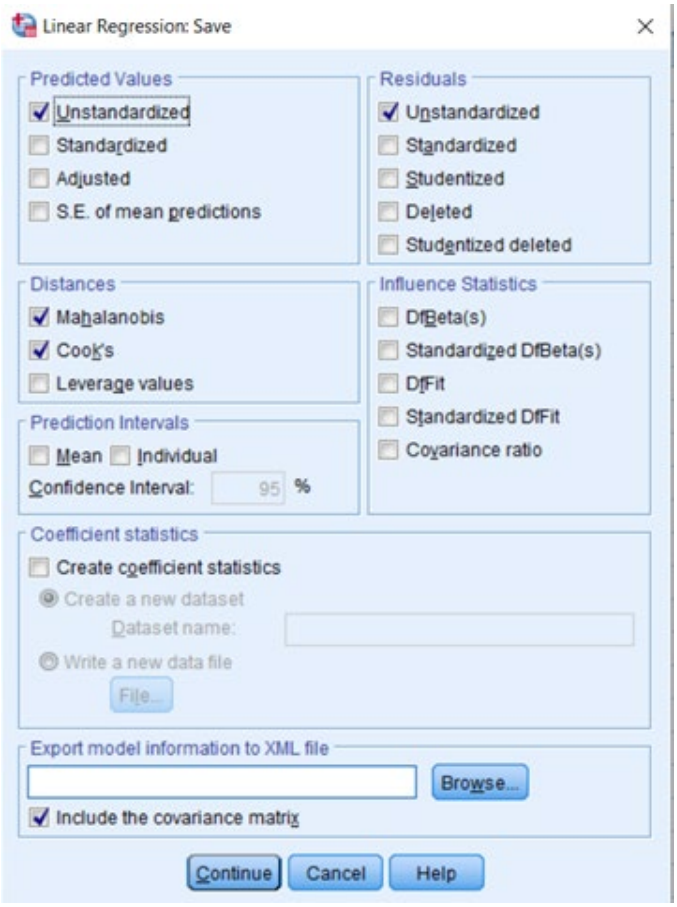


Figure 2.5: Settings for the "Save" submenu.

Figure 2.6 shows where to find the R^2, F statistic, coefficients, and residual standard deviations values in the output file. The R square is the coefficient of determination (R^2) and the F Change is the Fischer's F-statistic. The Standard Error of the Estimate is the standard deviation of the entire regression. R^2 can be calculated using Equation 2.2, and the Adjusted R^2 can be calculated using Equation 2.3.

$$R^2 = \frac{\sum \hat{y} - \bar{y}^2}{\sum y - \bar{y}^2} = 1 - \frac{\sum y - \hat{y}^2}{\sum y - \bar{y}^2} \quad \textbf{(Eq. 2.2)}$$

$$R^2_{adj} = 1 - \left(\frac{n-1}{n-k-1}\right)(1 - R^2) \quad \textbf{(Eq. 2.3)}$$

where $\hat{y}$ is the predicted value based on the regression, $\bar{y}$ is the average of the experimental value, and y is the experimental value, k is the total number of independent variables in the

regression and n is the sample size. The F-statistic is important because it is the ration of explained variance to unexplained variance in the regression. Equation 2.4 shows how one can calculate the F-statistic.

$$F = \frac{explained\ variance}{unexplained\ variance} = \frac{R^2}{1-R^2} \cdot \frac{n-(k+1)}{k} \qquad \textbf{(Eq. 2.4)}$$

Model Summary[b]

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate	Change Statistics: R Square Change	F Change	df1	df2	Sig. F Change
1	.994[a]	.988	.987	.1133267369	.988	908.476	5	54	.000

a. Predictors: (Constant), L, S, A, E, B

b. Dependent Variable: log K (KL)

Coefficients[a]

Model		Unstandardized Coefficients: B	Unstandardized Coefficients: Std. Error	Standardized Coefficients: Beta	t	Sig.	95.0% Confidence Interval for B: Lower Bound	95.0% Confidence Interval for B: Upper Bound	Correlations: Zero-order	Correlations: Partial	Correlations: Part
1	(Constant)	-1.105	.093		-11.906	.000	-1.291	-.919			
	E	.503	.100	.116	5.049	.000	.304	.703	.516	.566	.074
	S	3.287	.105	.804	31.401	.000	3.077	3.496	.779	.974	.463
	A	4.927	.131	.724	37.549	.000	4.664	5.190	.491	.981	.554
	B	.231	.113	.049	2.034	.047	.003	.458	.431	.267	.030
	L	.525	.026	.470	20.469	.000	.474	.577	-.157	.941	.302

a. Dependent Variable: log K (KL)

Residuals Statistics[a]

	Minimum	Maximum	Mean	Std. Deviation	N
Predicted Value	.5615388751	4.009130478	2.258611042	.9943703700	60
Std. Predicted Value	-1.707	1.760	.000	1.000	60
Standard Error of Predicted Value	.026	.067	.035	.008	60
Adjusted Predicted Value	.5573154688	3.966347694	2.258984763	.9943016367	60
Residual	-.234442636	.3036555350	.0000000000	.1084184659	60
Std. Residual	-2.069	2.679	.000	.957	60
Stud. Residual	-2.226	2.755	-.002	1.013	60
Deleted Residual	-.271379650	.3210691512	-.000373721	.1218633657	60

Figure 2.6: The locations of the (left to right, top to bottom) R^2 value, F-statistic, coefficient values, and the standard deviation respectively.

Meaningful analysis of Abraham solvation model coefficients can be determined with a minimum of 30 values, as there are six variables which need to be solved.[64] Analysis can be performed with fewer solutes if they cover a range of chemical types such as alkanes, alcohols, and aromatics.[65]

Occasionally, a coefficient will be set to zero.[13] This is because those values contributed so little to the equation that they were within the standard error of the parameter.[13] This happens most often with the variables *e* and *s*, although the *a* and *b* parameters can also be removed if their values are negative for log *K*. That would indicate that hydrogen bond acidity (*a*) and hydrogen bond basicity (*b*) would be less than that of the gas phase, which is unrealistic as hydrogen bond acidity and basicity in the gas phase is zero.[14] Throughout the dissertation the anion $[NTf_2]^-$ is used. $[NTf_2]^-$ was chosen as the reference ion for anion-specific coefficients because of its ubiquity among ILs.[17,28] Therefore, all of its ion parameters are always zero.

At the time the ion-specific equation coefficient version of the Abraham model was first proposed, Sprunger and coworkers addressed how ion-specific equation coefficients for new anions and cations would be added to the compilation of existing equation coefficients as additional experimental data became available. The authors needed an approach that allowed values for new cations and anions to be added without changing the numerical values of existing ions in the compendium. According to their approach, ion-specific equation coefficients for a new cation would be obtained as the difference in the calculated IL-specific equation coefficients minus the respective anion-specific equation coefficients (e.g., $c_{K,cation} = c_{K,IL} - c_{K,anion}$; $e_{K,cation} = e_{K,IL} - e_{K,anion}$, and so forth) provided, of course, that the anion-specific equation coefficients are already known.

In the present case, not only are the anion-specific equation coefficients for $[NTf_2]^-$ known but the calculation proves to be trivial because all of the equation coefficients for the $[NTf_2]^-$ anion are set to zero. This arises because, in calculating equation coefficients for the individual ions, Sprunger and coworkers needed to define a reference point from which all

individual ion values would be calculated. The reference point that was established at the outset was to set every one of the equation coefficients for the $[NTf_2]^-$ anion to zero. In hindsight, this reference point turns out to be a very convenient choice in that $[NTf_2]^-$ is the most popular choice of anion when deriving ILs based on novel, emergent, or underexplored cations.[24]

2.4 Validation of the Regression

A regression can be verified by comparing the regression results against a training set and test set. This method relies on internal consistency: half of the data is randomly split in half into the training and the test sets respectively. If there are an odd number of data points then the odd point is always included in the training set. A linear regression is performed on the training set and its results are used to predict values in the test set. The average error (AE), the absolute average error (AAE), and the standard deviation of the residual are computed from the test set. The AE will reveal inherent bias in the regression. A value of zero indicates no bias, a value above zero indicates a bias above the experimental value and a negative value indicates the opposite. The AAE reveals inherent deviations in the regression from experimental data.[3] Equations 2.5 and 2.6 show how to calculate AE and AAE.

$$AE = \frac{\sum(x_{observed} - x_{predicted})}{n} \quad \textbf{(Eq. 2.5)}$$

$$AAE = \frac{\sum |x_{observed} - x_{predicted}|}{n} \quad \textbf{(Eq. 2.6)}$$

CHAPTER 3

CHARACTERIZATION OF THE SOLUBILIZING ABILITY OF TETRAALKYLAMMONIUM IONIC LIQUIDS CONTAINING A PENDANTALKYL CHAIN BEARING A BASIC N,N-DIMETHYLAMINOETHOXY FUNCTIONALITY*

3.1 Introduction

Chapter 1 covered the theory and the applications of the ABSM. The use of the ABSM for various systems is one of its strongest attributes. However, the predictive power of the ABSM lies with the variety of solvents and solutes which have ABSM parameters. In this chapter the ABSM parameters were calculated for functionalized tetraalkylammonium bis(trifluoromethylsulfonyl)imide ILs that contain either a terminal N,N-dimethylamino functionality or an N,N-dimethylamino functional group pendant to an ether chain. The molecular structures of the four ILs studies are given in Table 3.1. Dr. Fabrice Mutelet's group calculated the infinite dilution of activity coefficients for >40 different organic solutes and the gas-to-ionic liquid partition coefficients in the temperature range from 323.15 K to 373.15 K.[18]

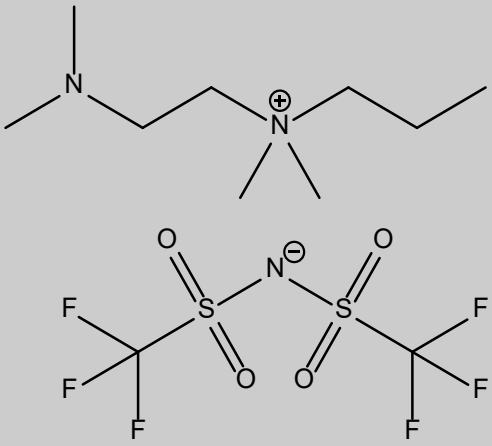
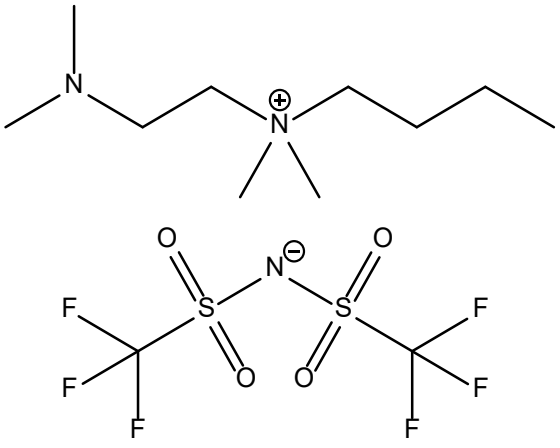
There is particular interest in obtaining correlations for solute transfer processes at 298 K as this is the temperature at which previous Abraham model correlations have been reported. Certainly, direct comparison of the solubilizing properties of different ILs is possible only if the values pertain to a common temperature. The numerical log *K* (at 298.15 K) values used in the present study were calculated from the standard thermodynamic log *K* versus T^{-1} linear

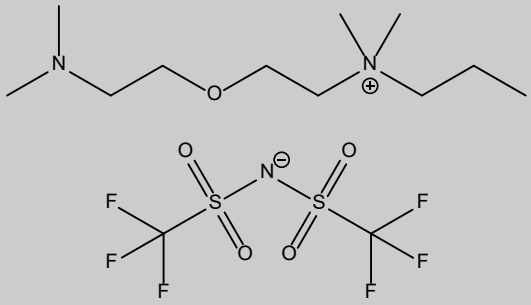
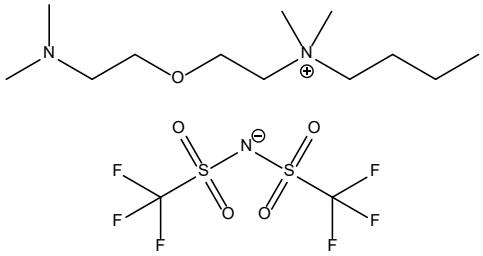
* This chapter is reproduced from Rabhib, F, Mutelet, F, Sifaoui, H, Wagle, DV, Baker, GA, Churchill, B, & Acree Jr, WE. (2019). Characterization of the solubilizing ability of tetraalkylammonium ionic liquids containing a pendant alkyl chain bearing a basic N,N-dimethylamino or N,N-dimethylaminoethoxy functionality. **Journal of Molecular Liquids, 283**, 380-390, with permission from Elsevier.

relationship, based on the measured values at 323.15 K and 333.15 K, as these represent the lowest two temperatures studied for these ILs. The linear extrapolation is acceptable in this instance because these measurements were performed at temperatures proximal to the desired temperature of 298.15 K (within ~35 K in the worst-case scenario).

Significantly, the results of the experimental measurements provided by Mutelet were further used to derive Abraham model ionic liquid-specific correlations for $[N_{112}N_{113}]^+$ $[NTf_2]^-$, $[N_{112}N_{114}]^+$ $[NTf_2]^-$,$[N_{112}O_2N_{113}]^+$ $[NTf_2]^-$,and $[N_{112}O_2N_{114}]^+[NTf_2]^-$ that permit the prediction of infinite dilution activity coefficients and gas-to-ionic liquid partition coefficients for additional organic solutes beyond those studied as part of the present communication.

Table 3.1: List of ionic liquids analyzed in this study.

Abbreviation	Name	Structure
$[N_{112}N_{113}]^+[NTf_2]^-$	N-[2-(N',N'-dimethylamino)ethyl]-N,N-(dimethyl)-1-Propanaminium bis(trifluoromethylsulfonyl)imide	
$[N_{112}N_{114}]^+[NTf_2]^-$	N-[2-(N',N'-dimethylamino)ethyl]-N,N-(dimethyl)-1-Butanaminium bis(trifluoromethylsulfonyl)imide	

Abbreviation	Name	Structure
$[N_{112}O_2N_{113}]^+[NTf_2]^-$	N-[2-(N',N'-dimethylamino)-ethoxyethyl]-N,N- (dimethyl)-1-Propanaminium bis(trifluoromethylsulfonyl)imide	
$[N_{112}O_2N_{114}]^+[NTf_2]^-$	N-[2-(N',N'-dimethylamino)ethoxyethyl]-N,N-(dimethyl)-1-Butanaminium bis (trifluoromethylsulfonyl)imide	

3.2 Development of IL-Specific Abraham Model Correlations for Solute Transfer into ILs

Infinite dilution activity coefficient data facilitate the design of chemical separation processes. Explicitly, the $\gamma^{\infty}_{1,\mathrm{IL}}$ values found in Rabhi et. al. can be used to calculate separation factors for 900 or more pairs of organic solutes for each of the four IL solvents studied.[18] While this appears a considerable number of prospective separations, it represents only a tiny fraction of the chemical separations practicing analytical chemists and chemical engineers routinely encounter. The approach that has been promoted [6,13,15–17,27,45,66–75] is based on the Abraham general solvation model, which predicts water-to-IL partition coefficients (log *P*) and gas-to-IL partition coefficients (log *K*) using Equations 1.1 and 1.2, which are related to $\gamma^{\infty}_{1,\mathrm{IL}}$ values through Equations 2.1 and 1.8.

The calculated log *K* and log *P* values for solute transfer into $[N_{112}N_{113}]^+[NTf_2]^-$, $[N_{112}N_{114}]^+[NTf_2]^-$, $[N_{112}O_2N_{113}]^+[NTf_2]^-$, and $[N_{112}O_2N_{114}]^+[NTf_2]^-$ are respectively reported in the eighth and ninth columns of Table B.1-Table B.4. For the convenience of the reader, Table B.1-

Table B.4 also contain the numerical solute descriptor values of the organic compounds studied in the present communication. Analysis of the experimental log *P* and log *K* data in Table B.1 gave the following Abraham model correlations for solute transfer into $[N_{112}N_{113}]^+[NTf_2]^-$:

$$log\ P\ (298K) = -0.205(0.133) - 0.053(0.129)E + 0.584(0.151)S$$
$$-1.037(0.182)A - 4.475(0.151)B + 3.508\ (0.106)V$$
$$(SD = 0.124, N = 45, R^2 = 0.996, and\ F = 1852.3) \quad \textbf{(Eq. 3.1)}$$

and

$$\log K\ (298\mathrm{K}) = -0.436(0.079) - 0.108(0.096)\mathrm{E} + 2.270(0.101)\mathrm{S}$$
$$-2.505(0.128)\mathrm{A} + 0.435(0.107)\mathrm{B} + 0.707\ (0.021)\mathrm{V}$$
$$(SD = 0.089, N = 45, R^2 = 0.980, and\ F = 391.6) \quad \textbf{(Eq. 3.2)}$$

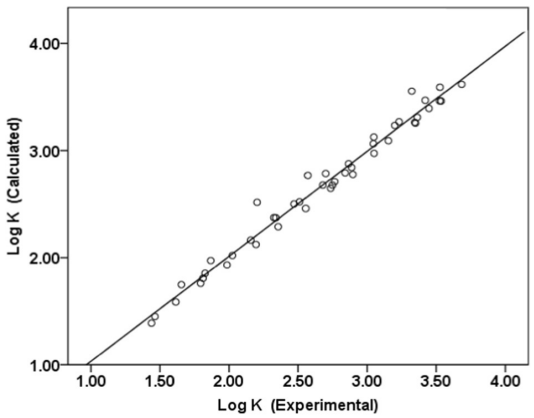


Figure 3.1: Comparison between the observed log K data and calculated log K values based on Equation 3.2 for 45 representative organic solutes dissolved in anhydrous $[N_{112}N_{113}]^+[NTf_2]^-$ at 298.15 K.

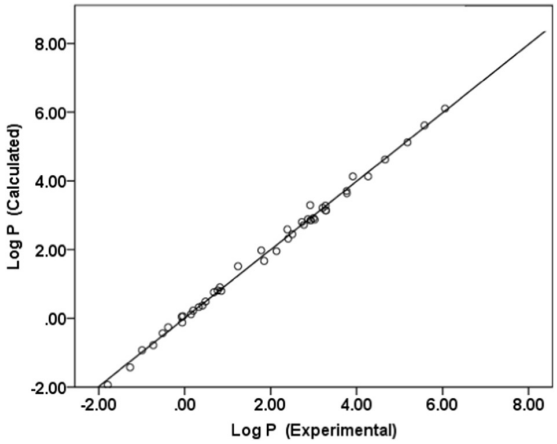


Figure 3.2: Comparison between the observed log P data and calculated log P values based on Equation 3.1 for 45 organic solutes dissolved in anhydrous $[N_{112}N_{113}]^+[NTf_2]^-$ at 298.15 K.

The two regression analyses were performed using the commercial IBM SPSS® Statistical 25 software. The statistical information associated with Equations 3.1 and 3.2 includes the standard deviation (SD), the number of experimental data points used in the regression analysis (N), the squared correlation coefficient (R^2), and the Fisher F-statistic (F). Standard errors in the calculated equation coefficients are given parenthetically immediately following the respective equation coefficient. Careful examination of the statistical information reveals that both mathematical expressions provide a reasonably accurate description of solute transfer into $[N_{112}N_{113}]^+[NTf_2]^-$, as evidenced by standard deviations of 0.124 log units (Equation 3.1) and 0.089 log units (Equation 3.2), respectively. Figure 3.1 compare the observed log *K* values against the back- calculated values based on Equation 3.2. The experimental values span a range of approximately 2.2 log units, from log *K* = 1.439 for 3-methylpentane to log *K* = 3.638 for o-xylene. A comparison of the back-calculated versus experimental log *P* data is graphically depicted in Figure 3.2. As an information note, Equations 3.1 and 3.2 are comparable in descriptive ability to Abraham model correlations previously obtained for solute transfer into other ILs. Standard deviations for published Abraham model correlations for IL solvents typically fall in the range of 0.12-0.16 log units, with the standard deviations of the log *K* correlations being slightly smaller than for log *P* correlations. This is to be expected as log *K* values represent actual measured quantities whereas “experimental” log *P* values contain the additional experimental uncertainty associated with the log K_w values needed in the log *K* to log *P* conmethods.

The log *P* and log *K* datasets (see Table B.1-Table B.4) for solute transfer Into $[N_{112}N_{114}]^+[NTf_2]^-$, $[N_{112}O_2N_{113}]^+[NTf_2]^-$, and $[N_{112}O_2N_{114}]^+[NTf_2]^-$ were analyzed in similar fashion.

Table 3.2: Equation coefficients for log P and log K Abraham model correlations for $[N_{112}N_{113}]^+[NTf_2]^-$, $[N_{112}N_{114}]^+[NTf_2]^-$, $[N_{112}O_2N_{113}]^+[NTf_2]^-$, and $[N_{112}O_2N_{114}]^+[NTf_2]^-$ at 298.15 K.

IL/Property	*c*	*e*	*s*	*a*	*b*	*v*	*l*	N	SD	R^2	F
$[N_{112}N_{113}]^+[NTf_2]^-$											
log *P*	-0.205	-0.053	0.584	-1.037	-4.475	3.508		45	0.124	0.996	1852
	-0.133	-0.129	-0.151	-0.182	-0.151	-0.106					
log *K*	-0.436	-0.108	2.279	2.505	0.435		0.707	45	0.089	0.980	392
	-0.079	-0.096	-0.101	-0.128	-0.107		-0.021				
$[N_{112}N_{114}]^+[NTf_2]^-$											
log *P*	-0.339	-0.149	0.748	-0.945	-4.542	3.605		43	0.125	0.996	1758
	-0.136	-0.131	-0.139	-0.182	-0.124	-0.108					
log *K*	-0.613	-0.225	2.440	2.608	0.420		0.748	43	0.098	0.978	332
	-0.089	-0.105	-0.100	-0.138	-0.097		-0.024				
$[N_{112}O_2N_{113}]^+[NTf_2]^-$											
log *P*	-0.397	0.000	0.779	0.712	-4.181	3.291		44	0.128	0.995	1776
	-0.132		-0.133	-0.184	-0.135	-0.107					
log *K*	-0.725	0.053	2.522	2.863	0.751		0.656	45	0.090	0.985	524
	-0.073	-0.101	-0.111	-0.125	-0.115		-0.019				
$[N_{112}O_2N_{114}]^+[NTf_2]^-$											
log *P*	-1.042	0.143	1.160	-0.335	-3.910	3.643		45	0.138	0.993	1082
	-0.143	-0.135	-0.149	-0.200	-0.159	-0.114					
log *K*	-1.338	0.044	2.865	3.280	1.041		0.762	47	0.114	0.984	509
	-0.087	-0.110	-0.112	-0.153	-0.131		-0.020				

Numerical values of the calculated equation coefficients alongside the associated statistical information are collected in Table 3.2. Each derived Abraham model correlation provides a very robust mathematical description of the observed solute partitioning behavior into the respective IL solvent, as evidenced by the low standard deviations and near-unity values for the squared correlation coefficients. Graphical comparisons of the descriptive abilities of the log *P* and log *K* correlations for $[N_{112}N_{114}]^+[NTf_2]^-$, $[N_{112}O_2N_{113}]^+[NTf_2]^-$,and $[N_{112}O_2N_{114}]^+[NTf_2]^-$ are provided in Figure 3.3-Figure 3.8. Based on past experience using the Abraham solvation parameter models, it is expected that the calculated IL-specific equation coefficients (tabulated within Table 3.2) will allow the reliable prediction of log *P*, log *K* and $\gamma^{\infty}_{1,\mathrm{IL}}$ values for additional organic solutes dissolved in $[N_{112}N_{113}]^+[NTf_2]^-$, $[N_{112}N_{114}]^+[NTf_2]^-$, $[N_{112}O_2N_{113}]^+[NTf_2]^-$,and $[N_{112}O_2N_{114}]^+[NTf_2]^-$, provided that the solute descriptors of the additional organic compounds fall within the range of numerical values used in calculating the equation coefficients. It should be pointed out that a great many volatile organic compounds have solute descriptors that will fall within this range of values.[76]

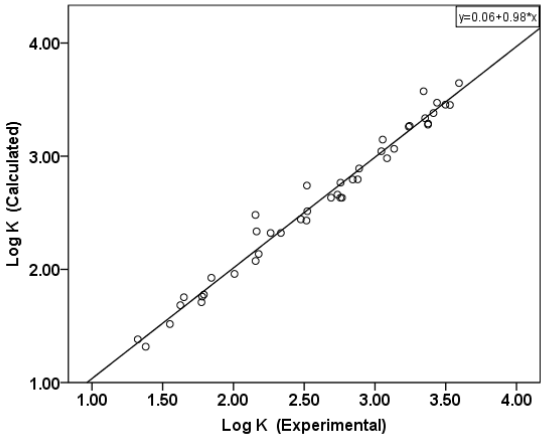


Figure 3.3: Comparison between the observed log K data and calculated log K values based on Eq. 1.2 for the 43 organic solutes dissolved in anhydrous $[N_{112}N_{114}]^+[NTf_2]^-$ at 298.15 K. Equation coefficients used in the Abraham model calculations were taken from Table 3.2.

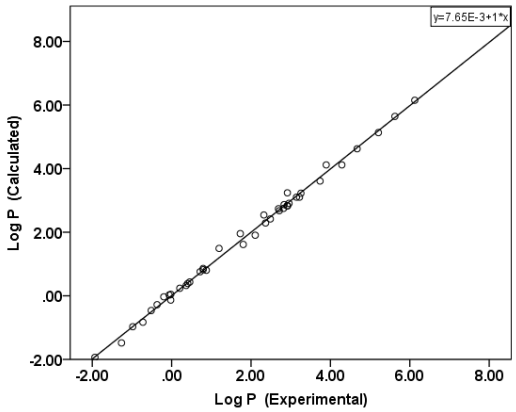


Figure 3.4: Comparison between the observed log P data and calculated log P values based on Eq. 1.1 for the 43 organic solutes dissolved in anhydrous $[N_{112}N_{114}]^+[NTf_2]^-$ at 298.15 K Equation coefficients used in the Abraham model calculations were taken from Table 3.2.

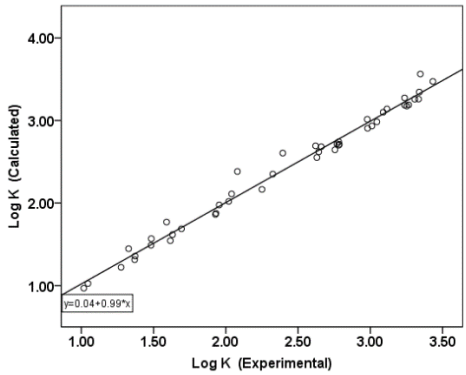


Figure 3.5: Comparison between the observed log K data and calculated log K values based on Eq. 1.2 for the 45 organic solutes dissolved in anhydrous $[N_{112}O_2N_{113}]^+[NTf_2]^-$ at 298.15 K. Equation coefficients used in the Abraham model calculations were taken from Table 3.2.

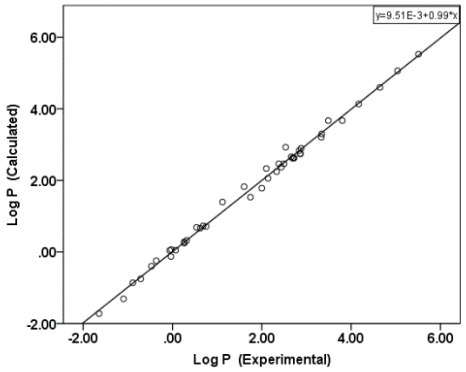


Figure 3.6: Comparison between the observed log P data and calculated log P values based on Eq. 1.1 for the 44 organic solutes dissolved in anhydrous $[N_{112}O_2N_{113}]^+[NTf_2]^-$ at 298.15 K. Equation coefficients used in the Abraham model calculations were taken from Table 3.2.

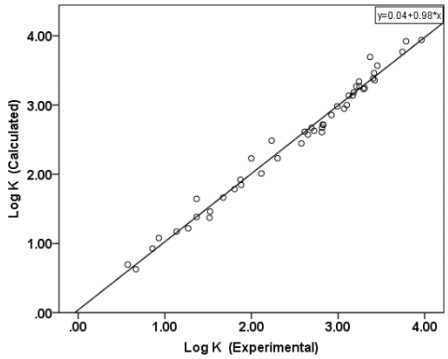


Figure 3.7: Comparison between the observed log K data and calculated log K values based on Eq. 1.2 for the 47 organic solutes dissolved in anhydrous $[N_{112}O_2N_{114}]^+[NTf_2]^-$ at 298.15 K. Equation coefficients used in the Abraham model calculations were taken from Table 3.2.

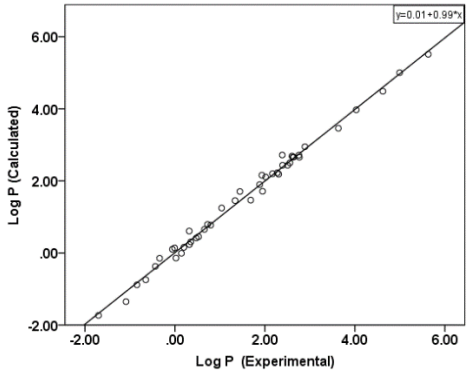


Figure 3.8: Comparison between the observed log *P* data and calculated log P values based on Eq. 1.1 for the 45 organic solutes dissolved in anhydrous $[N_{112}O_2N_{114}]^+[Tf_2N]^-$ at 298.15 K. Equation coefficients used in the Abraham model calculations were taken from Table 3.2.

3.3 Development of Ion-Specific Abraham Model Correlations for Solute Transfer into IL Solvents

The Abraham model correlations presented in the preceding section apply only to the four specific ILs introduced here: $[N_{112}N_{113}]^+[NTf_2]^-$, $[N_{112}N_{114}]^+[NTf_2]^-$, $[N_{112}O_2N_{113}]^+[NTf_2]^-$,and $[N_{112}O_2N_{114}]^+[NTf_2]^-$. Greater predictive capability can be achieved by resolving each calculated equation coefficient into individual cation- and anion-specific contributions given in Equations 1.3 and 1.4. Once calculated, individual cation- and anion-specific coefficients can be pairwise

summed to yield overall equation coefficients for additional ILs. Suppose a researcher wishes to predict log *P* and log *K* values for organic solutes dissolved in the tetrafluoroborate or dicyanamide salts of N-[2-(N',N'-dimethylamino)ethyl]-N,N-(dimethyl)-1-propanaminium (i.e., $[N_{112}N_{113}]^+$ $[BF_4]^-$ and $[N_{112}N_{113}]^+$ $[N(CN)_2]^-$, respectively). In this instance, the anion-specific equation coefficients for both $[BF_4]^-$ and $[N(CN)_2]^-$ are available from a previous study.[77] Although equation coefficients for the $[N_{112}N_{113}]^+$ cation have not yet been determined, fortunately these can be easily calculated from the log *P* and log *K* experimental values tabulated in Table 3.2.

The numerical values of the coefficients of Equations 3.1 and 3.2 are thus the respective cation-specific coefficients for $[N_{112}N_{113}]^+$. Similarly, cation-specific equation coefficients for the $[N_{112}N_{114}]^+$, $[N_{112}O_2N_{113}]^+$ and $[N_{112}O_2N_{114}]^+$ cations are the tabulated equation coefficients provided in Table 3.2 for the ILs $[N_{112}N_{114}]^+[NTf_2]^-$, $[N_{112}O_2N_{113}]^+[NTf_2]^-$,and $[N_{112}O_2N_{114}]^+[NTf_2]^-$, respectively. The cation-specific equation coefficients determined in the current study for $[N_{112}N_{113}]^+$, $[N_{112}N_{114}]^+$, $[N_{112}O_2N_{113}]^+$ and $[N_{112}O_2N_{114}]^+$ cations can be combined with existing equation coefficients for 20 different IL anions[12,64,74,77] to allow one to estimate log *P*, log *K*, and $\gamma_{1,\mathrm{IL}}^{\infty}$ values for solutes dissolved in an additional 80 IL solvents.

A major question with this method is can splitting coefficients into cation- and anion-specific parameters provide accurate results? Studies have demonstrated that Abraham model correlations constructed from summing calculated cation- and anion-specific equation coefficients indeed have predictive ability. For example, Lu and co- workers[78] constructed Abraham model correlations for predicting log *K* and log *P* values for solutes dissolved in 1-butyl-3-methylimidazolium dicyanamide, $([BMIm]^+[N(CN)_2]^-)$ by combining known ion-specific

equation coefficients for the $[BMIm]^+$ cation and the $[N(CN)_2]^-$ anion. Equations 3.3 and 3.4 were found to predict the partition coefficient data of 67 organic solutes dissolved in $[BMIm]^+[N(CN)_2]^-$ with a standard error of 0.16 and 0.11 log units for log *P* and log *K*, respectively.

$$log\ P\ (298K) = -0.305 + 0.492\ E + 0.742\ S + 0.835\ A - 4.593\ B + 3.147\ V \quad \textbf{(Eq. 3.3)}$$

$$log\ K\ (298K) = -0.793 + 0.378\ E + 2.610\ S + 4.551\ A + 0.405\ B + 0.657\ L \quad \textbf{(Eq. 3.4)}$$

Paduszynski and Domanska[79] similarly performed an Abraham model analysis for log *K* correlations of solute partitioning into 1-butyl-1-methylpiperidinium thiocyanate ($[BMPip]^+[SCN]^-$) using the previously-determined cation- and anion-specific coefficients for $[BMPip]^+$ and $[SCN]^-$. The constructed log *K* correlation performed well, predicting the experimental gas-to-IL partition coefficients to within a standard deviation of 0.122 log units.

CHAPTER 4

DEVELOPMENT OF ABRAHAM MODEL EXPRESSIONS FOR PREDICTING THE STANDARD MOLAR ENTHALPIES OF VAPORIZATION OF ORGANIC COMPOUNDS AT 298.15K*

4.1 Introduction

Chapter 1 explained the application of the ABSM for solvent parameters such as $\Delta_{vap}H^0_m$. This chapter elucidates the process of how $\Delta_{vap}H^0_m$ ABSM paramaters were calculated. Past studies have shown that the ABSM provides reasonably accurate mathematical descriptions of the enthalpies of solvation of organic vapors and inorganic gases dissolved in both water and a wide range of organic solvents that include five hydrocarbon (hexane, heptane, octane, hexadecane, cyclohexane), four chloroalkane (dichloromethane, chloroform, carbon tetrachloride, 1,2-dichloroethane), one dialkyl ether (dibutyl ether) and three cyclic ether (tetrahydrofuran, 1,4-dioxane, 1,3-dioxolane), twelve alcohol (methanol, ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-octanol, 2-propanol, 2-butanol, 2-methyl-1-propanol, 2-methyl-2-propanol, 1,2-ethylene glycol), two alkanone (acetone, 2-butanone), two alkyl acetate (methyl acetate, ethyl acetate), three dialkyl carbonate (dimethyl carbonate, diethyl carbonate, propylene carbonate), aromatic hydrocarbon (benzene, toluene, p-xylene, mesitylene), two chloroaromatic hydrocarbon (chlorobenzene, 1,2-dichlorobenzene) and seven miscellaneous organic solvents (pyridine, acetonitrile, dimethyl sulphoxide, formamide, N,N-dimethylacetatemide, N,N-dimethylformamide, acetic acid) used in industrial manufacturing processes[80–96].

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* This chapter is reproduced from Churchill, B, Acree Jr, WE, & Abraham, MH. (2019). Development of Abraham model expressions for predicting the standard molar enthalpies of vaporization of organic compounds at 298.15 K. **Thermochimica Acta, 681**, 178372, with permission from Elsevier.

Derived Abraham model correlations described the experimental $\Delta_{solv}H_m^0$ data to better than 3.5 kJ mol^{-1}. The documented success of the Abraham model in describing $\Delta_{solv}H_m^0$ data suggests that the model will also provide reasonably accurate mathematical correlations/predictions for $\Delta_{vap}H_m^0$ values as well. For liquid solutes the standard molar enthalpy of vaporization is the major contributor to the enthalpy of solvation.

4.2 Construction of Standard Molar Enthalpy of Vaporization Database

The standard molar enthalpy of vaporization database was constructed by extracting experimental $\Delta_{vap}H_m^0$ values from the large enthalpy of transition compilation of Acree and Chickos [88], supplemented by recently published data for several N,N-dialkylformamides[97]. The compilation contains experimental values reported over the time period of 1880-2015 with a few references from 2016. Multiple experimental entries were found for many of the organic compounds. The experimental values were determined by both direct and indirect methods. Direct methods include calorimetric measurements and indirect methods usually include a direct or indirect measure of vapor pressure over a range of temperatures. In the case of vapor pressure measurements the numerical value of $\Delta_{vap}H_m^0$ is computed from the vapor pressure dependency on temperature according to the integrated form of Clausius-Clapeyron equation (for temperature intervals < 30) or more complex mathematical forms that take into account heat capacity effects. Enthalpies of vaporization have also been obtained by correlations of changes in gas chromatographic net retention times[98,99]. Almeida and Monte[100] reviewed the different experimental methods for measuring enthalpies of sublimation. Several of the methods also apply to $\Delta_{vap}H_m^0$ determinations.

The enthalpy of transition compilation of Acree and Chickos covers approximately 130 years of the published literature, and as one might expect the compilation contains multiple $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ entries for many of the listed organic compounds. In deciding which of the multiple entries to include in the database the following were selected: (a) only values that pertained to 298.15 K; (b) values based on direct experimental measurements over indirect measurements; (c) values that did not require large temperature extrapolations back to 298.15 K; and (d) values that showed internal thermodynamic consistency provided that experimental enthalpy of fusion and enthalpy of sublimation data were also available. No attempt was made to select the $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ values that would yield the best Abraham model correlations. Using the above criterion, $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ values were compiled for 703 different organic and organometallic compounds for which Abraham model solute descriptors were available. The $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ values are given in Table C.1, along with the numerical values of the Abraham model solute descriptors that will be used in developing the predictive Abraham model $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ correlations. Most of the $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ values pertain to compounds that are liquid at 298.15 K; however, there are a few values that pertain compounds that are crystalline at 298.15 K. These later values were determined using correlation gas chromatography, or were calculated using measured $\Delta_{\mathrm{fus}}\mathrm{H}_{\mathrm{m}}^{0}$ and $\Delta_{\mathrm{sub}}\mathrm{H}_{\mathrm{m}}^{0}$values through Equation 4.1.

$$\Delta_{sub}H_m^0 = \Delta_{fus}H_m^0 + \Delta_{vap}H_m^0 \qquad \textbf{(Eq. 4.1)}$$

4.3 Development of Abraham Model Correlations for Molar Enthalpies of Vaporization

The Abraham solvation parameter model for molar enthalpies of solvation takes the following mathematical forms:

$$\Delta_{solv}H_m^0 = c_{h,l} + e_{h,l} \cdot E + s_{h,l} \cdot S + a_{h,l} \cdot A + b_{h,l} \cdot B + l_{h,l} \cdot L \quad \textbf{(Eq. 4.2)}$$

$$\Delta_{solv}H_m^0 = c_{h,v} + e_{h,v} \cdot E + s_{h,v} \cdot S + a_{h,v} \cdot A + b_{h,v} \cdot B + v_{h,v} \cdot V \quad \textbf{(Eq. 4.3)}$$

Each term on the right-hand side of Equations 4.2 and 4.3 represent a different type of molecular interaction just like that from Equations 1.1 and 1.2. In applying the Abraham model to enthalpies of vaporization, two additional terms, ss ·S·S and ab ·A·B, will be added to the model:

$$\Delta_{vap}H_m^0 = c_{h,l} + e_{h,l} \cdot E + s_{h,l} \cdot S + a_{h,l} \cdot A + b_{h,l} \cdot B + l_{h,l} \cdot L + ss_{h,l} \cdot SS + ab_{h,l} \cdot AB \quad \textbf{(Eq. 4.4)}$$

$$\Delta_{vap}H_m^0 = c_{h,v} + e_{h,v} \cdot E + s_{h,v} \cdot S + a_{h,v} \cdot A + b_{h,v} \cdot B + v_{h,v} \cdot V + ss_{h,v} \cdot SS + ab_{h,v} \cdot AB \quad \textbf{(Eq. 4.5)}$$

To account for any additional compound-compound interactions that might be present in the "pure" organic compound. The ab·A·B term has been used previously by Abraham and coworkers [101,102] in solubility correlations of liquid and solid solutes dissolved in water and in 1-octanol. The authors found that inclusion of the term yielded significantly better mathematical correlations. The preliminary regression analyses showed that this is also the case for enthalpy of vaporization correlations. Analysis of the experimental $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ data in the last column of Table C.1 in accordance with Equations 4.4 and 4.5 yielded the following Abraham model correlations:

$$\Delta_{vap}H_m^0(kJ\ mol^{-1}) = 5.938(0.313) - 7.667(0.456)\mathrm{E} + 9.983(0.876)\mathrm{S} + 15.483(1.200)\mathrm{A} + 1.694(0.558)\mathrm{B} + 9.608(0.067)\mathrm{L} - 1.541(0.618)\mathrm{SS} + 43.483(1.964)\mathrm{AB} \quad \textbf{(Eq. 4.6)}$$

(with N = 703, SD = 2.55, R^2 = 0.979, F = 4710.9)

$$\Delta_{vap}H_m^0(kJ\ mol^{-1}) = -3.246(0.412) + 5.114(0.515)\mathrm{E} + 19.635(0.955)\mathrm{S} + 20.131(1.355)\mathrm{A} + 1.266(0.629)\mathrm{B} + 34.388(0.271)\mathrm{V} - 2.487(0.698)\mathrm{SS} + 42.350(2.215)\mathrm{AB} \quad \textbf{(Eq. 4.7)}$$

(with N=703, SD=2.87, R2=0.974, F=3685.6)

where the standard error in each calculated equation coefficient is given in parenthesis following the respective coefficient. The statistical information associated with each correlation includes the number of experimental data points used in the regression analysis (N), the standard deviation (SD), the squared correlation coefficient (R^2) and the Fisher F-statistic (F). All regression analyses were performed using IBM SPSS Version 22 Statistic Software. The large $ab_{h,l}$ and $ab_{h,v}$ coefficients in Equations 4.4 and 4.5 indicate the importance of including this term in the model. The relatively small standard deviations and the near unity squared correlation coefficients suggest that both equations provide a reasonable accurate mathematical description of the observed $\Delta_{vap}H^0_m$ data. In fact the correlations are comparable to (if not slightly better than) the predictive expressions discussed in the introduction. A comparison of the experimental $\Delta_{vap}H^0_m$ data versus back-calculated values is depicted in Figure 4.1 and Figure 4.2.

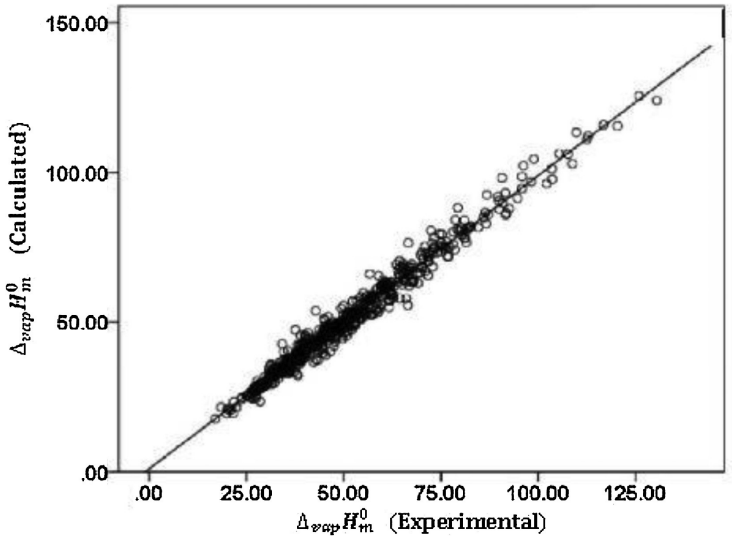

Figure 4.1: Comparison between experimental $\Delta_{vap}H^0_m$ data (in kJ mol^{-1}) and back-calculated values based on Equation 4.6.

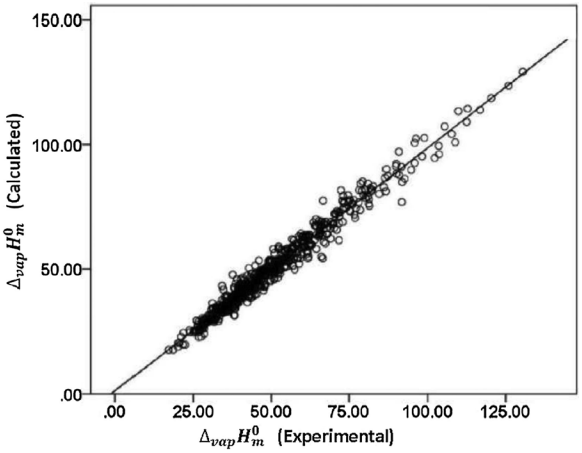

Figure 4.2: Comparison between experimental $\Delta_{vap}H_m^0$ data (in kJ mol^{-1}) and back-calculated values based on Equation 4.7.

A more careful point-by-point comparison of the experimental versus back-calculated values reveals that Equations 4.6 and 4.7 over-predicted the $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ values for the 28 alkylamines in the dataset. Relatively large deviations were observed for several of the alkanediols. Elimination of these compounds from the regression analysis led to Figure 4.1 and Figure 4.2 with much better mathematical correlations having standard deviations of SD = 1.95 kJ mol^{-1} and SD = 2.44 kJ mol^{-1} for Equations 4.8 and 4.9, respectively. The large reduction in standard deviation accompanying the removal of alkylamines and alkane-diols shows just how poor the back-calculations were for these two classes of organic compounds. While the reduced standard deviations are gratifying from a predictive point-of-view, it is preferred that the Abraham model correlations include the widest range of chemical diversity as possible.

$$\Delta_{vap}H_m^0(kJ\ mol^{-1}) = 6.192(0.243) - 7.688(0.361)\mathrm{E} + 10.222(0.684)\mathrm{S} + 3.068(1.366)\mathrm{A} + 1.341(0.506)\mathrm{B} + 9.517(0.052)\mathrm{L} - 1.038(0.483)SS + 81.336(3.314)\mathrm{AB} \quad \textbf{(Eq. 4.8)}$$

(with N = 658, SD = 1.95, R^2 = 0.986, F = 6759.9)

$$\Delta_{vap}H_m^0(kJ\ mol^{-1}) = -2.960(0.356) + 4.688(0.452)\mathrm{E} + 20.076(0.863)\mathrm{S} + 8.803(1.711)\mathrm{A} + 0.328(0.633)\mathrm{B} + 34.145(0.236)\mathrm{V} - 1.861(0.606)SS + 77.495(4.147)\mathrm{AB} \quad \textbf{(Eq. 4.9)}$$

(with N = 658, SD = 2.44, R^2 = 0.979, F = 4286.1)

To include alkylamines and alkanediols into the Abraham model correlations it was decided that three additional indicator variables would be added to both equations. The first indicator variable is for the 28 alkylamines (I_{amine} = 1 for alkylamines, I_{amine} = 0 for all other compounds). The last two indicator variables are for the 16 alkanediols and one alkanetriol (glycerol) ($I_{non\text{-}\alpha,\omega\text{-}diol}$ = 1 for non-α,ω-diols. $I_{\alpha,\omega\text{-}diol}$ = 1 for α,ω-diols, for nondiols $I_{non\text{-}\alpha,\omega\text{-}diol}$ = $I_{\alpha,\omega\text{-}diol}$ = 0). Glycerol is treated as having adjacent -OH groups. The large differences in the enthalpies of vaporization for propane-1,2-diol ($\Delta_{vap}H_m^0$ =67.5 kJ mol^{-1}) versus propane-1,3-diol ($\Delta_{vap}H_m^0$ = 72.4 kJ mol^{-1}), for butane-1,2-diol ($\Delta_{vap}H_m^0$ =73.3 kJ mol^{-1}) versus butane-1,3-diol ($\Delta_{vap}H_m^0$ =72.8 kJ mol^{-1}) versus butane-1,4-diol ($\Delta_{vap}H_m^0$ = 79.3 kJ mol^{-1}), and for pentane-1,2-diol ($\Delta_{vap}H_m^0$ =74.6 kJ mol^{-1}) versus pentane-1,5-diol ($\Delta_{vap}H_m^0$ = 86.8 kJ mol^{-1}) suggests that the relative placement of the two OH groups is an important factor in determining the compound's enthalpy of vaporization. The difference in the $\Delta_{vap}H_m^0$ appears to become larger with increasing alkyl chain length.

One final analysis of the experimentally $\Delta_{vap}H_m^0$ data in the last column of Table C.1, this time with the three indicator variables included in the model, yielded the following two Abraham model correlations:

$$\Delta_{vap}H_m^0(kJ\ mol^{-1}) = 6.100(0.257) - 7.363(0.380)\mathrm{E} + 9.733(0.733)\mathrm{S} + 4.025(1.351)\mathrm{A} + 2.123(0.521)\mathrm{B} + 9.537(0.055)\mathrm{L} - 1.180(0.515)\mathrm{SS} + 77.871(3.233)\mathrm{AB} - 5.781(0.441)\mathrm{I_{amine}} - 14.783(1.235)\mathrm{I_{non-\alpha\omega-diol}} - 17.873(1.431)\mathrm{I_{\alpha,\omega-diol}} \quad \textbf{(Eq. 4.10)}$$

(with N = 703, SD = 2.09, R^2 = 0.986, F = 4925.6)

$$\Delta_{vap}H_m^0(kJ\ mol^{-1}) = -3.008(0.368) + 5.226(0.465)\mathrm{E} + 18.422(0.892)\mathrm{S} + 8.978(1.661)\mathrm{A} + 1.363(0.637)\mathrm{B} + 34.141(0.242)\mathrm{V} - 2.045(0.631)\mathrm{SS} + 75.728(3.952)\mathrm{AB} - 4.888(0.543)\mathrm{I_{amine}} - 13.297(1.510)\mathrm{I_{non-\alpha\omega-diol}} - 17.619(1.748)\mathrm{I_{\alpha,\omega-diol}} \quad \textbf{(Eq. 4.11)}$$

(with N=703, SD=2.54, R2=0.979, F=3274.7)

Both correlations provide a reasonably accurate mathematical description of the observed enthalpy of vaporization data. Inclusion of the three indicator variables significantly reduced the standard deviations to the point where the descriptive abilities of Equations 4.10 and 4.11 are comparable to those of Equations 4.8 and 4.9. Figure 4.3 and Figure 4.4 compare the experimental $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ to values back-calculated using Abraham model Equations 4.10 and 4.11.

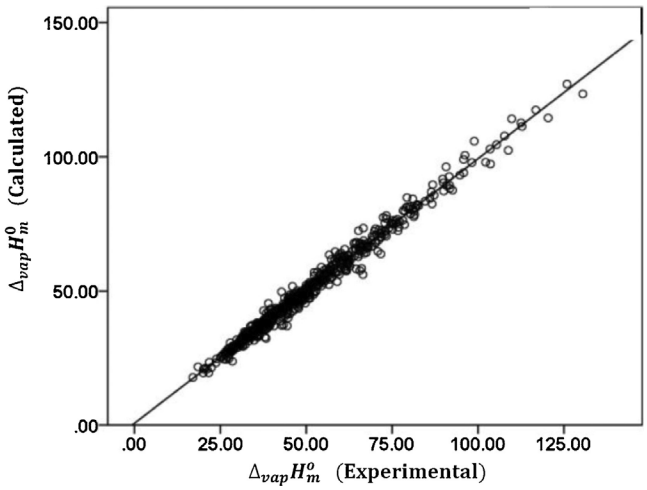

Figure 4.3: Comparison between experimental $\Delta_{vap}H_m^0$ data (in kJ mol^{-1}) and back-calculated values based on Equation 4.10.

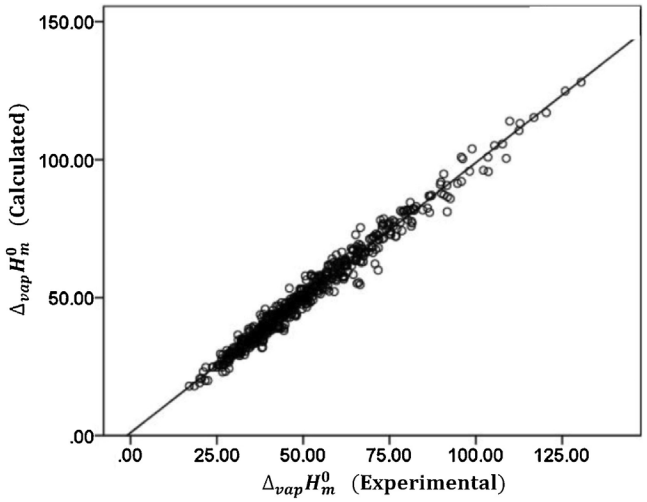

Figure 4.4: Comparison between experimental $\Delta_{vap}H_m^0$ data (in kJ mol^{-1}) and back-calculated values based on Equation 4.11.

As an informational note calculations based on the derived Abraham model correlations are comparable to, if not better than, those obtained from many of the existing methods used to predict enthalpies of vaporization. The method is limited to those 8000 or so organic and organometallic compounds for which Abraham model solute descriptors are known[76]. Group contribution methods will provide $\Delta_{\mathrm{vap}}\mathrm{H}_{\mathrm{m}}^{0}$ predictions for more compounds; however, the calculation error is likely to be somewhat larger. Approximate standard deviation errors of SD = 4.0 to 4.5 kJ mol^{-1} and of SD = 3.0 to 3.5 kJ mol^{-1} were noted in the group contribution methods proposed by Gharagheizi *et al*.[103] and by Naef and Acree[104].

CHAPTER 5

ABRAHAM MODEL CORRELATION FOR DIRECT WATER-TO-2,2,5,5-TETRAMETHYLOXOLANE SOLUTE TRANSFER PARTITIONING PROCESS REVISITED*

5.1 Introduction

Chapter 3 expanded on the ABSM by calculating ABSM parameters for recently discovered ILs which had modified tetraalkylimidazolium cations. This chapter covers the calculation of log *P* ABSM parameters for more traditional solvent systems: log $P_{toluene/water}$ and log $P_{tetramethyloxolane/water}$. 2,2,5,5-tetramethyloxoxlane (TMO) has been suggested as a replacement solvent for non-polar hydrocarbon solvents, particularly toluene, especially in systems with water. Unlike other greener ether solvents (such as methyl cyclopentyl ether and 2-methyltetra-hydrofuran) TMO has been shown to be inherently resistant to peroxide formation. Acidity stability tests have further shown that DMO can resist acid attacks at room temperature[105]. Byrne and co-workers[106] reported water-to-toluene and water-to-2,2,5,5-tetramethyloxolane partition coefficients of a chemically diverse set of 66 different organic compounds of varying polarity and hydrogen-bonding character. The authors used their measured partition coefficient data to develop model correlations for describing solute transfer into both water-saturated organic solvents through the general Abraham equation, Equation 1.2.

Byrne and co-workers[106] derived Equations 5.1 and 5.2 where log $P_{toluene/water}$ and log $P_{tetramethyloxolane/water}$ are the respective logarithms of the water-to-organic solvent partition

* This chapter is reproduced from Churchill, B, Acree, WE & Abraham, MH. (2019). Abraham model correlation for direct water-to-2,2,5,5-tetramethyloxolane solute transfer partitioning process revisited. **Physics and Chemistry of Liquids, 58**(6), 833-838, with permission from Taylor & Francis Online.

coefficients, and used the coefficients in these equations to compare the two water-solvent systems.

$$log\ P_{toluene/water} = 0.642 + 0.430E - 0.755S - 3.180A - 4.945B + 4.298V \quad \textbf{(Eq. 5.1)}$$

$$log\ P_{tetramethyloxolane/water} = 0.374 + 0.057E - 0.766S + 0.275A - 5.178B + 4.396V \quad \textbf{(Eq. 5.2)}$$

Unfortunately there were numerous errors in the tabulated solute descriptors that were given in Table 5.1 of reference 2. For example, Byrne and co-workers incorrectly gave the A solute descriptor of phenol, m-cresol, p-cresol, 3-fluorophenol, 4-fluorophenol and resorcinol as either zero or as a value less than A = 0.10. The A solute descriptor of each of the fore-mentioned phenol derivatives is much larger. Also, the authors gave different McGowan volumes for two pairs of isomeric compounds, namely 4-fluorophenol (V = 0.424) and 3-fluorophenol (V = 0.891), and for m-cresol (V = 0.970) and p-cresol (V = 0.545). Tabulated McGowan volumes for phenol (V = 0.404) and resorcinol (V = 0.565) were also incorrect. Given the number of incorrect entries for the solute descriptors, the question naturally arises regarding whether the coefficients for Equation 5.2 were correctly determined. We are not as concerned about the coefficients for Equation 5.1 as Stephens and co-workers[107] determined Abraham model log $P_{toluene/water}$ correlations for solute partition into toluene based upon experimental partition coefficients and molar solubility ratios for 204 compounds. The published log $P_{toluene/water}$ correlation is based on three times more experimental data points and has a much lower standard deviation (SD = 0.124 log units) than Equation 5.1 derived by Byrne and co-workers.[106] Attention is focused on the log $P_{tetramethyloxolane/water}$ correlation for solute transfer into 2,2,5,5-tetramethyloxolane because this is the first time that an Abraham model correlation has been reported for this green organic solvent.

Table 5.1: Logarithms of experimental water-to-2,2,5,5-tetramethyloxolane partition coefficients, log $P_{tetramethyloxolane/water}$, and solute descriptors for the 66 organic solutes considered in the current commentary.

Solute	E	S	A	B	V	log $P_{tetramethyloxolane/water}$
Benzoic acid	0.730	0.900	0.590	0.400	0.932	2.248
Butanoic acid	0.210	0.640	0.610	0.450	0.747	0.830
Acetic acid	0.265	0.640	0.620	0.440	0.465	-0.276
Diethyl carbonate	0.061	0.690	0.000	0.500	0.946	1.494
Cyclopentanol	0.427	0.540	0.260	0.570	0.763	0.782
2-Propanol	0.212	0.360	0.330	0.560	0.590	-0.301
1-Butanol	0.224	0.420	0.370	0.480	0.731	0.793
tert-Butanol	0.180	0.300	0.310	0.600	0.731	0.096
Ethanol	0.246	0.420	0.370	0.480	0.449	-0.673
1-Propanol	0.236	0.420	0.370	0.480	0.590	0.009
Methanol	0.278	0.440	0.430	0.470	0.308	-0.967
Benzaldehyde	0.820	1.000	0.000	0.390	0.873	1.899
Vanillin	0.990	1.300	0.310	0.680	1.131	1.037
Octane	0.000	0.000	0.000	0.000	1.236	5.739
Cyclohexene	0.395	0.280	0.000	0.090	0.802	3.681
1-Hexene	0.078	0.080	0.000	0.070	0.911	4.057
N,N-Dimethylacetamide	0.363	1.380	0.000	0.800	0.788	-1.621
Pyridine	0.631	0.840	0.000	0.520	0.675	-0.065
Triethylamine	0.101	0.150	0.000	0.790	1.054	0.949
Dipropylamine	0.124	0.300	0.080	0.690	1.054	1.907
Dibutylamine	0.107	0.300	0.080	0.690	1.336	1.947[a]
Butylamine	0.224	0.350	0.160	0.610	0.772	0.069
Hexylamine	0.197	0.350	0.160	0.610	1.054	1.530
Naphthylamine	1.670	1.270	0.190	0.510	1.185	2.292
Aniline	0.955	0.960	0.260	0.410	0.816	1.197
Benzene	0.610	0.520	0.000	0.140	0.716	2.507
Xylenes	0.623	0.520	0.000	0.160	0.998	3.663
Fluorene	1.588	1.060	0.000	0.250	1.357	3.320[a]
Propyelne carbonate	0.319	1.370	0.000	0.600	0.697	-0.840
Butyl acetate	0.071	0.600	0.000	0.450	1.028	2.304
Butyl benzoiate	0.668	0.800	0.000	0.460	1.495	3.539[a]
Ethyl acetate	0.106	0.620	0.000	0.450	0.747	0.882
Propyl acetate	0.092	0.600	0.000	0.450	0.888	1.557
tert-Butyl methyl ether	0.024	0.220	0.000	0.550	0.872	1.340
tert-Butyl ethyl ether	0.000	0.160	0.000	0.570	1.013	1.929

Solute	E	S	A	B	V	log $P_{tetramethyl\ oxolane/water}$
Anisole	0.708	0.750	0.000	0.290	0.916	2.784
Diethyl ether	0.041	0.250	0.000	0.450	0.731	1.264
1,4-Dioxane	0.329	0.750	0.000	0.640	0.681	-0.418
Methyl formate	0.192	0.680	0.000	0.380	0.465	-0.971[a]
Chlorocyclohexane	0.448	0.480	0.000	0.100	0.968	3.681
Iodomethane	0.676	0.430	0.000	0.120	0.508	2.506[a]
1,2-Dichloroethane	0.416	0.640	0.100	0.110	0.635	2.269
Chloroform	0.425	0.490	0.150	0.020	0.617	3.157
Bromobenzene	0.882	0.730	0.000	0.090	0.891	2.679[a]
Chlorobenzene	0.718	0.650	0.000	0.070	0.839	3.116
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	0.961	2.728[a]
Iodobenzene	1.188	0.820	0.000	0.120	0.975	3.482
3-Pentanone	0.154	0.660	0.000	0.510	0.829	1.105
Acetophenone	0.818	1.010	0.000	0.480	1.014	1.875
2-Butanone	0.166	0.700	0.000	0.510	0.688	0.397
3-Hexanone	0.136	0.660	0.000	0.510	0.970	1.619
Propionitrile	0.162	0.900	0.020	0.360	0.545	0.162
Acetonitrile	0.237	0.900	0.070	0.320	0.404	-0.453
Nitrobenzene	0.871	1.110	0.000	0.280	0.891	2.055
Nitroethane	0.270	0.950	0.020	0.330	0.565	0.669
Nitromethane	0.313	0.950	0.060	0.310	0.424	0.117
4-Nitroaniline	1.220	1.920	0.460	0.350	0.990	1.913
m-Cresol	0.822	0.880	0.570	0.340	0.916	2.827
p-Cresol	0.820	0.870	0.570	0.310	0.916	2.728
Phenol	0.805	0.890	0.600	0.300	0.775	2.122
3-Fluorophenol	0.667	0.980	0.680	0.170	0.793	2.479
4-Fluorophenol	0.670	0.970	0.630	0.230	0.793	2.320
3-Hydroxybenzldehyde	0.990	1.380	0.730	0.400	0.932	1.745
4-Nitrophenol	1.070	1.720	0.820	0.260	0.949	2.268
Resorcinol	0.980	1.110	1.090	0.520	0.834	0.360
Ethylene glycol	0.404	0.900	0.580	0.780	0.508	-2.216

5.2 Development of Abraham Model Correlation

In Table 5.1 of this chapter, the Abraham model solute descriptors of the 66 organic solutes studied by Byrne and co-workers were tabulated, as well as the experimental log

$P_{\text{tetramethyloxolane/water}}$ data reported in reference 2. Numerical values of the solute descriptors can be found in earlier publications, [107–111] and are conveniently available on a public website for over 8,000 organic, organometallic and inorganic compounds[112]. As an informational note the numerical values are periodically updated as more experimental data becomes available.

Preliminary regression analysis of the experimental log $P_{\text{tetramethyloxolane/water}}$ in Table 5.1 of this communication in accordance with the Abraham model indicated that the experimental values for seven compounds appeared to be outliers as evidenced by large differences between the experimental data and values back-calculated by the preliminary Abraham model correlation. These seven compounds were removed from the dataset. Our final regression analysis yielded the following Abraham model correlation:

$$P_{\underline{tetramethyloxolane}}_{water} = 0.242(0.157) + 0.116(0.114)\mathrm{E} - 0.757(0.120)\mathrm{S} + 0.151(0.128)\mathrm{A} - 5.415(0.170)\mathrm{B} + 4.760(0.173)\mathrm{V} \quad \textbf{(Eq. 5.3)}$$

(N = 59, SD = 0.222, R^2 = 0.978, F 478.2)

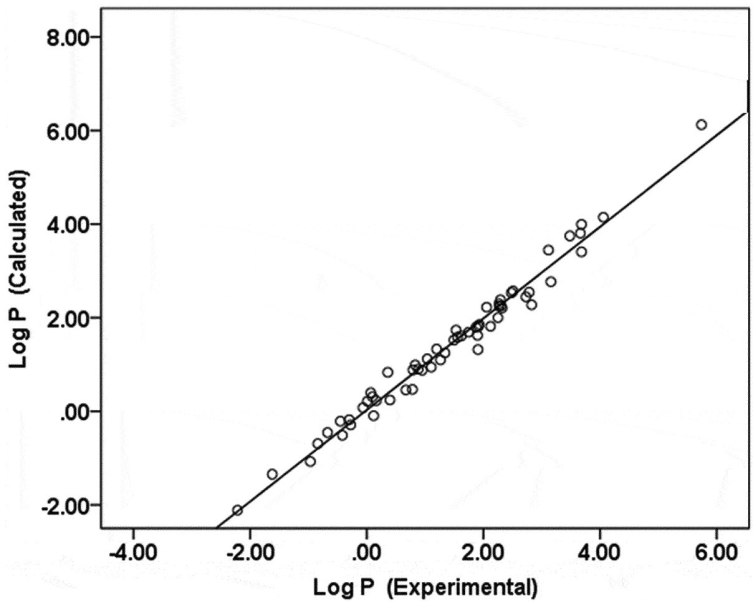

Figure 5.1: Comparison of the experimental $P_{\text{tetramethyloxolane/water}}$ and back-calculated values based on Equation 5.3.

The correlations were obtained using the IBM SPSS® Statistical 22 commercial software. Removal of the seven experimental data points from the regression analysis significantly reduced the standard deviation from SD = 0.358 log units to SD = 0.222 log units. Figure 5.1 compares the experimental log $P_{tetramethyloxolane/water}$ to back-calculated values based on Equation 5.3. We believe that the derived correlation is more representative of the solubilizing character of 2,2,5,5-tetramethyloxolane than the correlation reported by Byrne and co-workers.[106] The correlation has a much lower standard error that the correlation derived by Byrne and co-workers (SE = 0.232 log units versus 0.424 log units), and there is no concern that incorrect numerical values of the solute descriptors may have been used in determining the equation coefficients. Values which were considered questionable were removed from the regression analysis of log $P_{tetramethyloxolane/water}$. For example, it is highly unlikely that the log $P_{tetramethyloxolane/water}$ values for dipropylamine and for dibutylamine, log $P_{tetramethyloxolane/water}$ =1.907and log $P_{tetramethyloxolane/water}$ = 1.945, respectively, should be nearly identical. The longer alkyl chain length on dibutylamine should lead to much greater partitioning into the organic solvent than is indicated by the experimental data. We also believe that the log $P_{tetramethyloxolane/water}$ values for bromobenzene, 1,2-dichlorobenzene and fluorene are too small when compared to the solubility of other similar organic molecules in the dataset. In the case of chlorobenzene versus 1,2-dichlorobenzene the presence of the second chlorine atom should lead to greater (not less) partitioning into 2,2,5,5-tetramethyloxolane as would be expected from 1,2-dichlorobenzene's lower aqueous solubility[113,114].

CHAPTER 6

ABRAHAM MODEL CORRELATIONS FOR DESCRIBING SOLUTE TRANSFER PROCESSES INTO DIETHYL CARBONATE*

6.1 Introduction

In recent years[105–119] there has been renewed interest in performing solubility measurements for crystalline organic compounds dissolved both in organic mono-solvents and in binary solvent mixtures. The primary objective of these studies has been to identify suitable solvents for purifying medicinal and cosmetic compounds, pesticides and herbicides, and other synthesised chemical products through recrystallisation. For the most part, the fore-mentioned studies have been limited to only a handful of different organic mono-solvents and solvent mixtures. This chapter explores diethyl carbonate and its ABSM parameters. Diethyl carbonate is an important organic co-solvent used in lithium-ion batteries[120] and as an extraction solvent for the removal of carboxylic acids from aqueous solutions.[121–123]

6.2 Chemical Materials and Experimental Methodology

In assembling the crystalline organic compounds for the solubility determinations compounds selected exhibit a wide range of chemical diversity and that span a wide range of solute descriptors values. All chemicals used in the solubility measurements were purchased from commercial sources. The commercial suppliers and chemical purities of the chemicals used in the solubility measurements are summarized in Table 6.1.

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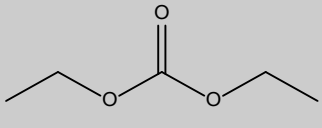
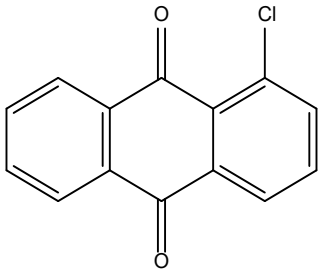
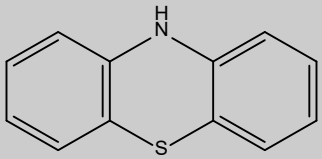
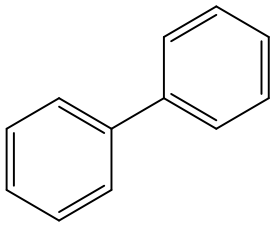
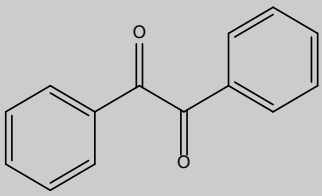
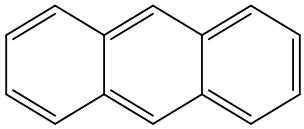
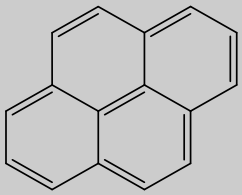
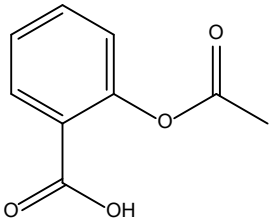
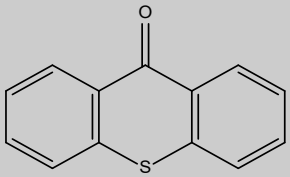
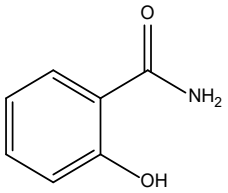
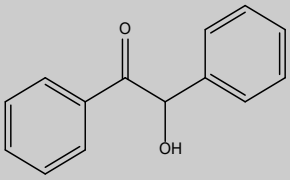
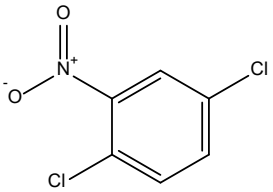
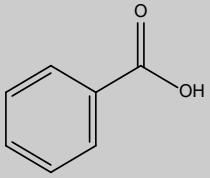
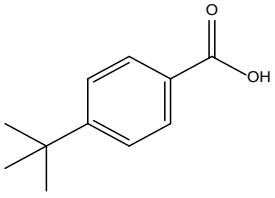
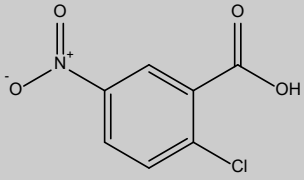
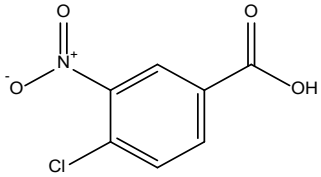
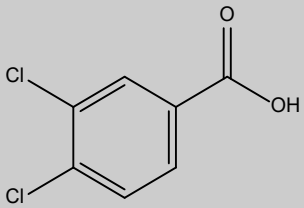
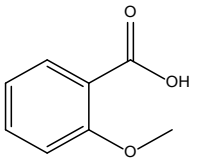
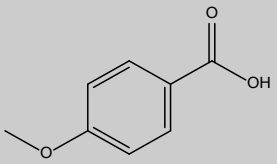
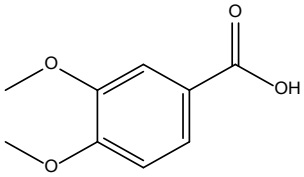
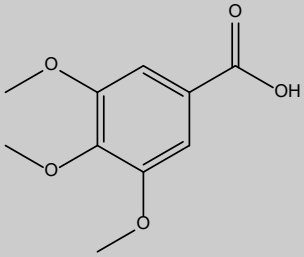
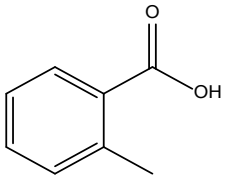
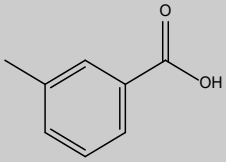
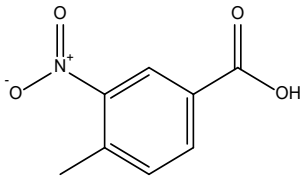
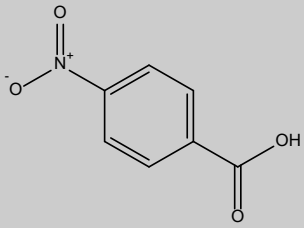
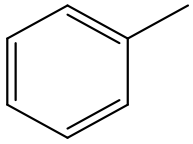
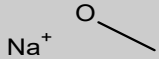
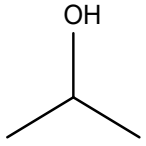
* This chapter is reproduced from Dai, J, Eddula, S, Jiang, C, Zhang, A, Liu, K, Zhu, S, Wang, S, Gupta, A, Churchill, B, Garcia, E, Acree Jr, WE & Abraham, MH. (2019). Abraham model correlations for describing solute transfer processes into diethyl carbonate. **Physics and Chemistry of Liquids,** 10.1080/00319104.2019.1675159, with permission from Taylor & Francis Online.

Table 6.1: Chemical sources and mass fraction purities of chemicals used in the solubility studies.

Chemical	Structure	Supplier	Purification Method	Purity (mass fraction)
Diethyl carbonate		Acros Organics, Morris Plains, New Jersey, USA	Stored over molecular and distilled	0.997
1-Chloroanthraquinone		Aldrich Chemical Company, Milwaukee, Wisconsin, USA	Recrystallization from anhydrous methanol	0.997
Phenothiazine		Acros Organics	Used as received	0.99
Biphenyl		Aldrich Chemical Company	Recrystallization from anhydrous methanol	0.997
Benzil		Aldrich Chemical Company	Recrystallization from anhydrous methanol	0.997
Anthracene		Aldrich Chemical Company	Recrystallization from anhydrous methanol	0.997
Pyrene		Aldrich Chemical Company	Recrystallization from anhydrous methanol	0.997

Chemical	Structure	Supplier	Purification Method	Purity (mass fraction)
Acetylsalicylic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
Thioxanthen-9-one		Aldrich Chemical Company	Recrystallization from anhydrous methanol	0.997
Salicylamide		Aldrich Chemical Company	Recrystallization from anhydrous methanol	0.997
Benzoin		Aldrich Chemical Company	Recrystallization from anhydrous methanol	0.997
1,4-Dichloro-2-Nitrobenzene		TCI America Chemical Company, Portland, Oregon, USA	Recrystallization from anhydrous methanol	0.997
Benzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
4-tert-Butylbenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998

Chemical	Structure	Supplier	Purification Method	Purity (mass fraction)
2-Chloro-5-nitrobenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
4-Chloro-3-Nitrobenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
3,4-Dichlorobenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
2-Methoxybenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
4-Methoxybenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
3,4-Dimethoxybenzoic acid		Acros Organics	Dried for two days at 333 K	0.998
3,4,5-Trimethoxybenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998

Chemical	Structure	Supplier	Purification Method	Purity (mass fraction)
2-Methylbenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
3-Methylbenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
4-Methyl-3-nitrobenzoic acid		Aldrich Chemical Company	Dried for two days at 333 K	0.998
4-Nitrobenzoic acid		Acros Organics	Dried for two days at 333 K	0.998
Toluene		Aldrich Chemical Company	None	Anhydrous
Sodium methoxide, 25 mass % solution in methanol		Aldrich Chemical Company	None	Anhydrous
2-Propanol		Aldrich Chemical Company	None	0.99

Solubilities of the 24 crystalline organic compounds were measured using a static equilibration method followed by a spectroscopic determination of the concentration of the dissolved solute in the saturated solution based on the Beer-Lambert law. Aliquots of the saturated solutions were transferred by syringe into weighed volumetric flasks after the

samples had equilibrated in sealed amber glass bottles in a constant temperature water bath at 298.15 ± 0.05 K for at least 3 days. The samples were periodically agitated to facilitate dissolution and mixing. The volumetric flasks containing the transferred aliquots were weighed on an electronic analytical balance. The transferred solutions were diluted quantitatively with 2-propanol. Absorbances of the diluted solutions and of the nine standard solutions of known solute concentrations were recorded on a Milton Roy Spectronic 1000 Plus spectrophotometer (Milton Roy, Rochester, NY, USA). The concentration of each diluted solution was computed from a Beer-Lambert law plot of absorbance versus concentration curve obtained from the measured absorbances of nine standard solutions of known solute molarity. The analysis wavelengths and concentration ranges used for each solute have been given in earlier publications.[124–142] We checked to make sure that diethyl carbonate did not absorb light at the analysis wavelengths and at the diethyl carbonate concentrations in the diluted solutions.

Molar concentrations of the diluted samples deduced from the Beer-Law law graph were converted into mole fraction solubilities using the volume of the volumetric flasks that the sample was transferred into, the mass of the sample analyzed, molar masses of the solvent and the respective solutes, and any dilutions that may have been needed in order for the sample's measured absorbance to fall on the Beer-Lambert law curve.

The experimental mole fraction solubilities, x_{solute}^{sat}, of the crystalline organics solutes in diethyl carbonate are tabulated in the second column of Table 6.2. The numerical values represent the average of 4 to 10 independent experimental determinations, which were reproducible to within ± 2% (relative error). The data for x_{solute}^{sat} was gathered and initially calculated by TAMS students and was checked by Dr. Acree and myself. I also showed the

students how to prepare the standard solution, how to perform the absorbance measurements and assisted with several of the actual solubility determinations.

Table 6.2: Mole fraction solubilities, x_{solute}^{sat}, of 24 crystalline organic compounds dissolved in diethyl carbonate at a temperature of 298.15 K.

Crystalline organic compound	x_{solute}^{sat}
1-Chloroanthraquinone	0.00775
Phenothiazine	0.0376
Biphenyl	0.234
Benzil	0.133
Anthracene	0.00547
Pyrene	0.0451
Acetylsalicylic acid	0.0226
Thioxanthen-9-one	0.00323
Salicylamide	0.0364
Benzoin	0.109
1,4-Dichloro-2-nitrobenzene	0.438
Benzoic acid	0.112
4-tert-Butylbenzoic acid	0.0332
2-Chloro-5-nitrobenzoic acid	0.0309
4-Chloro-3-nitrobenzoic acid	0.0133
3,4-Dichlorobenzoic acid	0.00809
2-Methoxybenzoic acid	0.0366
4-Methoxybenzoic acid	0.006
3,4-Dimethoxybenzoic acid	0.00401
3,4,5-Trimethoxybenzoic acid	0.00698
2-Methylbenzoic acid	0.0996
3-Methylbenzoic acid	0.0951
4-Methyl-3-nitrobenzoic acid	0.0123
4-Nitrobenzoic acid	0.00614

6.3 Development of Abraham Model Correlations for Solute Transfer into Diethyl Carbonate

Development of Abraham model correlations to describe solute transfer into diethyl carbonate requires constructing an Equation 1.1 and Equation 1.2 for each of the 50 individual organic and inorganic solutes considered in the current study. The solute descriptors needed for the right-hand sides of the two equations are tabulated in Table 6.3. The transfer properties needed on the left-hand side of Equations 1 and 2 are calculated from the experimental mole fraction solubility data given in or from the experimental solubility data and activity coefficients retrieved from the published chemical and engineering. Mole fraction-based solubilities are converted into molar solubilities by dividing x_{solute}^{sat} by the ideal molar volume of the saturated solution

$$C_{solute,org\ solv}^{sat} = \frac{x_{solute}^{sat}}{(1-x_{solute}^{sat})V_{solvent}+x_{solute}^{sat}V_{solute}} \quad \textbf{Eq. 6.1}$$

The subscripts 'org solv', 'water' and 'gas phase' associated with the molar solubilities indicate the phase to which the molar solubility pertains. For example $\mathrm{C}_{\mathrm{solute,org\ solv}}^{\mathrm{sat}}$ and $\mathrm{C}_{\mathrm{solute,water}}^{\mathrm{sat}}$ denote the molar solubility of the solute in the organic solvent and in water, respectively. The quantity $\mathrm{C}_{\mathrm{solute,gas}}^{\mathrm{gas}}$ is the molar concentration of the solute in the gas phase whose numerical value is often determined as part of the solute descriptor calculations.

The log *K* and log *P* values for the liquid and gases were tabulated from the eighth and ninth columns of Table 6.3. As the column headings indicate, the tabulated numerical values for the crystalline organic solutes pertain to the two respective solubility ratios, $\log\left(\frac{\mathrm{C}_{\mathrm{solute,org\ solv}}^{\mathrm{sat}}}{\mathrm{C}_{\mathrm{solute,gas\ phase}}^{\mathrm{sat}}}\right)$ and $\log\left(\frac{\mathrm{C}_{\mathrm{solute,org\ solv}}^{\mathrm{sat}}}{\mathrm{C}_{\mathrm{solute,water}}^{\mathrm{sat}}}\right)$.

Table 6.3: Logarithms of experimental partition coefficients, log P and log K, logarithms of molar solubility ratios, $log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right)$ and $log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right)$ and solute descriptors for organic compounds and inorganic gases dissolved in diethyl carbonate at 298.15 K.

Solute	E	S	A	B	L	V	log *K*[a]	log *P*[b]	Ref.
Helium	0.000	0.000	0.000	0.000	-1.741	0.068	-1.504	0.516	[143]
Neon	0.000	0.000	0.000	0.000	-1.575	0.085	-1.378	0.582	[143]
Argon	0.000	0.000	0.000	0.000	-0.688	0.190	-0.571	0.899	[143]
Krypton	0.000	0.000	0.000	0.000	-0.211	0.246	-0.132	1.078	[143]
Xenon	0.000	0.000	0.000	0.000	0.378	0.329	0.420	1.390	[143]
Hydrogen	0.000	0.000	0.000	0.000	-1.200	0.109	-1.107	0.613	[143]
Nitrogen	0.000	0.000	0.000	0.000	-0.978	0.222	-0.813	0.987	[143]
Oxygen	0.000	0.000	0.000	0.000	-0.723	0.183	-0.713	0.787	[144]
Sulphur hexafluoride	-0.600	-0.200	0.000	0.000	-0.120	0.464	0.018	2.238	[143]
Tetrafluoromethane	-0.580	-0.260	0.000	0.000	-0.817	0.320	-0.667	1.623	[143]
Carbon dioxide	0.000	0.280	0.050	0.100	0.058	0.281	0.713	0.793	[145]
Hydrogen sulphide	0.350	0.310	0.100	0.070	0.723	0.272	1.056	0.656	[145]
Methane	0.000	0.000	0.000	0.000	-0.323	0.250	-0.261	1.199	[143]
Ethane	0.000	0.000	0.000	0.000	0.492	0.390	0.495	1.835	[143]
Ethene	0.107	0.100	0.000	0.070	0.289	0.347	0.499	1.439	[143]
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	2.887	4.707	[20]
Octane	0.000	0.000	0.000	0.000	3.677	1.236	3.437	5.547	[20]
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	5.441	7.971	[20]
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.845	2.610	3.510	[20]

Solute	E	S	A	B	L	V	log K^a	log P^b	Ref.
1,1,1,2-Tetrafluoroethane	-0.410	0.410	0.060	0.020	0.530	0.461	1.562	1.972	[146]
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.739	3.134	3.194	[20]
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	3.232	2.602	[20]
Methyl tert-butyl ether	0.024	0.220	0.000	0.590	2.380	0.872	2.674	1.084	[20]
Dimethyl carbonate	0.142	0.540	0.000	0.570	2.328	0.664	3.308		[20,147]
Diethyl carbonate	0.060	0.580	0.000	0.530	3.412	0.946	4.099	1.659	Unity
Diphenyl carbonate	1.280	1.530	0.000	0.590	7.843	1.598	9.374	4.242	[148]
1-Chloroanthraquinone	1.900	1.790	0.000	0.570	9.171	1.651	10.376	4.342	[20]
Anthracene	2.290	1.340	0.000	0.280	7.568	1.454	8.111	5.081	[20]
Biphenyl	1.360	0.990	0.000	0.260	6.014	1.324	6.540	4.590	[20]
Pyrene	2.808	1.710	0.000	0.280	8.833	1.585	9.211	5.711	[20]
Benzil	1.445	1.590	0.000	0.620	7.611	1.637	8.930	4.060	[20]
Benzoic acid	0.730	0.900	0.590	0.400	4.657	0.932	6.660	1.520	[20]
Acetylsalicylic acid	0.781	1.690	0.710	0.670	6.279	1.288	9.446	0.946	[20]
4-tert-Butylbenzoic acid	0.730	1.111	0.551	0.443	6.547	1.495	8.553	3.329	[20]
3,4-Dichlorobenzoic acid	0.950	0.920	0.670	0.260	5.623	1.177	7.542	2.802	[20]
2-Chloro-5-nitrobenzoic acid	1.250	1.400	0.670	0.460	6.513	1.228	8.941	1.991	[20]
4-Chloro-3-nitrobenzoic acid	1.250	1.470	0.700	0.440	6.685	1.228	9.249	2.039	[20]
2-Methoxybenzoic acid	0.899	1.410	0.450	0.620	5.636	1.131	7.831	1.031	[20]
4-Methoxybenzoic acid	0.899	1.250	0.620	0.520	5.741	1.131	8.192	1.492	[20]
3,4-Dimethoxybenzoic acid	0.950	1.646	0.570	0.755	6.746	1.331	9.459	1.012	[20]
3,4,5-Trimethoxybenzoic acid	1.001	1.760	0.603	0.850	7.711	1.531	10.562	1.307	[20]

Solute	E	S	A	B	L	V	log *K*[a]	log *P*[b]	Ref.
2-Methylbenzoic acid	0.730	0.840	0.420	0.440	4.677	1.073	6.272	1.972	[20]
3-Methylbenzoic acid	0.730	0.890	0.600	0.400	4.819	1.073	7.012	2.032	[20]
4-Methyl-3-nitrobenzoic acid	1.040	1.461	0.659	0.521	6.434	1.247	8.972	1.687	[20]
4-Nitrobenzoic acid	0.990	1.520	0.680	0.400	5.770	1.106	8.582	1.682	[20]
Thioxanthen-9-one	1.940	1.441	0.000	0.557	8.436	1.536	9.031	3.963	[20]
Benzoin	1.585	2.115	0.196	0.841	9.159	1.680	11.351	2.620	[20]
Salicylamide	1.160	1.650	0.630	0.480	5.910	1.032	8.912	1.227	[20]
1,4-Dichloro-2-nitrobenzene	1.120	1.289	0.000	0.199	5.783	1.135	6.747	3.846	[20]
Phenothiazine	1.890	1.560	0.310	0.300	8.389	1.479	9.987	4.584	[20]

[a]For crystalline solutes the tabulated value is $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right)$.

[b]For crystalline solutes the tabulated value is $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right)$.

The experimental measurements, combined with a search of the published literature, have experimental partition coefficients and solubility ratios for 50 different organic and inorganic compounds. The solutes are chemically diverse, they cover a wide range of solute polarities and hydrogen-bonding capability, and include several fairly strong H-bond donors (acetylsalicylic acid, A = 0.710; 4-chloro-3-nitrobenzoic acid, A = 0.700) and several fairly strong H-bond acceptors (3,4,5-trimethoxybenzoic acid, B = 0.850; benzoin, B = 0.841). Regression analysis of the experimental values yielded the following two Abraham model expressions:

$$log\ P\ and log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right) = \quad \textbf{(Eq. 6.2)}$$

$$0.133(0.044) + 0.135(0.075)\mathrm{E} - 0.309(0.121)\mathrm{S} - 1.532(0.103)\mathrm{A} - 4.816(0.183)\mathrm{B} + 4.398(0.069)\mathrm{V}$$

(with N = 49, SD = 0.134, R^2 = 0.994, F = 1333)

$$log\ K and log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right) = \quad \textbf{(Eq. 6.3)}$$

$$0.092(0.027) - 0.598(0.027)\mathrm{E} + 1.527(0.087)\mathrm{S} + 1.942(0.088)\mathrm{A} + 0.948(0.014)\mathrm{L}$$

(with N = 50, SD = 0.117, R^2 = 0.999, F = 13898)

The correlations were obtained using the IBM SPSS® Statistical 22 commercial software. As an informational note the $b_k \cdot B$ is removed from Equation 6.3 because diethyl carbonate lacks an acidic hydrogen and therefore cannot act as a hydrogen-bond donor. Removal of the $b_k \cdot B$ led to an insignificant increase in the standard deviation, from SD = 0.115 to SD = 0.117. The $b_p \cdot B$ term is retained in Equation 6.2, however, as the expression pertains to solute transfer into diethyl carbonate from water. Here the b_p equation coefficient represents the difference in the acidity of diethyl carbonate and water, which does possess two acidic hydrogens capable of engagement in hydrogen-bond formation.

As noted in Chapter 1 a major advantage that the Abraham model offers is that the

derived correlations can be used to predict the solubility and/or infinite dilution activity coefficient of many additional organic, organometallic and inorganic solutes dissolved in the given solvent media. An indication of Equations 6.2 and 6.3 ability to estimate partition coefficients and solubility ratios can be obtained by examining each correlation's ability to describe the 50 experimental values given in Table 6.3. The small standard deviations, SD = 0.134 log units and SD = 0.117 log units, and near-unity squared correlation coefficients, R^2 = 0.994 and R^2 = 0.999, indicate that Equations 6.2 and 6.3 provide reasonably accurate mathematical descriptions of the observed experimental data used in both regression analyses. Figure 6.1 and Figure 6.2 provide a graphical comparison of the experimental data versus back-calculated values based on Equations 6.2 and 6.3, respectively. As an informational note the experimental $\log K$and $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right)$ data span a range of just under 13 log units, from log *K*= -1.504 for helium to $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right)$ = 11.351 for benzoin. A slightly smaller range of approximately 7.5 log units is covered by the experimental log *P* and $\log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right)$ data.

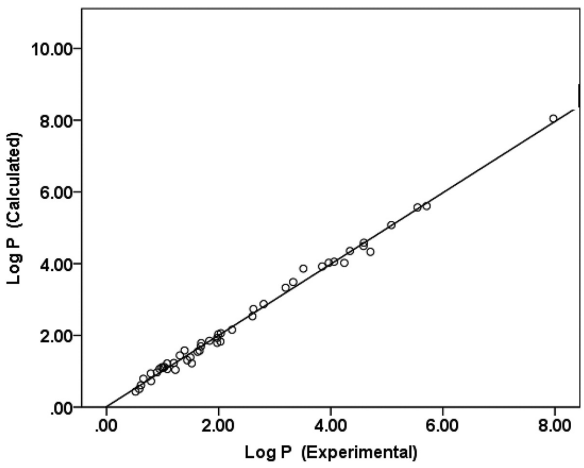


Figure 6.1: Comparison between the experimental log P and $log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,water}}\right)$ data and back-calculated values based on Equation 6.2.

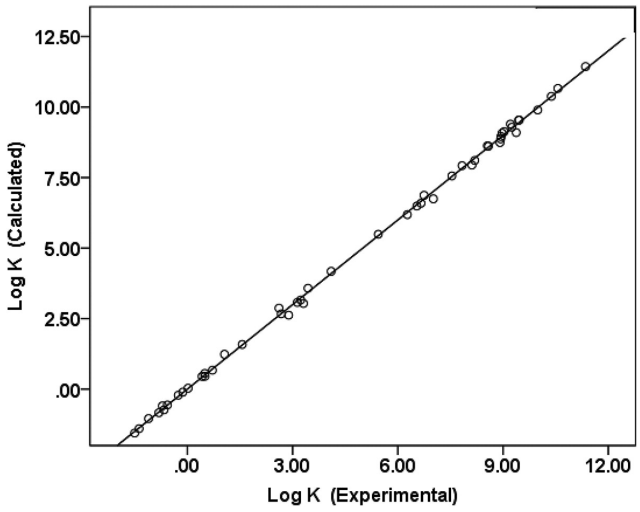


Figure 6.2: Comparison between the experimental log K an $log\left(\frac{C^{sat}_{solute,org\ solv}}{C^{sat}_{solute,gas\ phase}}\right)$ data and back-calculated values based on Equation 6.3.

CHAPTER 7

CHARACTERIZATION OF THE SOLUBILIZING ABILITY OF SHORT-CHAINED GLYCOL-GRAFTED AMMONIUM AND PHOSPHONIUM IONIC LIQUIDS*

7.1 Introduction

Chapter 1 showed that ILs can have different solubilization characteristics by changing their cation or anion. There still exist a very large number of cations and anions present in IL solvents for which Abraham model ion-specific coefficients have not yet been determined. Chapter 7, Chapter 8, and Chapter 9 all discuss calculating ABSM parameters for new ionic liquids. In this chapter, the ABSM parameters for glycol-pendant ILs (2-methoxyethyl)triethylphosphonium bis(trifluoromethylsulfonyl)imide ($[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$), (2-methoxyethyl)tributylphosphonium bis(trifluoromethylsulfonyl)imide ($[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$), and (2-methoxyethyl)triethylammonium bis(trifluoromethylsulfonyl)imide ($[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$) were measured from the densities of the ILs as well as the infinite dilution activity coefficients and gas-to- liquid partition coefficients of >40 different organic solutes provided by Dr. Fabrice Mutelet's group.[22] Molecular structures of the glycol- functionalized ILs are shown in Table 7.1

The cation-specific equation coefficients determined in the in this chapter, when combined with previously existing anion-specific equation coefficients, enable researchers to estimate infinite dilution activity coefficients and partition coefficients for an additional 60 ILs.

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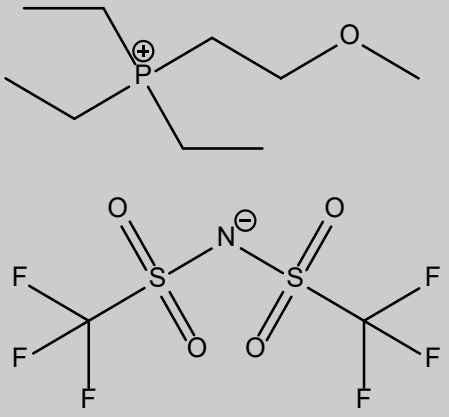
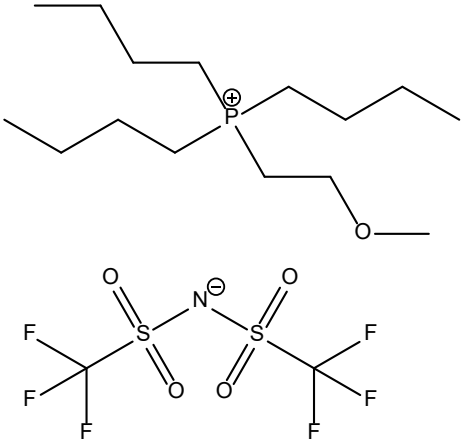
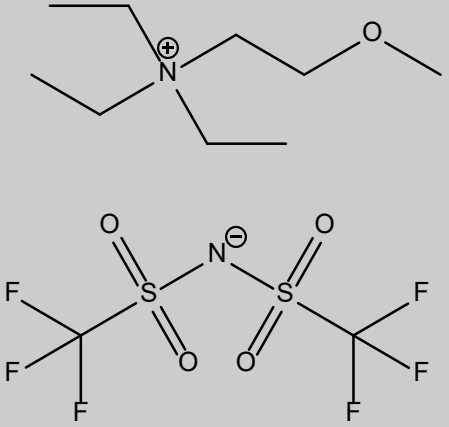
* This chapter is reproduced from Mutelet, F, Hussard, C, Baker, GA, Zhao, H, Churchill, B & Acree Jr, WE. (2020). Characterization of the solubilizing ability of short-chained glycol-grafted ammonium and phosphonium ionic liquids. **Journal of Molecular Liquids, 304**, 112786, 10.1016/j.molliq.2020.112786, with permission from Elsevier.

Table 7.1: Molecular structures (2-methoxyethyl)triethylphosphonium bis(trifluoromethylsulfonyl)imide, (2-methoxyethyl)tributylphosphonium bis(trifluoromethylsulfonyl)imide, (2-methoxyethyl)triethylammonium bis(trifluoromethylsulfonyl)imide.

Abbreviation	Name	Structure
$[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$	(2-methoxyethyl)Triethylphosphonium bis(trifluoromethylsulfonyl)imide	
$[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$	(2-methoxyethyl)Tributylphosphonium bis(trifluoromethylsulfonyl)imide	
$[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$	(2-methoxyethyl)Triethylammonium bis(trifluoromethylsulfonyl)imide	

7.2 Linear Solvation Energy Relationship (LSER) Correlations

In Table 7.2-Table 7.4, the log *K* and log *P* values for solutes dissolved in $[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$, $[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$, and $[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$, respectively, were tabluated at 298.15 K. Numerical values of the logarithm of the solute's gas-to-water partition coefficient, log K_w, were taken from earlier publications.[149–154] Also tabulated in Table 7.2-Table 7.4 are the numerical values of E, S, A, B, V and L for the solutes considered in the current study.

Table 7.2: Logarithm of the gas-to-IL partition coefficients (log K) and logarithm of water-to-IL partition coefficients (log P) for solutes dissolved in anhydrous $[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$ at 298.15 K.

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.372	3.192
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.332	3.172
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.733	3.693
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	1.719	3.839
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.083	4.193
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.418	4.568
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.748	5.068
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	3.061	5.441
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	3.380	5.910
Tridecane	0.000	0.000	0.000	0.000	6.200	1.940	3.701	
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	1.648	2.818
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.797	2.667
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	1.979	3.229
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.317	2.907
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.910	2.280
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.274	2.624
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.545	2.965
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.614	2.774
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	1.967	3.207

Solute	E	S	A	B	L	V	log *K*	log *P*
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.305	3.715
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.264	2.474
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.606	3.046
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.787	-0.045
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.089	0.369
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.379	0.799
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.383	0.883
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.485	-0.225
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.551	-1.189
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.756	-0.914
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.073	-0.487
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.825	-0.655
2-Methyl-1-Propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.248	-0.052
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.446	-0.015
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.688	0.398
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.849	0.799
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.616	1.826
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.325	1.365
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.393	2.583
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.190	0.340
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.054	2.230	-0.130
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	3.048	2.081
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.875	0.715
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.809	-1.840

Table 7.3: Logarithm of the gas-to-IL partition coefficients (log K) and logarithm of water-to-IL partition coefficients (log P) for solutes dissolved in anhydrous $[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$ at 298.15 K.

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.506	3.326
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.436	3.276
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.881	3.841
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	1.846	3.966

Solute	E	S	A	B	L	V	log *K*	log *P*
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.209	4.319
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.624	4.774
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.993	5.313
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	3.343	5.723
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	3.604	6.134
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	1.784	2.954
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.931	2.831
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	2.093	3.343
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.412	3.002
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.933	2.303
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.293	2.643
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.581	3.001
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.669	3.059
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.635	3.045
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	3.770	3.110
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.689	2.849
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	2.011	3.251
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.412	3.822
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.286	2.496
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.668	3.108
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.786	-0.044
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.098	0.378
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.423	0.843
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.384	0.884
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.746	0.196
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.405	-0.305
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.542	-1.198
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.755	-0.915
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.114	-0.446
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.852	-0.628
2-Methyl-1-Propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.314	0.014

Solute	E	S	A	B	L	V	log *K*	log *P*
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.497	0.037
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.721	0.431
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.932	0.882
Methyl butyl ether	0.045	0.250	0.000	0.440	2.658	0.872	2.240	1.110
Methyl tert-butyl ether	0.024	0.220	0.000	0.590	2.380	0.872	2.056	0.466
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.708	1.918
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.336	1.376
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.435	2.625
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.144	0.294
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.424	3.466	0.516
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	3.061	2.031
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.606	2.631	0.331
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.886	0.726
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.816	-1.824
Methyl propionate	0.128	0.600	0.000	0.450	2.431	0.747	2.933	0.783

Table 7.4: Logarithm of the gas-to-IL partition coefficients (log K) and logarithm of water-to-IL partition coefficients (log P) for solutes dissolved in anhydrous $[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$ at 298.15 K.

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.804	3.264
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.764	3.604
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	2.206	4.166
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	2.190	4.310
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.605	4.715
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	3.004	5.154
Decane	0.000	0.000	0.000	0.000	4.686	1.518	3.375	5.695
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	2.030	3.200
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	2.174	3.074
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	2.402	3.652
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.720	3.310
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.872	2.242
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.273	2.623

Solute	E	S	A	B	L	V	log *K*	log *P*
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.615	3.035
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.678	3.068
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.675	3.085
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	3.820	3.160
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.909	3.069
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	2.314	3.554
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.710	4.120
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.388	2.598
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.791	3.231
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.708	-0.122
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.075	0.355
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.206	0.626
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.198	0.698
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.773	0.223
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.325	-0.385
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.368	-1.372
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.618	-1.052
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.028	-0.532
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.717	-0.763
2-Methyl-1-Propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.253	-0.047
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.222	-0.238
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.801	0.511
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	2.096	1.096
Methyl butyl ether	0.045	0.250	0.000	0.440	2.658	0.872	2.364	1.234
Methyl tert-butyl ether	0.024	0.220	0.000	0.590	2.380	0.872	2.149	0.559
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.703	1.913
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.314	1.354
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.510	2.700
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	2.974	0.124
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.424	3.273	0.323
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.980	1.950

Solute	E	S	A	B	L	V	log *K*	log *P*
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.606	2.554	0.254
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.883	0.723
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.450	-2.190
Methyl propionate	0.128	0.600	0.000	0.450	2.431	0.747	2.923	0.773

Analysis of the experimental log *P* and log *K* data in Table 7.2-Table 7.4 was performed using the commercial IBM SPSS® Statistical 25 software. The Abraham model correlations for solute transfer are:

- Anhydrous $[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$:

$$log\ P\ (298K) = -0.129(0.146) + 0.080(0.155)\mathrm{E} + 0.682(0.156)\mathrm{S} - 1.084(0.191)\ \mathrm{A} - 4.538(0.134)\ \mathrm{B} + 3.370(0.118)\ \mathrm{V} \quad \textbf{(Eq. 7.1)}$$

N = 42, SD = 0.131, R^2 = 0.995, F = 1531

$$log\ K\ (298K) = -0.399(0.077) + 0.086(0.105)\ \mathrm{E} + 2.376(0.100)\ \mathrm{S} + 2.397(0.125)\ \mathrm{A} + 0.452(0.094)\ \mathrm{B} + 0.670(0.020)\ \mathrm{L} \quad \textbf{(Eq. 7.2)}$$

N = 43, SD = 0.092, R^2 = 0.980, F = 370.3

- Anhydrous $[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$:

$$log\ P\ (298K) = -0.177(0.118) + 0.103(0.117)\mathrm{E} + 0.582(0.129)\mathrm{S} - 1.022(0.156)\ \mathrm{A} - 4.516(0.126)\ \mathrm{B} + 3.546(0.095)\ \mathrm{V} \quad \textbf{(Eq. 7.3)}$$

N = 50, SD = 0.116, R^2 = 0.996, F = 2295

$$log\ K\ (298K) = -0.437(0.069) + 2.291(0.059)\ \mathrm{S} + 2.503(0.106)\ \mathrm{A} + 0.431(0.076)\ \mathrm{B} + 0.725(0.018)\ \mathrm{L} \quad \textbf{(Eq. 7.4)}$$

N = 50, SD = 0.082, R^2 = 0.984, F = 678.0

- Anhydrous $[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$:

$$log\ P\ (298K) = -0.045(0.146) + 0.041(0.124)\mathrm{E} + 0.218(0.145)\mathrm{S} - 1.396(0.177)\ \mathrm{A} - 4.650(0.132)\ \mathrm{B} + 3.708(0.128)\ \mathrm{V} \quad \textbf{(Eq. 7.5)}$$

N = 48, SD = 0.121, R^2 = 0.996, F = 2024

$$log\ K\ (298K) = \quad \textbf{(Eq. 7.5)}$$
$$-0.233(0.084) - 0.176(0.094)\ \mathrm{E} + 1.902(0.090)\ \mathrm{S} + 2.121(0.119)\ \mathrm{A} + 0.239(0.089)\ \mathrm{B} + 0.769(0.026)\ \mathrm{L}$$
N = 48, SD = 0.082, R^2 = 0.976, F = 341.1

Careful examination of the statistical information reveals that Equations 7.1-7.6 provide a reasonably accurate mathematical description of the observed partition coefficient data, evidenced by the relatively small standard deviations and near-unity values of the squared correlation coefficients. Figure 7.1-Figure 7.6 provide a graphical comparison of the observed log *P* and log *K* data versus back-calculated values based on derived Abraham model correlations. It should be noted that Equations 7.1-7.6 are comparable in descriptive ability to Abraham model correlations which were previously obtained for solute transfer into other ILs. Standard deviations for published Abraham model correlations for IL solvents typically fall in the range of 0.12-0.16 log units, with the standard deviations of the log *K* correlations being slightly smaller than for log *P* correlations. This is to be expected as log *K* values represent actual measured quantities whereas "experimental" log *P* values contain the additional experimental uncertainty associated with the gas-to-water partition coefficient used in the log *K* to log *P* conversion. Based on previous chapters, it is expected that Equations 7.1-7.6 will allow the reliable prediction of log *P*, log *K*, and values for additional organic solutes dissolved in $[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$, $[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$, and $[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$, provided that the solute descriptors for additional organic solutes fall within the range of numerical values of E, S, A, B, V and L used in generating the equation coefficients.

In Chapter 2 the anion-specific equation coefficient for $[NTf_2]^-$ was set to zero. Consequently, the log *P* and log *K* equation coefficients for the $[MeOCH_2CH_2NEt_3]^+$ cation are simply the equation coefficients in Equations 7.1 and 7.2; the log *P* and log *K* equation

coefficients for the $[MeOCH_2CH_2PEt_3]^+$ cation are the equation coefficients in Equations 7.3 and 7.4;and the log *P* and log *K* equation coefficients for the $[MeOCH_2CH_2PBu_3]^+$ cation are the equation coefficients in Equations 7.5 and 7.6. With these cation-specific equation coefficients for $[MeOCH_2CH_2NEt_3]^+$,$[MeOCH_2CH_2PEt_3]^+$, and $[MeOCH_2CH_2PBu_3]^+$ in hand, they can now be combined with the 20 established anion-specific coefficients to yield overall equation coefficients for some 60 ILs not previously known or reported.

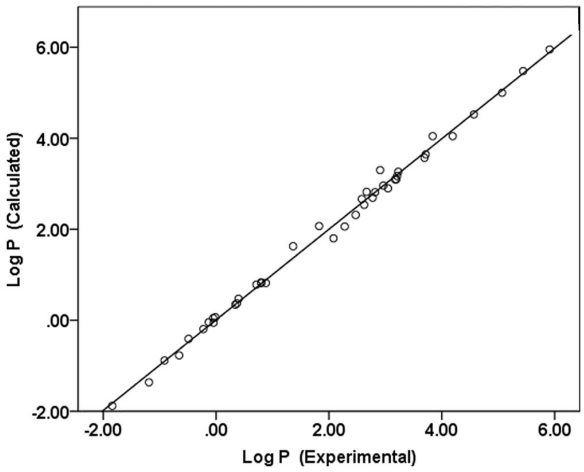


Figure 7.1: Comparison of experimental log P data for solutes dissolved in $[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$ versus back-calculated values based on Equation 7.1.

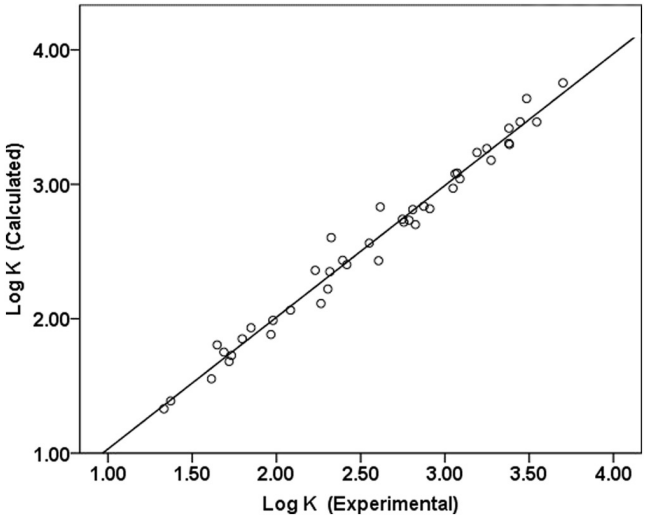


Figure 7.2: Comparison of experimental log K data for solutes dissolved in $[MeOCH_2CH_2NEt_3]^+[NTf_2]^-$ versus back-calculated values based on Equation 7.2.

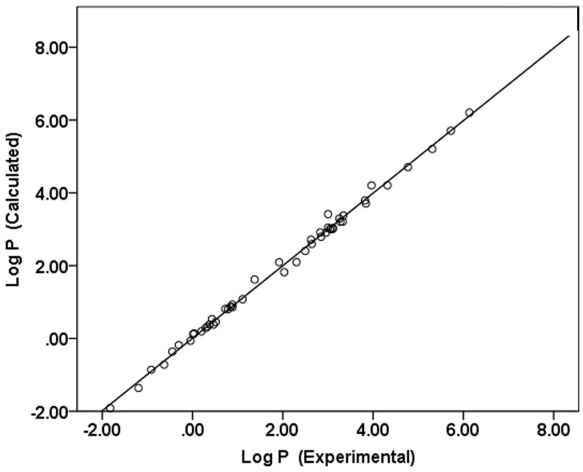


Figure 7.3: Comparison of experimental log P data for solutes dissolved in $[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$ versus back-calculated values based on Equation 7.3.

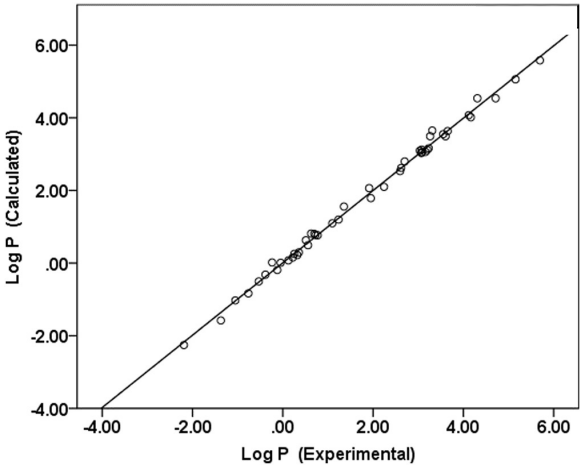


Figure 7.4: Comparison of experimental log K data for solutes dissolved in $[MeOCH_2CH_2PEt_3]^+[NTf_2]^-$ versus back-calculated values based on Equation 7.4.

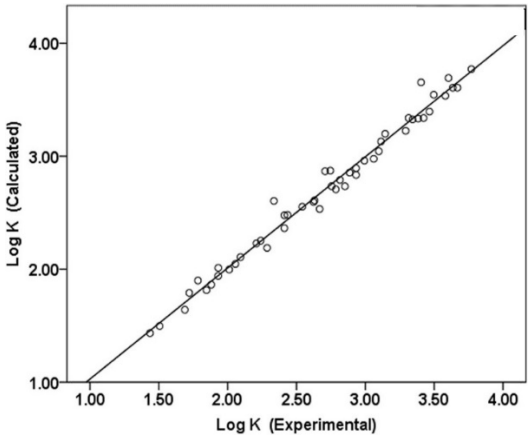


Figure 7.5: Comparison of experimental log P data for solutes dissolved in $[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$ versus back-calculated values based on Equation 7.5.

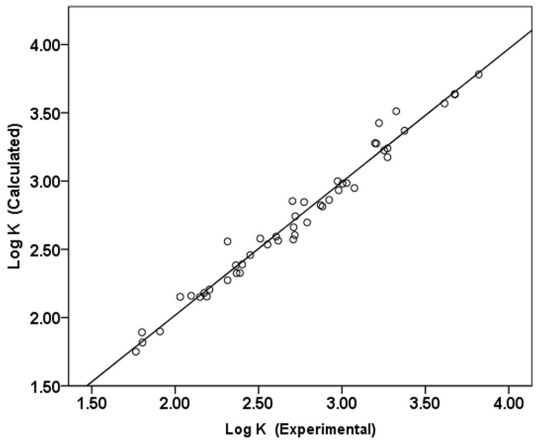


Figure 7.6: Comparison of experimental log K data for solutes dissolved in $[MeOCH_2CH_2PBu_3]^+[NTf_2]^-$ versus back-calculated values based on Equation 7.6.

CHAPTER 8

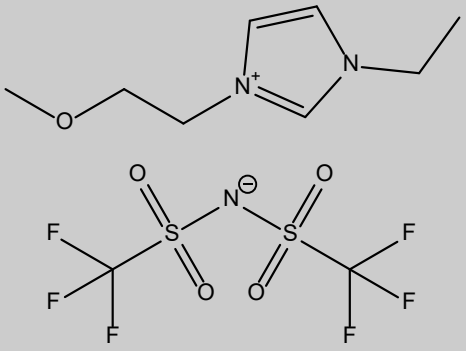
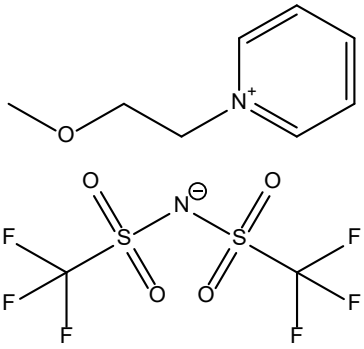
DEVELOPMENT OF ABRAHAM MODEL CORRELATIONS FOR SHORT-CHAIN GLYCOL GRAFTED IMIDAZOLIUM PYRIDINIUM IONIC LIQUIDS FROM INVERSE GAS-CHROMATOGRAPHIC MEASUREMENTS*

8.1 Introduction

In Chapter 3 the ABSM parameters of tetraalkylammonium ILs were measured. Chapter 7 expanded on ammonium cations by including glycol groups. In this chapter, the ABSM parameters of two new ILs with glycol groups were measured, however they are cyclic in nature. Infinite dilution activity coefficients and gas-to-liquid partition coefficients of more than 40 different organic solutes dissolved in the glycol-pendant ILs 1-ethyl-3-(2-methoxyethyl)imidazolium bis(trifluoromethylsulfonyl)imide ($[MeOCH_2CH_2EtIm]^+[NTf_2]^-$) and N-(2-methoxyethyl)pyridinium bis(trifluoromethylsulfonyl)imide ($[MeOCH_2CH_2Py]^+[NTf_2]^-$) over the temperature range from 323.15 to 373.15 K using inverse gas chromatography were provided by Mutelet *et al* and extrapolated to 298 K.[55] Molecular structures of these glycol-functionalized ILs are provided in Table 8.1. The densities for this work are available in previously published work.[55]

* This chapter is reproduced from Mutelet, F, Baker, GA, Zhao, H, Churchill, B & Acree Jr, WE. (2020). Development of Abraham model correlations for short-chain glycol-grafted imidazolium and pyridinium ionic liquids from inverse gas-chromatographic measurements, **Journal of Molecular Liquids, 317**, 113983, 10.1016/j.molliq.2020.113983, with permission from Elsevier.

Table 8.1: Molecular structures of 1-ethyl-3-(2-methoxyethyl)imidazolium bis(trifluoromethylsulfonyl)imide ($[MeOCH_2CH_2EtIm]^+[NTf_2]^-$) and N-(2-methoxyethyl)pyridinium bis(trifluoromethylsulfonyl)imide ($[MeOCH_2CH_2Py]^+[NTf_2]^-$).

Abbreviation	Name	Structure
$[MeOCH_2CH_2EtIm]^+$ $[NTf_2]^-$	1-Ethyl-3-(2-methoxyethyl)imidazolium bis(trifluoromethylsulfonyl)imide	
$[MeOCH_2CH_2Py]^+[NTf_2]^-$	N-(2-methoxyethyl)Pyridinium bis(trifluoromethylsulfonyl)imide	

8.2 Abraham Model Correlations for Predicting Partition Coefficients and Activity Coefficients

In Table 8.2 and Table 8.3, tabulated log *K* and log *P* values are given for solutes dissolved in $[MeOCH_2CH_2EtIm]^+[NTf_2]^-$ and $[MeOCH_2CH_2Py]^+[NTf_2]^-$, respectively, at 298.15 K. Numerical values of the logarithm of the solute's gas-to-water partition coefficient, log K_w, were taken from earlier publications.[150,152,155,156] Also tabulated in Table 8.2 and Table 8.3 are the numerical values of E, S, A, B, L and V for the 52 different organic solutes considered in the current study. We note that the solutes studied encompass a fairly wide range of solute descriptor values and include many of the volatile organic compounds of relevance in modern industrial manufacturing processes.

Table 8.2: Logarithms of gas-to-IL partition coefficients (log K) and logarithms of water-to-IL partition coefficients (log P) for solutes dissolved in anhydrous $[MeOCH_2CH_2EtIm]^+[NTf_2]^-$ at 298.15 K.

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.326	3.146
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.291	3.131
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.652	3.612
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	1.646	3.766
Octane	0.000	0.000	0.000	0.000	3.677	1.236	1.989	4.099
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.323	4.473
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.647	4.967
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	2.978	5.358
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	3.302	5.832
Tridecane	0.000	0.000	0.000	0.000	6.200	1.940	3.614	
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	1.583	2.753
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.744	2.644
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	1.929	3.179
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.248	2.838
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.816	2.186
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.179	2.529
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.468	2.888
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.528	2.918
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.502	2.912
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.538	2.698
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	1.884	3.124
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.207	3.617
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.216	2.426
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.543	2.983
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.874	0.044
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.163	0.443
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.433	0.853
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.409	0.909
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.794	0.244
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.536	-0.174

Solute	E	S	A	B	L	V	log *K*	log *P*
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.567	-1.173
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.776	-0.894
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.112	-0.448
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.840	-0.640
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.301	0.001
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.491	0.031
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.741	0.451
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.924	0.874
Methyl tert-butyl ether	0.024	0.220	0.000	0.590	2.380	0.872	2.089	0.499
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.632	1.842
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.290	1.330
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.352	2.542
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.227	0.377
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.054	2.081	-0.279
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.967	1.937
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.606	2.722	0.422
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.963	0.802
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.894	-1.746
Methyl propionate	0.128	0.600	0.000	0.450	2.431	0.747	2.993	0.843

Table 8.3: Logarithms of gas-to-IL partition coefficients (log K) and logarithms of water-to-IL partition coefficients (log P) for solutes dissolved in anhydrous $[MeOCH_2CH_2Py]^+[NTf_2]^-$ at 298.15 K.

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.153	2.973
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.114	2.954
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.470	3.430
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	1.456	3.576
Octane	0.000	0.000	0.000	0.000	3.677	1.236	1.795	3.905
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.108	4.258
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.427	4.747
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	2.731	5.110
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	3.057	5.587

Solute	E	S	A	B	L	V	log *K*	log *P*
Tridecane	0.000	0.000	0.000	0.000	6.200	1.940	3.327	
Tetradecane	0.000	0.000	0.000	0.000	6.705	2.081	3.699	
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	1.435	2.605
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.603	2.503
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	1.768	3.018
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.100	2.690
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.786	2.156
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.138	2.488
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.403	2.823
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.494	2.884
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.476	2.886
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	3.652	2.992
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.407	2.567
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	1.739	2.979
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.056	3.466
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.097	2.307
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.423	2.863
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.857	0.027
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.113	0.393
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.358	0.778
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.329	0.829
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.752	0.202
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.516	-0.194
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.511	-1.229
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.705	-0.965
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.048	-0.512
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.775	-0.705
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.198	-0.102
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.397	-0.063
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.654	0.364
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.804	0.754

Solute	E	S	A	B	L	V	log *K*	log *P*
Methyl butyl ether	0.045	0.250	0.000	0.440	2.658	0.872	2.123	0.993
Methyl tert-butyl ether	0.024	0.220	0.000	0.590	2.380	0.872	1.983	0.393
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.555	1.765
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.243	1.283
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.225	2.415
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.223	0.373
Pyridine	0.631	0.840	0.000	0.520	3.022	0.675	3.515	0.075
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.940	1.910
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.606	2.711	0.411
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.971	0.811
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.890	-1.750
Methyl propionate	0.128	0.600	0.000	0.450	2.431	0.747	2.957	0.807

The two sets of Abraham model log *P* and log *K* expressions constructed for each IL solvent by substituting the numerical values in Table 8.2 and Table 8.3 into Equations 1.1 and 1.2 are solved by regression analysis to yield:

- For anhydrous $[MeOCH_2CH_2EtIm]^+[NTf_2]^-$:

$$log\ P\ (298K) = -0.114(0.122) - 0.081(0.121)\mathrm{E} + 0.802(0.130)\mathrm{S} - 1.101(0.157)\mathrm{A} - 4.449(0.111)\mathrm{B} + 3.314(0.098)\mathrm{V} \quad \textbf{(Eq. 8.1)}$$

(with N = 48, SD = 0.117, R^2 = 0.996, F = 2003)

$$log\ K\ (298K) = -0.421(0.071) + 0.068(0.092)\mathrm{E} + 2.549(0.091)\mathrm{S} + 2.420(0.114)\mathrm{A} + 0.497(0.085)\mathrm{B} + 0.658(0.018)\mathrm{L} \quad \textbf{(Eq. 8.2)}$$

(with N = 49, SD = 0.089, R^2 = 0.992, F = 476.6)

- For anhydrous $[MeOCH_2CH_2Py]^+[NTf_2]^-$:

$$log\ P\ (298K) = -0.187(0.125) + 0.791(0.115)\mathrm{S} - 1.189(0.168)\mathrm{A} - 4.275(0.115)\mathrm{B} + 3.230(0.102)\mathrm{V} \quad \textbf{(Eq. 8.3)}$$

(with N = 50, SD = 0.127, R^2 = 0.995, F = 2061)

$$log\ K\ (298K) = \quad \textbf{(Eq. 8.4)}$$
$$-0.479(0.071) + 0.079(0.103)\mathrm{E} + 2.511(0.111)\mathrm{S} + 2.318(0.135)\mathrm{A} + 0.680(0.111)\mathrm{B} + 0.624(0.017)\mathrm{L}$$
(with N = 52, SD = 0.100, R^2 = 0.981, F = 481.7)

Regression analysis was performed using commercial IBM SPSS® Statistical 25 software. Careful examination of the statistical information reveals that Equations 8.1-8.4 provide a reasonably accurate mathematical description of the observed partition coefficient data, evidenced by the relatively small standard deviations and near-unity values of the squared correlation coefficients. Figure 8.1-Figure 8.4 depict graphical comparisons of the observed log *P* and log *K* data versus back-calculated values based upon derived Abraham model correlations. The descriptive ability of Equations 8.1-8.4 is comparable to other ABSM coefficients in previous chapters.

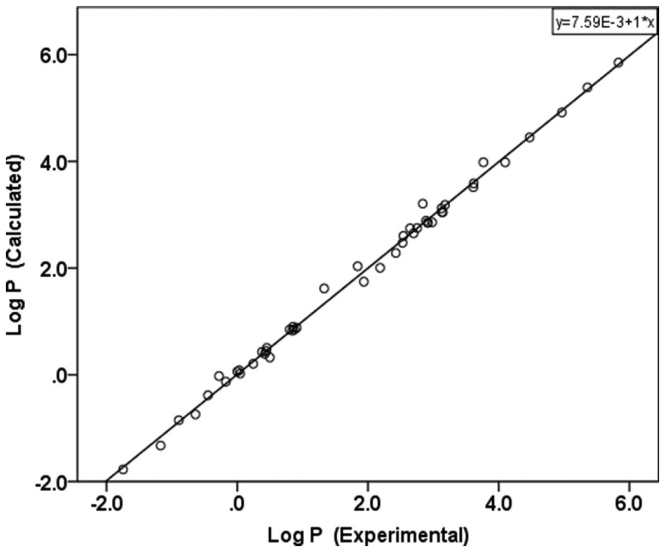


Figure 8.1: Comparison of logarithm of the experimental water-to-IL partition coefficient, log P, data for solutes dissolved in $[MeOCH_2CH_2EtIm]^+[NTf_2]^-$ versus back-calculated values based on Equation 8.1. [55]

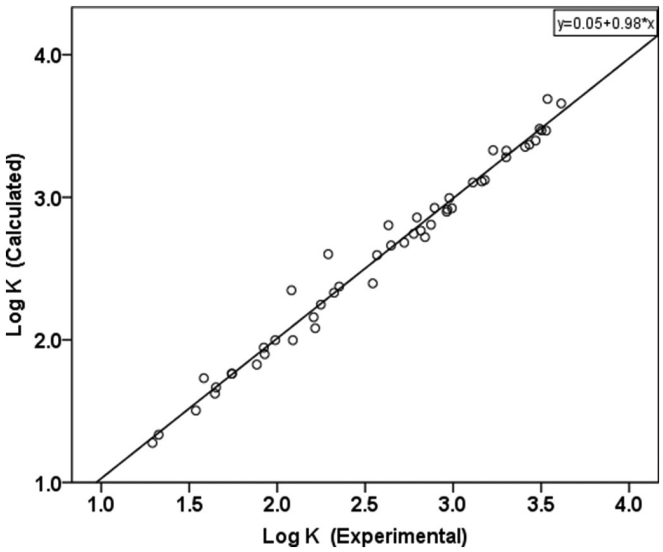


Figure 8.2: Comparison of logarithm of the experimental water-to-IL partition coefficient, log P, data for solutes dissolved in $[MeOCH_2CH_2EtPy]^+[NTf_2]^-$ versus back-calculated values based on Equation 8.3. [55]

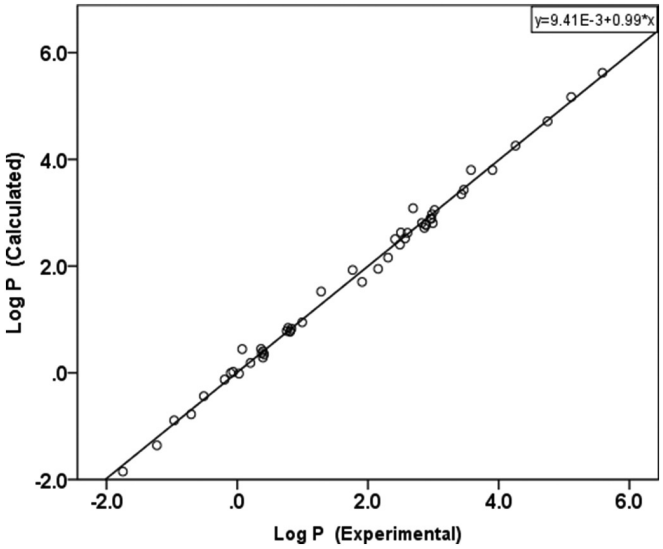


Figure 8.3: Comparison of logarithm of the experimental water-to-IL partition coefficient, log K, data for solutes dissolved in $[MeOCH_2CH_2EtIm]^+[NTf_2]^-$ versus back-calculated values based on Equation 8.2. [55]

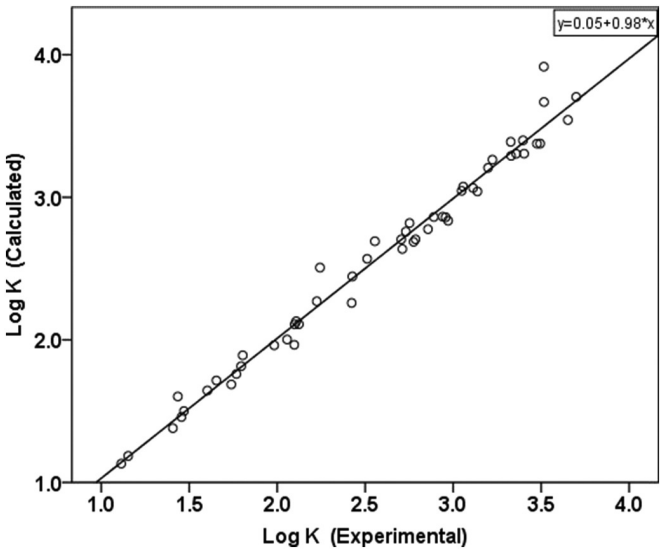


Figure 8.4: Comparison of logarithm of the experimental water-to-IL partition coefficient, log K, data for solutes dissolved in $[MeOCH_2CH_2EtPy]^+[NTf_2]^-$ versus back-calculated values based on Equation 8.4. [55]

CHAPTER 9

ABRAHAM SOLVATION PARAMETER MODEL: CALCULATION OF ION-SPECIFIC EQUATION COEFFICIENTS FOR THE N-ETHYL-N-METHYLMORPHOLINIUM AND N-OCTYL-N-MOETHYLMORPHOLINIUM CATIONS*

9.1 Introduction

A recent search of the chemical literature found published infinite dilution activity coefficient data, $\gamma^{\infty}_{1,\mathrm{solute}}$, for 48 different organic solutes dissolved in the IL solvents N-ethyl-N-methylmorpholinium bis(trifluoromethylsulfonyl)imide, $[EMMorp]^+[NTf_2]^-$, and N-octyl-N-methylmorpholinium bis(trifluoromethylsulfonyl)imide, $[OMMorp]^+[NTf_2]^-$, measured at six temperatures from 313.15 K to 363.15 K. Marcinkowski and co-workers[157] determined the $\gamma^{\infty}_{\mathrm{solute}}$ values based on inverse gas-chromatographic retention data. Gas-to-IL solvent partition coefficients can be calculated from γ_1 solute data through a standard thermodynamic relationship found in Equation 2.1. In this chapter, Abraham model correlations are calculated for $[EMMorp]^+[NTf_2]^-$ and $[OMMorp]^+[NTf_2]^-$ based on the published γ_1 solute data of Marcinkowski and co-workers.[157] Also determined are the Abraham model ion-specific equation coefficients for the $[EMMorp]^+$ and $[OMMorp]^+$ cations.

9.2 Construction of $[EMMorp]^+[NTf_2]^-$ and $[OMMorp]+[NTf_2]^-$ Data Sets

As in previous chapters, the published infinite dilution activity coefficient data for solutes dissolved in $[EMMorp]^+[NTf_2]^-$ and $[OMMorp]^+[NTf_2]^-$ were measured at temperatures

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* This chapter is reproduced from Churchill, B, Casillas, T, Acree Jr, WE & Abraham, MH. (2020). Abraham solvation parameter model: calculation of ion-specific equation coefficients for the N-Ethyl-N-methylmorpholinium and N-Octyl-N-methylmorpholinium cations, **Physics and Chemistry of Liquids. 10**, 1080/00319104.2020.1774879, with permission from Taylor & Francis Online.

above 298.15 K, from 313.15 K to 363.15 K. The numerical values of log *K* were computed using Equation 2.1 and the log $K = T^{-1}$ linear relationship was explained in Chapter 2.

In the eighth and ninth columns in Table 9.1 and Table 9.2 the log *K* and log *P* values at 298.15 K were tabulated the calculated. Tabulated in the second through seventh columns are the numerical values of the solute descriptors that were used in deriving the Abraham model correlations.

Table 9.1: Experimental log K and log P data for 46 different organic solutes dissolved in N-ethyl-N-methylmorpholinium bis(trifluoromethylsulfonyl)imide, $[EMMorp]^+[NTf_2]^-$ at 298.2 K, along with the numerical values of the solute descriptors.

Solute	E	S	A	B	L	V	log *K*	log *P*
Pentane	0.000	0.000	0.000	0.000	2.162	0.813	0.811	2.511
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.111	2.931
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.519	3.479
Octane	0.000	0.000	0.000	0.000	3.677	1.236	1.819	3.929
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.199	4.349
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.624	4.944
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.547	2.477
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.793	2.163
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.194	2.544
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.526	2.936
1,3,5-Trimethylbenzene	0.649	0.520	0.000	0.190	4.344	1.139	3.929	3.269
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.704	2.864
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	2.042	3.262
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.379	3.789
1-Nonene	0.090	0.080	0.000	0.070	4.073	1.334	2.776	4.286
1-Decene	0.093	0.080	0.000	0.070	4.533	1.475	3.170	4.810
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.133	2.343
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.596	3.036
1-Octyne	0.155	0.220	0.090	0.100	3.521	1.150	2.863	3.383
1-Nonyne	0.150	0.220	0.090	0.100	4.019	1.291	3.135	
1-Decyne	0.143	0.220	0.090	0.100	4.537	1.432	3.487	
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.475	0.895
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.422	0.922

Solute	E	S	A	B	L	V	log *K*	log *P*
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.720	4.126	0.676
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.861	4.332	0.732
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.828	0.278
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.661	-0.049
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.703	-1.037
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.892	-0.788
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.207	-0.353
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.909	-0.571
2-Methyl-2-Propanol	0.180	0.300	0.310	0.600	1.963	0.731	2.949	-0.331
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.490	0.030
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.872	3.788	0.438
1-Hexanol	0.210	0.420	0.370	0.480	3.610	1.013	4.135	0.905
1-Octanol	0.199	0.420	0.370	0.480	4.619	1.295	4.807	1.807
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.519	1.729
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.381	0.531
Pyridine	0.631	0.840	0.000	0.520	3.022	0.675	3.884	0.444
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.978	0.818
Acetaldehyde	0.208	0.670	0.000	0.450	1.230	0.406	2.376	-0.194
Propanal	0.196	0.650	0.000	0.450	1.815	0.547	2.661	0.141
Butanal	0.187	0.650	0.000	0.450	2.270	0.688	2.947	0.617
Pentanal	0.163	0.650	0.000	0.450	2.851	0.829	3.240	1.020
Hexanal	0.146	0.650	0.000	0.450	3.357	0.970	3.551	1.491
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.839	3.431	2.811

Table 9.2: Experimental log K and log P data for 46 different organic solutes dissolved in N-octyl-N-methylmorpholinium bis(Trifluoromethylsulfonyl)imide, $[OMMorp]^+[NTf_2]^-$ at 298.2 K, along with the numerical values of the solute descriptors.

Solute	E	S	A	B	L	V	log *K*	log *P*
Pentane	0.000	0.000	0.000	0.000	2.162	0.813	1.262	2.962
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.744	3.564
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	2.155	4.115
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.580	4.690
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	3.002	5.152
Decane	0.000	0.000	0.000	0.000	4.686	1.518	3.424	5.744
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	2.076	2.976
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.931	2.301

Solute	E	S	A	B	L	V	log *K*	log *P*
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.448	2.798
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.883	3.293
1,3,5-Trimethylbenzene	0.649	0.520	0.000	0.190	4.344	1.139	4.284	3.624
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.783	2.943
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	2.185	3.405
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.596	4.006
1-Nonene	0.090	0.080	0.000	0.070	4.073	1.334	3.035	4.545
1-Decene	0.093	0.080	0.000	0.070	4.533	1.475	3.463	5.103
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.147	2.357
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.677	3.117
1-Octyne	0.155	0.220	0.090	0.100	3.521	1.150	2.953	3.473
1-Nonyne	0.150	0.220	0.090	0.100	4.019	1.291	3.267	
1-Decyne	0.143	0.220	0.090	0.100	4.537	1.432	3.654	
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.786	1.206
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.877	1.377
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.720	4.382	0.932
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.861	4.541	0.941
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	3.071	0.521
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.659	-0.051
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.688	-1.052
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.949	-0.721
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.363	-0.197
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	3.027	-0.453
2-Methyl-2-Propanol	0.180	0.300	0.310	0.600	1.963	0.731	3.125	-0.155
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.782	0.322
1-Pentanol	0.219	0.420	0.370	0.480	3.106	0.872	4.118	0.768
1-Hexanol	0.210	0.420	0.370	0.480	3.610	1.013	4.501	1.271
1-Octanol	0.199	0.420	0.370	0.480	4.619	1.295	5.353	2.353
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.686	1.896
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.282	0.432
Pyridine	0.631	0.840	0.000	0.520	3.022	0.675	4.016	0.576
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	3.232	1.072
Acetaldehyde	0.208	0.670	0.000	0.450	1.230	0.406	2.355	-0.215
Propanal	0.196	0.650	0.000	0.450	1.815	0.547	2.764	0.244
Butanal	0.187	0.650	0.000	0.450	2.270	0.688	3.156	0.826

Solute	E	S	A	B	L	V	log *K*	log *P*
Pentanal	0.163	0.650	0.000	0.450	2.851	0.829	3.576	1.356
Hexanal	0.146	0.650	0.000	0.450	3.357	0.970	3.987	1.927
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.839	3.755	2.935

9.3 Development of IL-Specific Abraham Model Correlations for $[EMMorp]^+[NTf_2]^-$ and $[OMMorp]^+[NTf_2]^-$

Preliminary regression analyses gave a very small numerical value for the c-coefficient in Equation 9.1 for $[EMMorp]^+[NTf_2]^-$, and in the e-coefficients for Equation 9.2 and Equation 9.3 for $[EMMorp]^+[NTf_2]^-$ and $[OMMorp]^+[NTf_2]^-$, respectively. In all cases, the standard error in the calculated coefficient was much larger than the coefficient itself. These terms were eliminated and the final regression analyses of the experimental log *P* and log *K* datasets in accordance with Equations 1.1 and 1.2 of the Abraham model yielded the following mathematical correlations:

- $[EMMorp]^+[NTf_2]^-$:

$$log\ P\ (298K) = 0.150(0.164)\mathrm{E} + 0.415(0.186)\mathrm{S} - 1.335(0.194)\ \mathrm{A} - 4.133(0.213)\ \mathrm{B} + 3.247(0.033)\ \mathrm{V} \quad \textbf{(Eq. 9.1)}$$

N = 44, SD = 0.130, R^2 = 0.997, F = 2669

$$log\ K\ (298K) = -0.398(0.103) + 2.248(0.136)\ \mathrm{S} + 2.384(0.196)\ \mathrm{A} + 0.863(0.188)\ \mathrm{B} + 0.662(0.027)\ \mathrm{L} \quad \textbf{(Eq. 9.2)}$$

N = 46, SD = 0.140, R^2 = 0.972, F = 359.5

- $[OMMorp]^+[NTf_2]^-$:

$$log\ P\ (298K) = -0.062(0.114) + 0.319(0.131)\mathrm{S} - 1.435(0.177)\ \mathrm{A} - 4.037(0.163)\ \mathrm{B} + 3.695(0.092)\ \mathrm{V} \quad \textbf{(Eq. 9.3)}$$

N = 44, SD = 0.121, R^2 = 0.995, F = 2057

$$log\ K\ (298K) = \quad \textbf{(Eq. 9.4)}$$
$$-0.329(0.087) - 0.115(0.151)\ \mathrm{E} + 1.934(0.173)\ \mathrm{S} + 2.143(0.181)\ \mathrm{A} + 1.060(0.191)\ \mathrm{B} + 0.768(0.023)\ \mathrm{L}$$
N = 46, SD = 0.117, R^2 = 0.980, F = 390.7

Examination of the associated statistical information reveals that both sets of equations provide reasonably accurate mathematical descriptions of the observed partitioning behavior of the solutes into the respective IL solvent as evidenced by standard deviations of SD = 0.130 (Equation 9.1) and SD = 0.140 log units (Equation 9.2) for solutes transferred into $[EMMorp]^+[NTf_2]^-$ and SD = 0.121 (Equation 9.3) and SD = 0.117 log units (Equation 9.4) for solutes transferred into $[OMMorp]^+[NTf_2]^-$. Figure 9.1-Figure 9.4 provide further evidence of the descriptive ability of Equations 9.1-9.4 in the form of a graphical comparison of the logarithm of observed partition coefficient data versus back-calculated values based on derived mathematical expressions.

Equations 9.1-9.4 should provide reasonably accurate log *P* and log *K* estimates for additional volatile organic compounds dissolved in both $[EMMorp]^+[NTf_2]^-$ and $[OMMorp]^+[NTf_2]^-$ at 298.15 K. Solute descriptors of many volatile organic compounds will fall in the predictive area of chemical space defined by the solutes listed in Table 9.1 and Table 9.2. Caution should be exercised in using the equations to predict the partition coefficients of the small inorganic gases as these molecules were not contained in the datasets used in determining the equation coefficients. The L and V solute descriptors of carbon dioxide, carbon monoxide, hydrogen gas and other inorganic gases are much smaller than the used regression analyses.

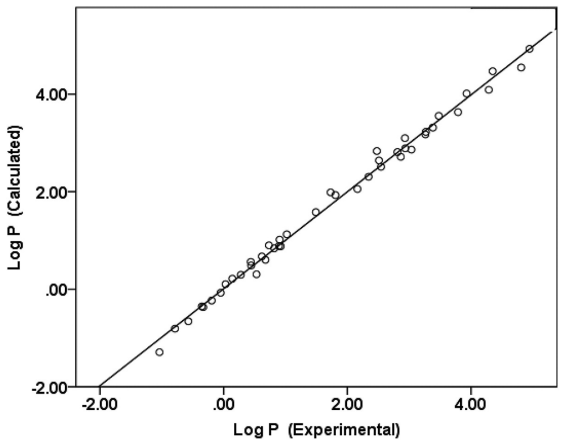


Figure 9.1: Comparison between the experimental log P data for $[EMMorp]^+[NTf_2]^-$ and back-calculated values based on Equation 9.1.

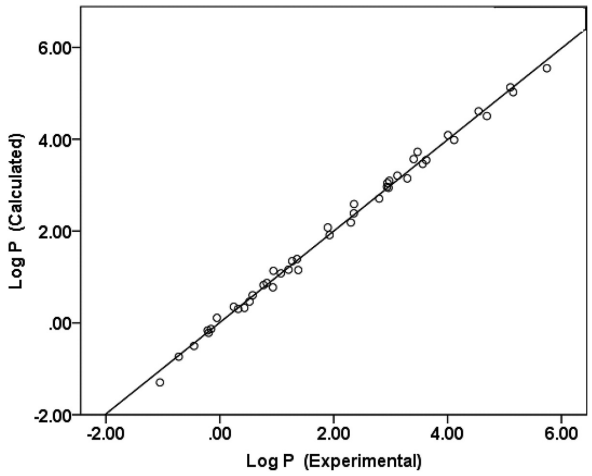


Figure 9.2: Comparison between the experimental log K data for $[EMMorp]^+[NTf_2]^-$ and back-calculated values based on Equation 9.2.

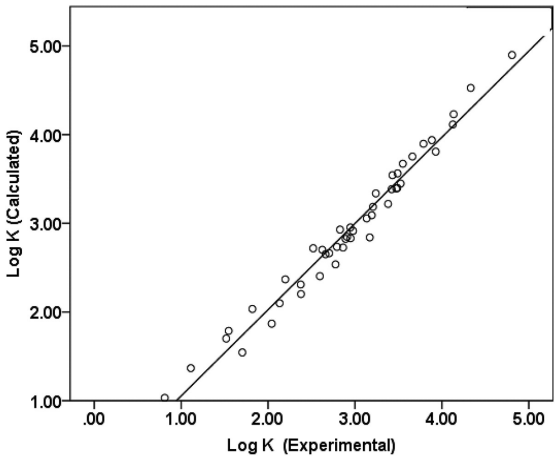


Figure 9.3: Comparison between the experimental log P data for $[OMMorp]^+[NTf_2]^-$ and back-calculated values based on Equation 9.3.

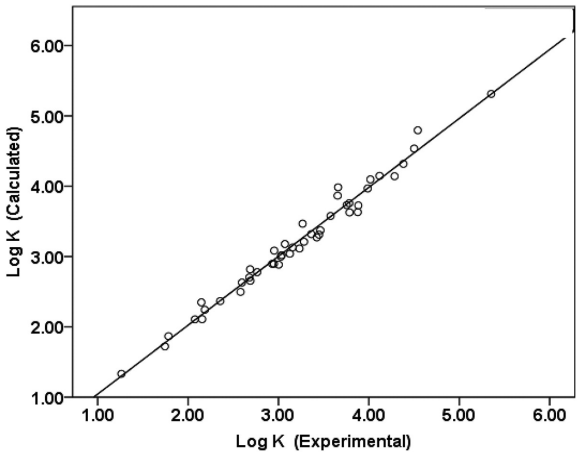


Figure 9.4: Comparison between the experimental log K data for $[OMMorp]^+[NTf_2]^-$ and back-calculated values based on Equation 9.4.

9.4 Calculation of Abraham Model Ion-Specific Equation Coefficients for the $[EMMorp]^+$ and $[OMMorp]^+$ Cations

Equations 9.1-9.4 permit one to estimate log *P* and log *K* values for additional solutes dissolved in $[EMMorp]^+[NTf_2]^-$ and $[OMMorp]^+[NTf_2]^-$; however, it would be more advantageous to also have predictive expressions for N-ethyl-N-methylmorpholinium and N-octyl-N-methylmorpholinium IL solvents containing anions other than bis(trifluoromethylsufonyl) imide. The physical and solubilising properties of IL solvents can be fine-tuned by judicious selection of cation-anion pair. Fortunately, the ion-specific equation coefficient version of the Abraham model (see Equations 1.3 and 1.4) allows one to write Abraham model expressions for unstudied IL solvents simply by summing the corresponding cation-specific and anion-specific equation coefficients. As in previous chapters, ion-specific equation coefficients for the $[EMMorp]^+$ and $[OMMorp]^+$ cations can easily be calculated from the equation coefficients given in Equations 9.1-9.4.

CHAPTER 10

A NOVEL METHOD FOR UPDATING ABRAHAM SOLVATION MODEL PARAMETERS USING PREVIOUSLY DETERMINED SOLVENT DESCRIPTORS

10.1 Introduction

The current method for updating ABSM descriptors for individual cations and anions of ionic liquids is tedious and time intensive. One must catalogue each individual $\log P$ and $\log K$ value available for a desired ion, correlate them with solutes and solute parameters, and run a linear regression to acquire new ABSM ion parameters. This process includes thousands of data points which can cause powerful tools such as Microsoft Excel and IBM SPSS to take upwards of 15 minutes for each parameter of each ion. With 87 individual ions for log *K* and log *P* already calculated (Table D.4 - Table D.7), and six parameters per ion, updating each ion's ABSM parameters would take 1305 minutes to complete, or 43.5 hours. As more ion parameters are measured and/or retrieved from the published literature, the analysis time for each ion will increase and updating the parameters will eventually become unteneable.

The first time the ABSM parameters were updated from originally published values was in 2011 when Grubbs *et al*. updated 1790 log *K* values and 1760 log *P* values.[77] In 2014 Stephens *et al*. updated the ABSM parameters again using over 3900 data points between log *K* and log *P* values.[77] In the past six years, those numbers have increased to 7473 log *K* values, and 6867 log *P* values across 146 and 132 ILs respectively. Given there are 6 terms per log *K*/log *P* value, updating the current ABSM database would catalogue 86,376 values. The amount of data to analyze means there is a significant chance that many incorrect values would be inputted into the calculation, causing uneeded error.

To help expedite the process of updating IL ion descriptors as well as attempt to eliminate potential transcription errors a new method to update ABSM ion parameters has been developed. This method utilized linear algebra to create a matrix which accounts for each IL ABSM parameter and the ions which make up the IL respectively. An example of such a matrix is shown in Equation 10.1.

$$\begin{bmatrix} c_{ion,IL_1} & \cdots & c_{IL_1} \\ \vdots & \ddots & \vdots \\ c_{ion,IL_n} & \cdots & c_{IL_n} \end{bmatrix} \quad \textbf{(Eq. 10.1)}$$

where c_{ion,IL_n} indicates whether an ion is present or absent and contributing to the value of c_{IL_n}. c_{IL_n}. represents the ABSM parameter for an IL (e.g. c, e, s, a, b, v, l) and exists only in the right-most column. The values to the left of the right-most column consist of a binary matrix where each column represents a different IL ion. A value of 1 indicates the ion is present and a value of zero indicates that the ion is absent. For example, the IL $[BMIM]^+[DCA]^-$ would have a 1 in the $[BMIM]^+$ and the $[DCA]^-$ columns and zeros in other columns. There is one anion which has a zero at all times: $[NTf_2]^-$. As discussed in Chapter 2, this is because the $[NTf_2]^-$ ion is the "standard" which all other ions are set to and therefore its value is always zero. This matrix is input in Microsoft® Excel® before being analyzed using IBM® SPSS® Statistics software.

For increasing accuracy of the expanding database of ILs, the solvent descriptors would need to expand respectively. Before 2020, there was no easily accessible database with values for solvent descriptors. For this work, a database was compiled with every IL found in literature up to August 2020 and their respective ABSM coefficients. The list of all cations and anions found in the ILs are listed in Table A.1 with their IUPAC names, other abbreviations, and their chemical structures. All solutes and their solute parameters can be found in *Table D.1*. The IL-

specific log *K* and log *P* ABSM parameters can be found in Table D.2 and Table D.3, the cation log *K* and log *P* parameters can be found in Table D.4 and Table D.5, and anion log *K* and log *P* values can be found in Table D.6 and Table D.7. Table D.2 - Table D.7 also note the number of solvents used (N), the standard deviation (SD), and the R^2 value for each IL pair, if provided in literature.

Several ILs found did not have ABSM parameters. Those IL parameters were compiled and calculated. Their log *K* and log *P* values can be found in Table D.2 and Table D.3. The solute descriptors for their analysis came from UFZ-LSER database and were from the LSER 2017 data set.[76] Some of these ILs have both log *K* values and $\log \gamma^{\infty}$ values which could be used to calculate ABSM parameters. For ILs with both log *K* and $\log \gamma^{\infty}$ values, the parameters were calculated and the equation with the lowest standard error was used for the rest of this work.

10.2 Methodology

Once all of the ILs were compiled together, several variations of the update method were implemented. Table 10.1 lists which methods were employed to update cation and anion ABSM parameters.

Table 10.1: The different methods applied to the new ABSM update method.

Method #	Parameters Calculated
1	All IL ABSM parameters
2	All IL ABSM parameters with N > 30
3	All IL ABSM parameters with parameters smaller than SD were set to zero
4	All IL ABSM parameters with N > 30 and parameters smaller than SD were set to zero

where N is the number of solutes used to calculate the IL-specific equation. Before implementing any of the methods in Table 10.1, all ILs which had log *K* ABSM parameters above or below 298 K were removed from the database. Log *K* and log *P* values are often reported at

298 K and limiting ABSM parameters to this temperature removes any effect temperature may have on the IL-specific equations.

The methods in Table 10.1 were chosen to determine which method, if any, would be suitable to updating IL ABSM parameters. Methods 2 and 4 take into account that a minimum of thirty values are needed in order to acquire a sufficiently low standard error[64]. Also, thirty different solutes reduces the likelihood of one "type" of solute (e.g. polar, nonpolar, aromatic, etc.) having too much of an impact on the IL-specific equation. This variety ensures that calculated parameters are more likely to represent the "actual" ABSM parameter value.[65] Rarely, an ABSM parameter will be set to zero if it is smaller than the standard error. This is done if the parameter is deemed to be insignificant to the equation by having a value smaller than its error as in Twu et. al., where the e parameter was 0.025 ± 0.084 and 0.040 ± 0.067 for log *K* and log *P* respectively and was omitted from the IL-specific equation. [158,159] Methods 3 and 4 employ this idea and all parameters smaller than the standard error are set to zero.

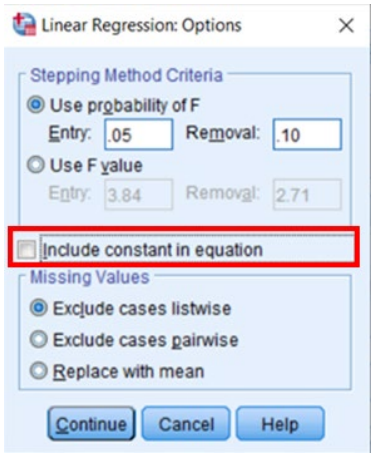


Figure 10.1: The "Include constant in equation" checkbox is left empty under the "options" section.

After importing the data from the Microsoft® Excel® file to IBM® SPSS® and ensuring that the variables were labeled correctly, the procedure from Chapter 2 was used except for one change, as shown in Figure 10.1. Under the "options" section the "Include constant in

equation" has been left unchecked.

10.3 Results

The data for Methods 1, 2, 3, 4 of data analysis are found in Table D.2 through Table D.15 in Appendix D. A comparison of known ABSM ion values and the values calculated can be seen in Table D.16-Table D.39 in Appendix D.

10.3.1 Cation Values

As previously explained in Chapter 1, the Abraham solvation parameter model allows one to predict a solute parameter given that they know solvent and solute descriptors. To determine the efficacy of this style of updating ABSM parameters, one would pick an IL and use its literature cation and anion values to calculate log *K* and log *P* using Equations 1.3 and 1.4. Those values would then be compared to log *K* and log *P* values calculated from Methods 1-4.

Table D.16 through Table D.39 show the data for cations and anions with known cation- and anion-specific parameters and their values for Methods 1-4. Table D.40-Table D.43 show data for cations and anions with more than one instance (appearance) in the updated model. This is important as the more instances an ion has, the more values which are analyzed and, theoretically, the more accurate the model should be.

The cations with the largest number of instances in Methods 1-4 were $[BMIM]^+$ and $[EMIM]^+$. $[BMIM]^+$ had 15 instances and $[EMIM]^+$ had 10 instances of both log *K* and log *P*. Table 10.2 shows the ion parameters for $[BMIM]^+$ from literature, ion parameters calculated from Methods 1-4 and the total number of log *K* and log *P* values used to calculate the ion parameters.

Table 10.2: log K and log P coefficients for $[BMIM]^+$.

	c	*e*	*s*	*a*	*b*	*l*	N
log *K*							
Lit. value	-0.421	0.033	2.134	2.281	0.603	0.712	485
Method 1	-0.512	-0.017	2.384	2.651	0.383	0.735	833
Method 2	-0.414	0.024	2.186	2.290	0.621	0.733	784
Method 3	-0.510	-0.045	2.385	2.651	0.383	0.735	833
Method 4	-0.415	-0.008	2.186	2.290	0.621	0.733	784
log *P*							
Lit. value	-0.048	0.328	0.296	-1.382	-4.337	3.390	509
Method 1	-0.235	0.340	0.558	-0.937	-4.040	3.470	818
Method 2	-0.106	0.133	0.679	-1.246	-4.126	3.442	770
Method 3	-0.188	0.242	0.632	-0.944	-4.217	3.481	818
Method 4	-0.079	0.105	0.666	-1.251	-4.126	3.442	770

There is a noticeable pattern in the models where Methods 1 and 3 and Methods 2 and 4 have similar results. For log *K*, the only parameters different between Methods 1 and 3 are *c* (-0.512 and -0.510), *e* (-0.017 and -0.045), and *s* (2.384 and 2.385). Coefficients *a*, *b*, and *l* are identical (2.651, 0.383, and 0.735 respectively). A similar pattern can also be seen with Methods 2 and 4 with *c* (-0.414 and -0.415) and *e* (0.024 and 0.-0.008) being different and *s* (2.186), *a* (2.290), *b* (0.621), and *l* (0.733) being identical. For log *P* all parameters are different for Methods 1 and 3 (*c* = -0.235 and -0.188, *e* = 0.340 and 0.242, *s* = 0.558 and 0.632, *a* = -0.937 and -0.944 , *b* = -4.040 and -4.217, *v* = 3.470 and 3.481). Methods 2 and 4 differ with *c* (-0.106 and -0.079), *e* (0.133 and 0.105), *s* (0.679 and 0.666), and *a* (-1.246 and -1.251) being different and *b* (-4.126), and *v* (3.442) being identical.

The other cation of interest is $[EMIM]^+$. Table 10.3 below shows the ion parameters for $[EMIM]^+$ from literature, ion parameters calculated from Methods 1-4 and the total number of

log *K* and log *P* values used to calculate the ion parameters.

Table 10.3: log K and log P coefficients for $[EMIM]^+$.

	c	*e*	*s*	*a*	*b*	*l*	N
log *K*							
Lit. value	-0.505	0.088	2.305	2.381	0.683	0.654	561
Method 1	-0.598	0.047	2.238	2.266	0.774	0.696	475
Method 2	-0.579	0.062	2.352	2.448	0.674	0.671	419
Method 3	-0.598	0.013	2.237	2.266	0.772	0.696	475
Method 4	-0.579	0.026	2.352	2.448	0.672	0.671	419
log *P*							
Lit. value	-0.049	0.215	0.428	-1.294	-4.209	3.163	552
Method 1	-0.130	0.190	0.338	-1.519	-4.096	3.228	462
Method 2	-0.117	0.184	0.434	-1.433	-4.237	3.164	407
Method 3	-0.144	0.153	0.373	-1.521	-4.188	3.234	462
Method 4	-0.134	0.198	0.428	-1.433	-4.237	3.164	407

As with $[BMIM]^+$, the $[EMIM]^+$ cation shows correlations between Methods 1 and 3 and Methods 2 and 4 for both log *K* and log *P*. For $[EMIM]^+$ the log *K* values of Methods 1 and 3 are different for *e* (0.047 and 0.013), *s* (2.238 and 2.237), and *b* (0.774 and 0.772) and are equal for values *c* (-0.598), *a* (2.266), and *l* (0.696). For Methods 2 and 3 the log K values of e (0.062 and 0.026) and b (0.674 and 0.672) are different while *c* (-0.579), *s* (2.352), *a* (2.448), and *l* (0.671) were identical. The log *P* values for Methods 1 and 3 were all different (*c* = -0.130 vs -0.144, *e* = 0.190 vs 0.153, *s* = 0.338 vs 0.373, *a* = -1.519 vs -1.521, *b* = -4.096 vs -4.188, *v* = 3.228 vs 3.234) while Methods 2 and 4 were only different for *c* (-0.117 and -0.134), *e* (0.184 and 0.198), and *s* (0.434 and 0.428) while *a* (-1.433), *b* (-4.237), and *v* (3.164) were the same.

10.3.2 Anion Values

Testing the new update methods with anions are more intensive. As previously

mentioned in Chapter 2, the $[NTf_2]^-$ anion is set to zero, which means all other anion coefficients can only be calculated if the cation coefficients are already known. To test the ability of this method to update anion values, the anion $[DCA]^-$ was chosen. $[DCA]^-$ has the most instances in the analysis, aside from $[NTf_2]^-$, with 12 instances of log *K* and 11 instances of log *P*. Table 10.4 shows these values.

Table 10.4: log *K* and log *P* coefficients for $[DCA]^-$.

	c	*e*	*s*	*a*	*b*	*l*	N
log *K*							
Lit. value	-0.372	0.345	0.476	2.270	-0.198	-0.055	150
Method 1	-0.373	0.441	0.257	2.436	-0.117	-0.084	668
Method 2	-0.357	0.375	0.291	2.257	-0.138	-0.066	668
Method 3	-0.373	0.461	0.258	2.436	-0.111	-0.084	668
Method 4	-0.357	0.395	0.291	2.257	-0.133	-0.066	668
log *P*							
Lit. value	-0.257	0.164	0.446	2.217	-0.256	-0.243	136
Method 1	-0.199	0.278	0.201	2.423	-0.211	-0.349	599
Method 2	-0.193	0.263	0.209	2.287	-0.123	-0.307	599
Method 3	-0.205	0.343	0.153	2.425	-0.097	-0.356	599
Method 4	-0.186	0.272	0.203	2.287	-0.123	-0.307	599

The log *K* and log *P* coefficients for the $[DCA]^-$ anion highlight the continuing pattern of Methods 1 and 3 and Methods 2 and 4 having similar parameters values. For Methods 1 and 3, log *K* coefficients *e* (0.441 and 0.461), *s* (0.257 and 0.291), and *b* (-0.117 and -0.111) were different while *c* (-0.373), *a* (2.463), and *v* (-0.084) were the same while for Methods 2 and 4, log *K* coefficients *e* (0.375 and 0.395) and *b* (-0.138 and -0.133) were different while *c* (-0.357), *s* (0.291), *a* (2.257), and *v* (-0.066) were the same. Log *P* coefficients show that all the parameters are different for Methods 1 and 3 (*c* = -0.199 and -0.205, *e* = 0.278 and 0.343, *s* = 0.201 and

0.153, *a* = 2.423 and 2.425, *b* = -0.211 and -0.097, *v* = -0.349 and -0.356) while coefficients *a* (2.287), *b* (-0.123), and *v* (-.307) remained the same and *c* (-0.193 and -0.186), *e* (0.263 and 0.272), and *s* (0.209 and 0.203) were different for Methods 3 and 4.

10.3.3 Comparison to Current Predictive Methods

To properly compare the log *K* and log *P* values using the ABSM, a solute must be chosen. For this section, the ILs $[BMIM]^+[NTf_2]^-$, $[EMIM]^+[NTf_2]^-$, $[BMIM]^+[DCA]^-$, $[EMIM]^+[DCA]^-$ and will be the solvent and the dichloromethane will be the solute. As discussed in Chapter 2, $[NTf_2]^-$ has ABSM parameters of zero. Using $[BMIM]^+[NTf_2]^-$ will allow one to compare the $[BMIM]^+$ coefficients more directly. Dichloromethane has non-zero ABSM parameters which can be found in Table D.1. It is important to have non-zero parameters to ensure that each of the ion parameters are compared fairly. Table 10.5 shows the ABSM coefficents for the $[BMIM]^+[NTf_2]^-$ and the calculated $[BMIM]^+[NTf_2]^-$/dichloromethane partitioning from water (log *P*) and from gas (log *K*).

Table 10.5: ABSM coefficients of $[BMIM]^+[NTf_2]^-$ for IL specific literature values, ion + cation literature values, values calculated from Methods 1, 2, 3, and 4, and calculated $[BMIM]^+[NTf_2]^-$/dichloromethane partitioning from water (log P) and from gas (log K).

	c	*e*	*s*	*a*	*b*	*l*	log *K*	Δ from IL Specific
log *K*								
IL Specific	-0.394	0.089	1.969	2.283	0.873	0.696	2.440	0.000
Lit (cation + anion)	-0.421	0.033	2.134	2.281	0.603	0.712	2.504	-0.064
Method 1	-0.512	-0.017	2.384	2.651	0.383	0.735	2.608	-0.168
Method 2	-0.414	0.024	2.186	2.29	0.621	0.733	2.581	-0.141
Method 3	-0.51	-0.045	2.385	2.651	0.383	0.735	2.600	-0.160
Method 4	-0.415	-0.008	2.186	2.29	0.621	0.733	2.568	-0.128

	c	*e*	*s*	*a*	*b*	*l*	log *K*	Δ from IL Specific
log *P*								
IL Specific	-0.018	0.416	0.153	-1.312	-4.187	3.347	1.545	0.000
Lit (cation + anion)	-0.048	0.328	0.296	-1.382	-4.337	3.390	1.569	-0.024
Method 1	-0.235	0.340	0.558	-0.937	-4.040	3.470	1.635	-0.090
Method 2	-0.106	0.133	0.679	-1.246	-4.126	3.442	1.703	-0.158
Method 3	-0.188	0.242	0.632	-0.944	-4.217	3.481	1.682	-0.137
Method 4	-0.079	0.105	0.666	-1.251	-4.126	3.442	1.712	-0.166

As can be seen in Table 10.5, the literature cation plus anion values are the closest to the IL specific values. This is expected as the literature values are calculated directly from solute log *K* and log *P* values while Methods 1-4 are calculated from predictive equation coefficients. The added calculation of using the predictive methods can lead to an increase in error due to the propagation of errors. From Table 10.5 it would be safe to say that Method 4 would be the best method with a difference of -0.128 for log *K* and Method 1 would be the best for log *P* with a difference of -0.090. However, these results may not apply to all ILs.

Table 10.6 shows the log *K* and log *P* parameters for the $[EMIM]^+[NTf_2]^-$ IL and their contribution to the $[EMIM]^+[NTf_2]^-$/dichloromethane partitioning from water (log *P*) and from gas (log *K*).

Table 10.6: ABSM coefficients of $[EMIM]^+[NTf_2]^-$ for IL specific literature values, ion + cation literature values, values calculated from Methods 1, 2, 3, and 4, and calculated $[BMIM]^+[NTf_2]^-$/dichloromethane partitioning from water (log P) and from gas (log K).

	c	*e*	*s*	*a*	*b*	*l*	log *K*	Δ from IL Specific
log *K*								
IL Specific	-0.486	0.068	2.296	2.278	0.988	0.651	2.441	0.000
Lit (cation + anion)	-0.505	0.088	2.305	2.381	0.683	0.654	2.436	0.005

	c	*e*	*s*	*a*	*b*	*l*	log *K*	Δ from IL Specific
Method 1	-0.598	0.047	2.238	2.266	0.774	0.696	2.367	0.074
Method 2	-0.579	0.062	2.352	2.448	0.674	0.671	2.419	0.022
Method 3	-0.598	0.013	2.237	2.266	0.772	0.696	2.353	0.088
Method 4	-0.579	0.026	2.352	2.448	0.672	0.671	2.405	0.036
log *P*								
IL Specific	0.029	0.351	0.202	-1.684	-3.585	3.059	1.445	0.000
Lit (cation + anion)	-0.049	0.215	0.428	-1.294	-4.209	3.163	1.502	-0.057
Method 1	-0.130	0.190	0.338	-1.519	-4.096	3.228	1.376	0.070
Method 2	-0.117	0.184	0.434	-1.433	-4.237	3.164	1.411	0.034
Method 3	-0.144	0.153	0.373	-1.521	-4.188	3.234	1.365	0.080
Method 4	-0.134	0.198	0.428	-1.433	-4.237	3.164	1.396	0.049

The $[EMIM]^+[NTf_2]^-$ results shows a completely different narrative than the $[BMIM]^+[NTF_2]^-$ results. For $[EMIM]^+[NTf_2]^-$, Method 2 is the method with the least difference between log *K* (0.022) and log *P* (0.034) when compared to the IL specific values, followed very closely by Method 4 (0.036 and 0.049 respectively).

Ideally, the calculated coefficients and calculated log *K* and log *P* values for cations would be identical to their literature values when paired with the $[NTf_2]^-$ anion. However, the cation values can appear to change for a few reasons: 1. The solute samples were limited in scope (e.g. only polar, only nonpolar, limited polar, limited nonpolar, limited aromatics, etc), 2. The interactions of the cation with the anion are different enough to create a significant difference in the values obtained with $[NTf_2]^-$. 3. There is not enough data for the cation with other anions to sufficiently determine a "true" ABSM parameter value.

The $[NTf_2]^-$ anion makes up only a fraction of anions which could be used. The following section will compare $[BMIM]^+[DCA]^-$ and $[EMIM]^+[DCA]^-$ ILs and their partitioning of the

dicholormethane solute. Table 10.7 show the predictive values for the $[BMIM]^+[DCA]^-$ IL and the calculated $[BMIM]^+[DCA]^-$/dichloromethane partitioning values respectively.

Table 10.7: ABSM coefficients of $[BMIM]^+[DCA]^-$ for IL specific literature values, ion + cation literature values, values calculated from Methods 1, 2, 3, and 4, and calculated $[BMIM]^+[NTf_2]^-$/dichloromethane partitioning from water (log P) and from gas (log K).

	c	*e*	*s*	*a*	*b*	*l*	log *K*	Δ from IL Specific
log *K*								
IL Specific	-0.773	0.435	2.553	4.844	0.505	0.658	2.690	0.000
Lit (cation + anion)	-0.793	0.378	2.61	4.551	0.405	0.657	2.644	0.046
Method 1	-0.885	0.424	2.641	5.087	0.266	0.651	2.622	0.068
Method 2	-0.771	0.399	2.477	4.547	0.483	0.667	2.622	0.068
Method 3	-0.883	0.416	2.643	5.087	0.272	0.651	2.622	0.068
Method 4	-0.772	0.387	2.477	4.547	0.488	0.667	2.617	0.073
log *P*								
IL Specific	-0.272	0.448	0.722	1.103	-4.437	3.131	1.750	0.000
Lit (cation + anion)	-0.305	0.492	0.742	0.835	-4.593	3.147	1.719	0.031
Method 1	-0.434	0.618	0.759	1.486	-4.251	3.121	1.718	0.032
Method 2	-0.299	0.396	0.888	1.041	-4.249	3.135	1.803	-0.053
Method 3	-0.393	0.585	0.785	1.481	-4.314	3.125	1.760	-0.009
Method 4	-0.265	0.377	0.869	1.036	-4.249	3.135	1.818	-0.068

The differences in log K for Methods 1-3 were all identical despite having different solute coefficients with a difference of 0.068 from the IL specific equation. When comparing this to the log *P* values, Method 3 is the most accurate update method with a difference of -0.009 from the IL specific equation. This is different from the results shown for $[BMIM]^+[NTf_2]^-$ and $[EMIM]^+[NTf_2]^-$ where Methods 4, 1, and 2 were the closest to the IL specific equations.

We then look at the $[EMIM]^+[DCA]^-$ IL partitioning dichloromethane with the ABSM parameters in Table 10.8. The $[BMIM]^+[DCA]^-$ results show that Method 2 is the method with the smallest difference from the IL specific equation with a difference of 0.085 for log *K* and

0.108 for log *P*. Altogether, this means that for any given IL any of the four methods could work as a way to update cation and anion parameters. However, these differences do not necessarily mean that the IL specific equation is more or less accurate than either the literature values or Methods 1-4. In the next section all of the predictive methods will be compared to experimental log *K* and log *P* values for solvents.

Table 10.8: ABSM coefficients of $[EMIM]^+[DCA]^-$ for IL specific literature values, ion + cation literature values, values calculated from Methods 1, 2, 3, and 4, and calculated $[BMIM]^+[NTf_2]^-$/dichloromethane partitioning from water (log P) and from gas (log K).

	c	*e*	*s*	*a*	*b*	*l*	log *K*	Δ from IL Specific
log *K*								
IL Specific	-0.990	0.379	2.880	4.789	0.421	0.617	2.545	0.000
Lit (cation + anion)	-0.877	0.433	2.781	4.651	0.485	0.599	2.576	-0.031
Method 1	-0.971	0.488	2.495	4.702	0.657	0.612	2.380	0.165
Method 2	-0.936	0.437	2.643	4.705	0.536	0.605	2.460	0.085
Method 3	-0.971	0.474	2.495	4.702	0.661	0.612	2.375	0.170
Method 4	-0.936	0.421	2.643	4.705	0.539	0.605	2.454	0.091
log *P*								
IL Specific	-0.329	0.326	0.909	0.933	-4.540	2.904	1.618	0.000
Lit (cation + anion)	-0.306	0.379	0.874	0.923	-4.465	2.920	1.652	-0.034
Method 1	-0.329	0.468	0.539	0.904	-4.307	2.879	1.459	0.159
Method 2	-0.310	0.447	0.643	0.854	-4.360	2.857	1.510	0.108
Method 3	-0.349	0.496	0.526	0.904	-4.285	2.878	1.443	0.175
Method 4	-0.320	0.470	0.631	0.854	-4.360	2.857	1.503	0.115

Table D.44 through Table D.47 found in Appendix D show other ILs and their comparison to other predictive values.

10.3.4 Comparison to Experimental Solute Log K and Log P Values

In the previous section the new update method for ABSM ion parameters were

compared to other predictive models. This section will compare all the predictive models to experimental log *K* and log *P* values for solutes to determine their accuracy. The ILs to be discussed in this section will be $[BMIM]^+[DCA]^-$, $[EMIM]^+[DCA]^-$, $[BMIM]^+[NTf_2]^-$, and $[EMIM]^+[NTf_2]^-$.

To check the accuracy of predictive models a wide variety of solutes must be compared and they must log *K* and log *P* values which have been experimentally determined with the chosen IL. For $[BMIM]^+[DCA]^-$, $[EMIM]^+[DCA]^-$, and $[BMIM]^+[NTf_2]^-$ the solvents hexane, benzene, ethanol, and pyridine chosen. For $[EMIM]^+[NTf_2]^-$ hexane, benzene, and ethanol will be chosen. These solutes were chosen because they encompass a variety of solutes (alkane, aromatic, alcohol, and heterocyclic aromatic) and all the solutes were used to create the ABSM parameters for the IL-specific predictive equation for each of the ILs (except pyridine and $[EMIM]^+[NTf_2]^-$).

The experimental values of solutes for log *K* and log *P* for $[BMIM]^+[DCA]^-$ were taken from Domanska *et al*.[160] and extrapolated to 298.15 K from log *K* values at 318.15-368.15 K. Table 10.9 below show the predictive ability of the $[BMIM]^+[DCA]^-$ models for hexane, benzene, ethanol, and pyridine. All of the solute parameters can be found in Table D.1.

Table 10.9: Comparison of all ABSM models for $[BMIM]^+[DCA]^-$ partitioning hexane, benzene, ethanol, and pyridine in water (log P) and gas (log K).

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Hexane				
Experimental	2.774	0.954	0.000	0.000
IL Specific	2.715	0.983	0.059	-0.029
Lit (cation + anion)	2.697	0.960	0.077	-0.006
Method 1	2.543	0.852	0.231	0.102
Method 2	2.692	1.009	0.082	-0.055

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Method 3	2.588	0.854	0.186	0.100
Method 4	2.726	1.008	0.048	-0.054
Benzene				
Experimental	2.112	2.742	0.000	0.000
IL Specific	1.999	2.724	0.113	0.018
Lit (cation + anion)	1.992	2.682	0.120	0.060
Method 1	1.978	2.598	0.134	0.144
Method 2	2.055	2.686	0.057	0.056
Method 3	2.007	2.597	0.105	0.145
Method 4	2.068	2.679	0.044	0.063
Ethanol				
Experimental	-0.293	3.377	0.000	0.000
IL Specific	-0.172	3.420	-0.121	-0.043
Lit (cation + anion)	-0.353	3.252	0.060	0.125
Method 1	-0.050	3.307	-0.243	0.070
Method 2	-0.073	3.274	-0.220	0.103
Method 3	-0.036	3.311	-0.257	0.066
Method 4	-0.054	3.272	-0.239	0.105
Pyridine				
Experimental	0.328	3.768	0.000	0.000
IL Specific	0.424	3.897	-0.096	-0.129
Lit (cation + anion)	0.365	3.834	-0.037	-0.066
Method 1	0.490	3.706	-0.162	0.062
Method 2	0.604	3.828	-0.276	-0.060
Method 3	0.502	3.708	-0.174	0.060
Method 4	0.610	3.822	-0.282	-0.054

What is interesting for $[BMIM]^+[DCA]^-$ are that all four methods show reasonable results. For hexane, the method closest to experimental log *K* and log *P* was Method 4 (-0.054 and 0.048 respectively). For benzene Method 2 had the lowest difference for log *K* (0.056) and Method 4 had the lowest difference for log *P* (0.044). Ethanol had Method 3 for the lowest

difference for log *K* (0.066) and Method 1 for the lowest difference for log *P* (-0.243). Pyridine had Method 4 for the lowest difference for log *K* (-0.054) and Method 1 for the lowest difference for log *P* (-0.162).

The experimental values of solutes for log *K* and log *P* for $[EMIM]^+[DCA]^-$ were taken from Mutelet *et al*.[45] Table 10.10 below show the predictive ability of the $[EMIM]^+[DCA]^-$ models for hexane, benzene, ethanol, and pyridine. All of the solute parameters can be found in Table D.1.

Table 10.10: Comparison of all ABSM models for $[EMIM]^+[DCA]^-$ partitioning hexane, benzene, ethanol, and pyridine in water (log P) and gas (log K).

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Hexane				
Experimental	2.436	0.616	0.000	0.000
IL Specific	2.441	0.656	-0.005	-0.040
Lit (cation + anion)	2.480	0.721	-0.044	-0.105
Method 1	2.418	0.662	0.018	-0.046
Method 2	2.416	0.678	0.020	-0.062
Method 3	2.397	0.662	0.039	-0.046
Method 4	2.406	0.678	0.030	-0.062
Benzene				
Experimental	1.963	2.593	0.000	0.000
IL Specific	1.787	2.517	0.176	0.076
Lit (cation + anion)	1.846	2.570	0.117	0.023
Method 1	1.696	2.421	0.267	0.172
Method 2	1.733	2.466	0.230	0.128
Method 3	1.689	2.413	0.274	0.180
Method 4	1.731	2.456	0.232	0.137
Ethanol				
Experimental	-0.385	3.285	0.000	0.000
IL Specific	-0.396	3.205	0.011	0.080
Lit (cation + anion)	-0.334	3.242	-0.051	0.043
Method 1	-0.426	3.163	0.041	0.122

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Method 2	-0.422	3.180	0.037	0.105
Method 3	-0.434	3.161	0.049	0.124
Method 4	-0.431	3.177	0.046	0.108
Pyridine				
Experimental	0.179	3.619	0.000	0.000
IL Specific	0.240	3.751	-0.061	-0.132
Lit (cation + anion)	0.317	3.794	-0.138	-0.175
Method 1	0.123	3.623	0.056	-0.004
Method 2	0.174	3.666	0.005	-0.047
Method 3	0.121	3.617	0.058	0.002
Method 4	0.168	3.658	0.011	-0.039

For $[EMIM]^+[DCA]^-$ there were three methods which had the lowest log *K* or log *P*, with Methods 1 and 2 occuring the most. For hexane, the method closest to experimental log *K* and log *P* was Method 1 (-0.046 and 0.018 respectively). For benzene Method 2 had the lowest difference for log *K* (0.128) and log *P* (0.230). Ethanol had Method 2 for the lowest difference for log *K* (0.105) and log *P* (0.037). Pyridine had Method 3 for the lowest difference for log *K* (0.002) and Method 1 for the lowest difference for log *P* (0.056).

The experimental values of solutes for log *K* and log *P* for $[BMIM]^+[NTf2]^-$ were taken from Sprunger *et al*.[30] Table 10.11 below show the predictive ability of the $[BMIM]^+[NTf_2]^-$ models for hexane, benzene, ethanol, and pyridine. All of the solute parameters can be found in Table D.1.

For $[BMIM]^+[NTf_2]^-$ all of the four methods had the lowest log *K* or log *P* for one solvent or another, Method 2 occuring the most. For hexane, Method 1 had the lowest difference for log *K* (-0.014) and Method 4 for the lowest difference for log *P* (0.050). For benzene, Method 2 had the lowest difference for log *K* (0.017) and Method 4 for log *P* (0.033). Ethanol had Method

2 for the lowest difference for log *K* (0.015) and log *P* (-0.231). Pyridine had Method 3 for the lowest difference for log *K* (-0.254) and log *P* (-0.462).

Table 10.11: Comparison of all ABSM models for $[BMIM]^+[NTf2]^-$ partitioning hexane, benzene, ethanol, and pyridine in water (log P) and gas (log K).

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Hexane				
Experimental	3.255	1.435	0.000	0.000
IL Specific	3.175	1.463	0.080	-0.028
Lit (cation + anion)	3.186	1.479	0.069	-0.044
Method 1	3.075	1.449	0.180	-0.014
Method 2	3.178	1.542	0.077	-0.107
Method 3	3.133	1.451	0.122	-0.016
Method 4	3.205	1.541	0.050	-0.106
Benzene				
Experimental	2.253	2.883	0.000	0.000
IL Specific	2.127	2.745	0.126	0.138
Lit (cation + anion)	2.127	2.777	0.126	0.106
Method 1	2.183	2.819	0.070	0.064
Method 2	2.216	2.866	0.037	0.017
Method 3	2.192	2.804	0.061	0.079
Method 4	2.220	2.846	0.033	0.037
Ethanol				
Experimental	-0.914	2.756	0.000	0.000
IL Specific	-0.842	2.753	-0.072	0.003
Lit (cation + anion)	-0.912	2.674	-0.002	0.082
Method 1	-0.643	2.741	-0.271	0.015
Method 2	-0.683	2.744	-0.231	0.012
Method 3	-0.672	2.737	-0.242	0.019
Method 4	-0.671	2.735	-0.243	0.021
Pyridine				
Experimental	0.191	3.631	0.000	0.000
IL Specific	0.456	3.873	-0.265	-0.242
Lit (cation + anion)	0.441	3.858	-0.250	-0.227
Method 1	0.690	3.900	-0.499	-0.269

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Method 2	0.727	3.975	-0.536	-0.344
Method 3	0.653	3.885	-0.462	-0.254
Method 4	0.725	3.954	-0.534	-0.323

The experimental values of solutes for log *K* and log *P* for $[EMIM]^+[NTf2]^-$ were taken from Sprunger *et al*.[30] Table 10.12 below show the predictive ability of the $[EMIM]^+[NTf_2]^-$ models for hexane, benzene, andethanol. All of the solute parameters can be found in Table D.1.

Table 10.12: Comparison of all ABSM models for $[EMIM]^+[NTf2]^-$ partitioning hexane, benzene, and ethanol in water (log P) and gas (log K).

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Hexane				
Experimental	3.062	1.242	0.000	0.000
IL Specific	2.947	1.251	0.115	-0.009
Lit (cation + anion)	2.969	1.240	0.093	0.002
Method 1	2.950	1.259	0.112	-0.017
Method 2	2.901	1.211	0.161	0.031
Method 3	2.941	1.259	0.121	-0.017
Method 4	2.884	1.211	0.178	0.031
Benzene				
Experimental	2.182	2.812	0.000	0.000
IL Specific	2.038	2.701	0.144	0.111
Lit (cation + anion)	1.981	2.665	0.201	0.147
Method 1	1.901	2.642	0.281	0.170
Method 2	1.894	2.646	0.288	0.166
Method 3	1.874	2.620	0.308	0.192
Method 4	1.883	2.623	0.299	0.189
Ethanol				
Experimental	-0.915	2.855	0.000	0.000
IL Specific	-0.768	2.779	-0.147	0.076

	log *P*	log *K*	Δ from exp log *P*	Δ from exp log *K*
Lit (cation + anion)	-0.894	2.665	-0.021	0.190
Method 1	-1.019	2.597	0.104	0.258
Method 2	-1.032	2.650	0.117	0.205
Method 3	-1.070	2.587	0.155	0.268
Method 4	-1.048	2.640	0.133	0.215

For $[EMIM]^+[NTf_2]^-$ all of the four methods were the best among the solvents, particularly Method 2. For hexane, Method 1 had the lowest difference for log *K* (-0.017) log *P* (0.112). For benzene, Method 2 had the lowest difference for log *K* (0.166) and Method 1 for log *P* (0.281). Ethanol had Method 2 for the lowest difference for log *K* (0.205) and Method 1 for log *P* (0.104).

10.4 Conclusion

There are two major advantages of this new ABSM update method: faster analysis time with more ABSM parameters and the ability to determine individual ion parameters for cations and anions which have not been specifically analyzed. The average time to calculate each ion parameter for all methods was 15 seconds, with multiple ions being calculated per run. This reduced the time to update cation and anion coefficients from a minium time of 43.5 hours (preparation of input into Excel spreadsheet) and 180 seconds to calculate the solvent coefficents, to a minimum time of 10 hours (preparation ofinput into Excel spreadsheet) and 180 seconds to calculate the solvent coefficients.

With all four methods used, new cation and anion parameters can be calculated. One can compare Table D.4 - Table D.7 which has literature values for cations and anions and

compare Table D.8 - Table D.15 and see new ions. For example, there are no literature values for the cation $[PDMIM]^+$, but there are cation coefficients calculated with this new method.

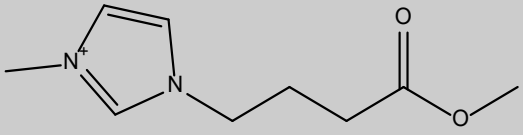
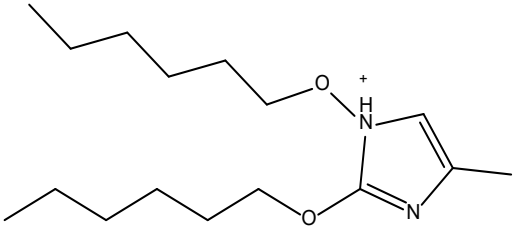
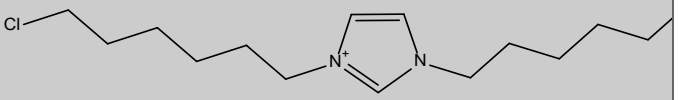
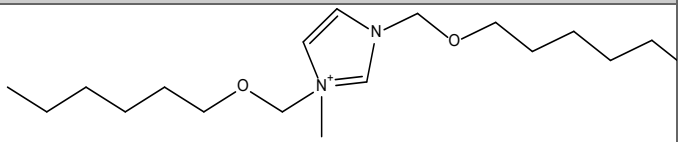
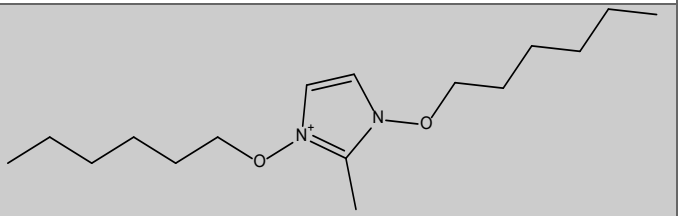
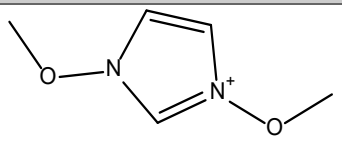
Table D.48 shows the predictive power of both the Abraham solvation model and the method of updating IL coefficients. It contains all the log K and log P values for $[BMIM]^+[DCA]^-$ for all solutes given in Table D.1 across the IL specific parameters, the literature (cation + anion) parameters, and the combined parameters from methods 1-4. Although a large number of the solutes in Table D.48 fall outside of the range of the solutes used to determine the equation coefficients for the the $[BMIM]^+[DCA]^-$ IL, they can be used to show the predictive power of the ion-specific Abraham solvation model as see with Equations 1.3 and 1.4.

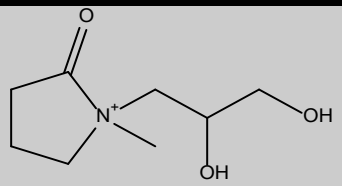
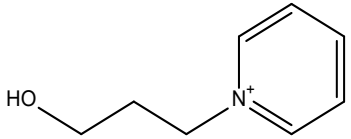
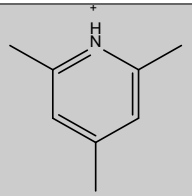
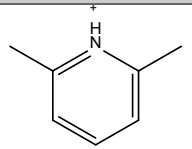
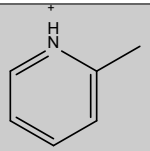
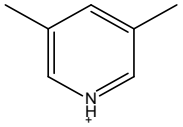
Although all of the methods showed promising results, especially when compared to the experimental log *K* and log *P* values for solutes as seen in Table 10.9 - Table 10.12, the method which consistently had the closest log *K* and log *P* values to experimental values were Methods 1 and 2. Out of the 30 different IL/solute combinations studied (15 log *K* and 15 log *P* for 30 total), Method 1 had the lowest log *K* or log *P* values for 8 of those combinations, with 2 of those IL/solute combinations having the lowest log *K* and log *P* values ($[EMIM]^+[DCA]^-$/hexane and $[EMIM]^+[NTf_2]^-$/hexane). Method 2 had the lowest log *K* or log *P* values for 7 of those combinations, with 3 of those IL/solute combinations having the lowest log *K* and log *P* values ($[EMIM]^+[DCA]^-$/benzene, $[EMIM]^+[DCA]^-$/ethanol, and $[BMIM]^+[NTf_2]^-$/ethanol). Method 3 had the lowest log *K* or log *P* values for 3 of those combinations, with 1 of those IL/solute combinations having the lowest log *K* and log *P* values ($[BMIM]^+[NTf_2]^-$/ethanol). Method 4 had the lowest log *K* or log *P* values for 5 of those combinations, with 1 of those IL/solute combinations having the lowest log *K* and log *P* values ($[BMIM]^+[DCA]^-$/hexane).

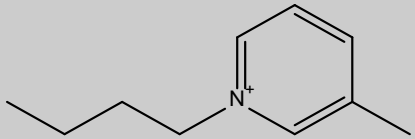
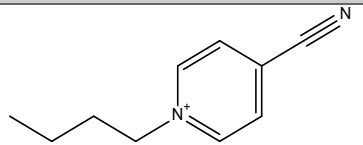
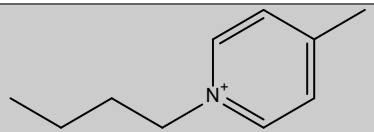
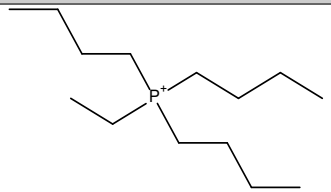
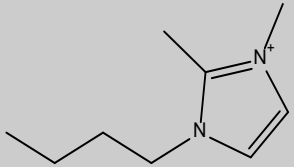
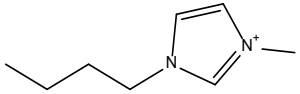
Ultimately, this new ABSM update method not only quickly updates the list of ABSM parameters, but it also updates old and new IL ABSM parameters when new data is acquired without significant loss to predictive power.

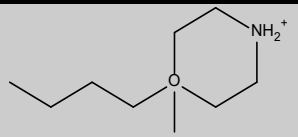
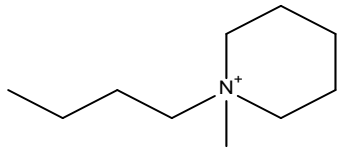
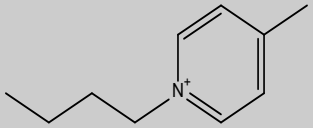
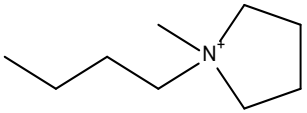
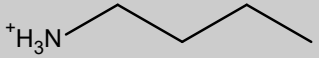
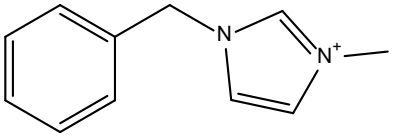
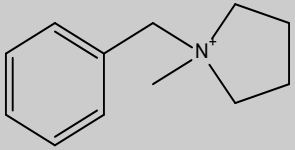
APPENDIX A

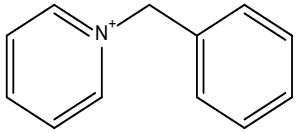
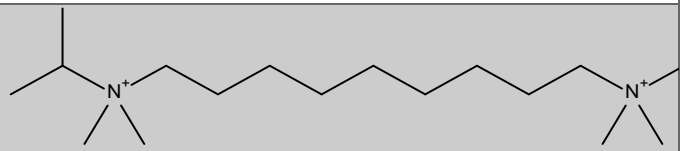
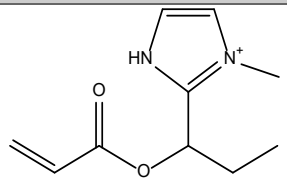
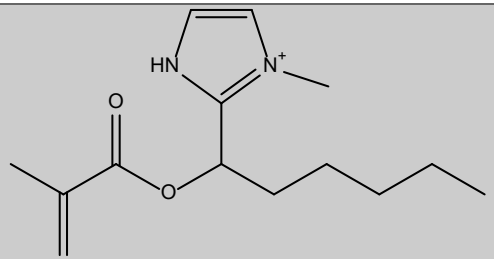
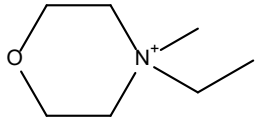
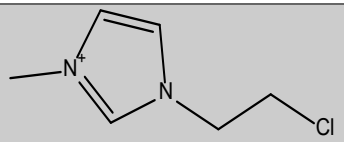
IONIC LIQUIDS AND THEIR ABSM PARAMETERS

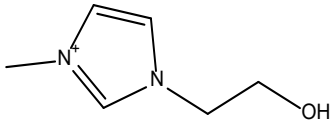
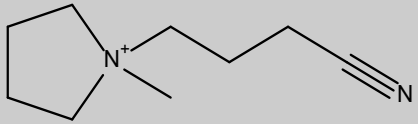
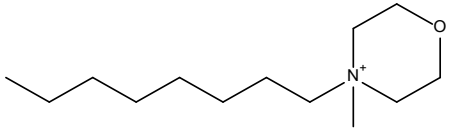
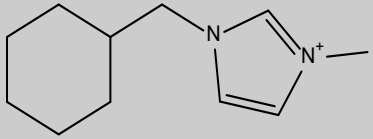
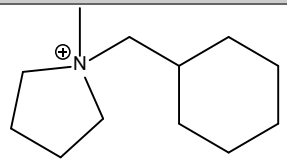
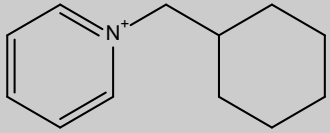
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[(C_3COOMe)MIM]^+$	1-(4-Methoxy-4-oxobutyl)-3-methylimidazolium		
$[(C6H13OCH2)2IM]^+$	1,2-Dihexyloxymethylimidazolium		
$[(ClH)2Im]^+$	1,3-Di(6-chlorohexyl)midazolium		
$[(Hexom)2Im]^+$	1,3-Dihexyloxymethyl-3-methylimidazolium		
$[(Hxom)2Im]^+$	1,3-Dihexyloxymethylimidazolium	$[Hexom2Im]^+$	
$[(Meo)2Im]^+$	1,3-Dimethoxyimidazolium	$[(OC1)2im]^+$	

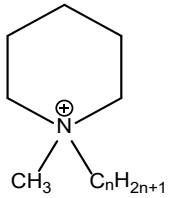
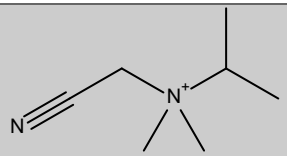
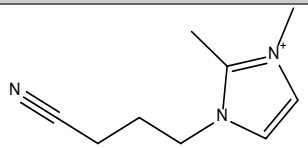
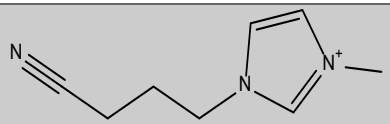
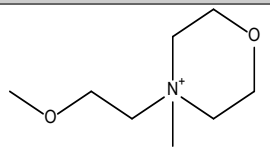
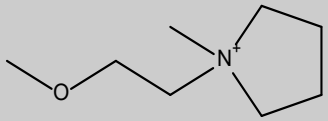
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[(OH)2C3MPyr]^+$	2,3-Dihydroxypropyl-N-methyl-2-oxopyrrolidinium		
$[1\text{-}PrOHPy]^+$	1-(3-Hydroxypropyl)pyridinium	$[PrOHPy]^+$, $[N\text{-}C3OHPY]^+$	
$[2,4,6\text{-}M3Py]^+$	2,4,6-Trimethylpyridinium		
$[2,6\text{-}M2Py]^+$	2,6-Dimethylpyridinium		
$[2\text{-}MPy]^+$	2-Methylpyridinium		
$[3,5\text{-}M2Py]^+$	3,5-Dimethylpyridinium		

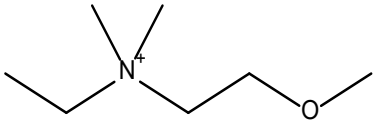
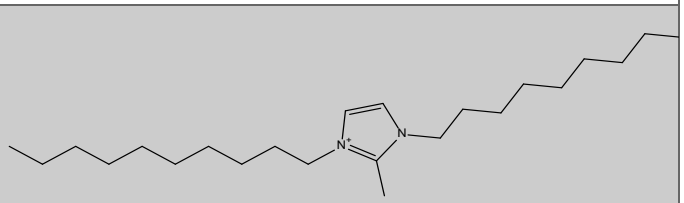
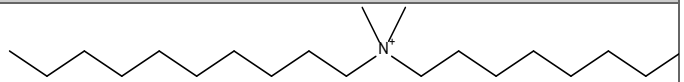
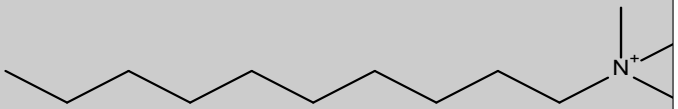
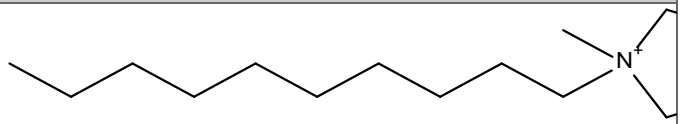
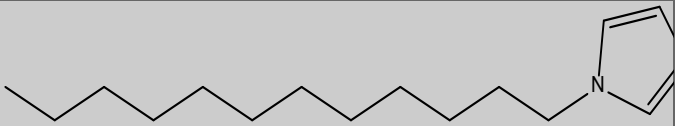
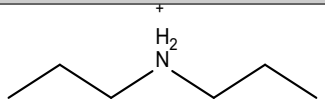
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[3\text{-MBPy}]^+$	3-Methyl-N-butylpyridinium; 3-Methyl-1-butylpyridinium	$[3\text{-BMPy}]^+$	
$[4\text{-CNBPy}]^+$	4-Cyano-1-butylpyridinium		
$[B3EP]^+$	Tributylethylphosphonium		
$[B4MPY]^+$	1-Butyl-4-methylpyridinium		
$[BM2Im]^+$	1-Butyl-2,3-dimethylimidazolium		
$[BMIm]^+$	1-Butyl-3-methylimidazolium, 1-methyl-3-butylimidazolium	$[MBIm]^+$, $[C4mim]^+$	

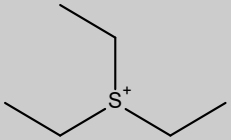
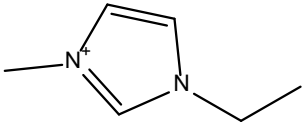
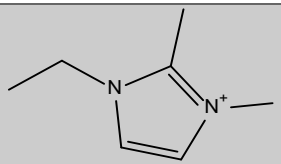
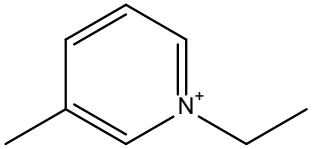
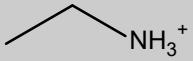
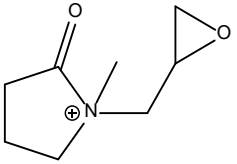
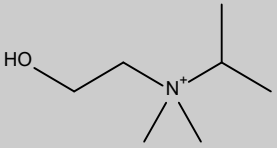
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[BMMOR]^+$	1-Butyl-1-methylmorpholinium	$[BMMorp]^+$	
$[BMPip]^+$	1-Butyl-1-methylpiperidinium		
$[BMPy]^+$	4-Methyl-N-butylpyridinium	$[4\text{-}MBPy]^+$, $[4\text{-}BMPy]^+$, $[MBPy]^+$	
$[BMPyrr]^+$	1-Butyl-1-methylpyrrolidinium; 1-Methyl-1-butylpyrrolidinium	$[BMPyr]^+$	
$[BNH3]^+$	n-Butylammonium		
$[BzMIM]^+$	1-Benzyl-3-methylimidazolium; 3-Methyl-1-benzylimidazolium	$[BeMIM]^+$	
$[BzmPyrr]^+$	1-Benzyl-1-methylpyrrolidinium		

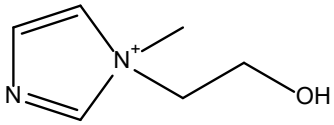
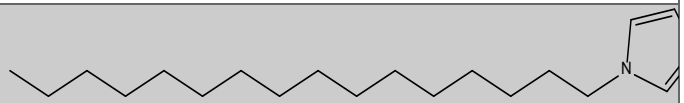
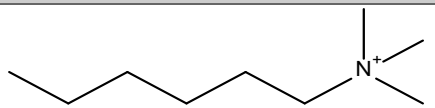
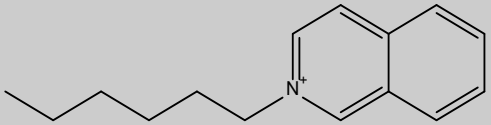
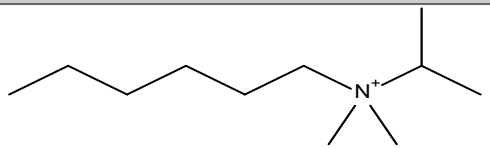
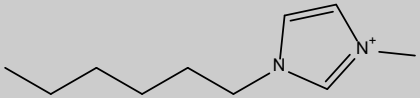
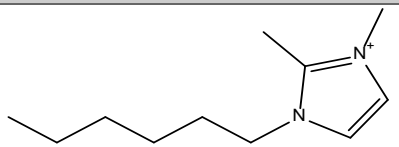
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[BzPy]^+$	1-Benzylpyridinium		
$[C1,9(M2iPAm)2]2^+$	N,N,N',N'-Tetramethyl-N,N'-diisopropyl-1,9-nonanediaminium		
$[C10H15O2MIM]^+$	n-Acryloyloxypropyl-N-methylimidazolium		
$[C10H17O2MIM]^+$	n-Methacryloyloxyhexyl-N-methylimidazolium		
$[C2C1Mor]^+$	N-Ethyl-N-methylmorpholinium		
$[C2ClC1Im]^+$	1-(2-Chloroethyl)-3-methylimidazolium		

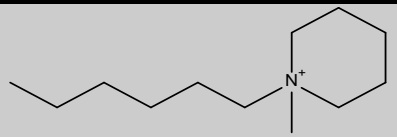
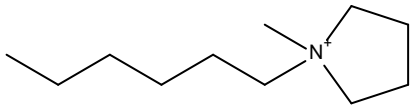
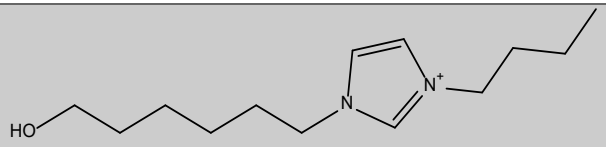
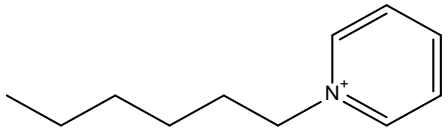
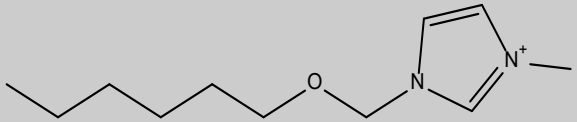
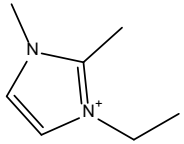
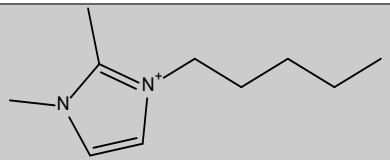
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[C2OHMim]^+$	1-(2-Hydroxyethyl)-3-methylimidazolium		
$[C3CNC1Pyr]^+$	1-(3-Cyanopropyl)-1-methyl pyrrolidinium		
$[C8C1Mor]^+$	N-Octyl-N-methylmorpholinium		
$[ChxmIm]^+$	1-Cyclohexylmethyl-3-methylimidazolium		
$[ChxmPyrr]^+$	1-Cyclohexylmethyl-1-methylpyrroldinium;1-(Cyclohexylmethyl)-1-methylpyrrolidin-1-ium		
$[ChxPy]^+$	N-Cyclohexylmethylpyridinium; 1-(Cyclohexylmethyl)pyridin-1-ium		

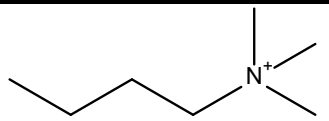
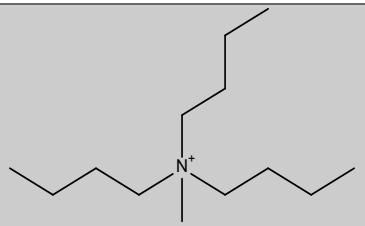
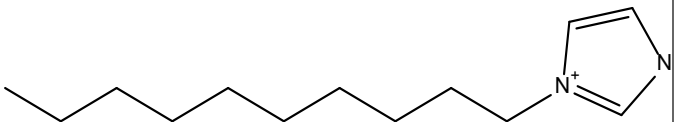
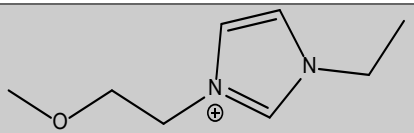
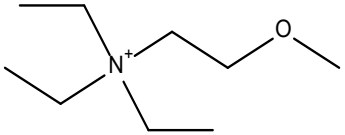
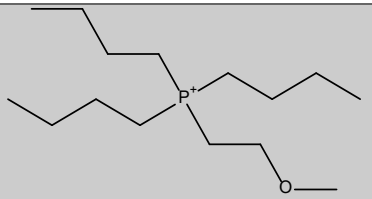
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[CnC1Pip]^+$	1-n-Alkyl-1-methylpiperidinium		
$[CNMeM2iPam]^+$	Cyanomethyl(dimethyl)isopropylammonium		
$[CnPrM2Im]^+$	1-(3-Cyanopropyl)-2,3-dimethylimidazolium		
$[CNPrMIm]^+$	1-(3-Cyanopropyl)-3-methylimidazolium	$[C3CNmim]^+$	
$[COC2mMOR]^+$	4-(2-Methoxyethyl)-4-methylmorpholinium		
$[COC2mPYR]^+$	1-(2-Methoxyethyl)-1-methylpyrrolidinium		

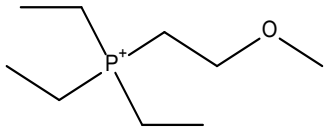
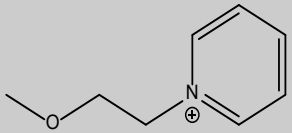
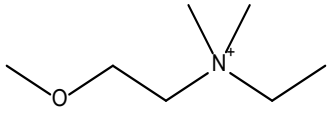
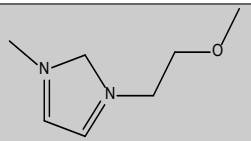
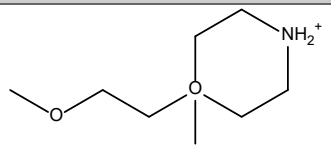
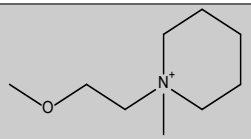
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[COC2N112]^+$	Ethyl-dimethyl-(2-methoxyethyl)ammonium		
$[D2MIm]^+$	1,3-Didecyl-2-methylimidazolium		
$[DDA]^+$	Didecyldimethylammonium		
$[DM3Am]^+$	Decyl(trimethyl)ammonium		
$[DMPyrr]^+$	1-Decyl-1-methylpyrrolidinium		
$[DoMIM]^+$	1-Dodecyl-3-methylimidazolium		
$[DPrNH3]^+$	Di-N-propylammonium		

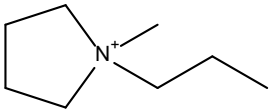
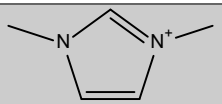
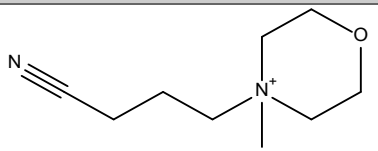
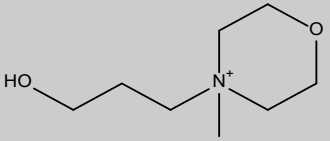
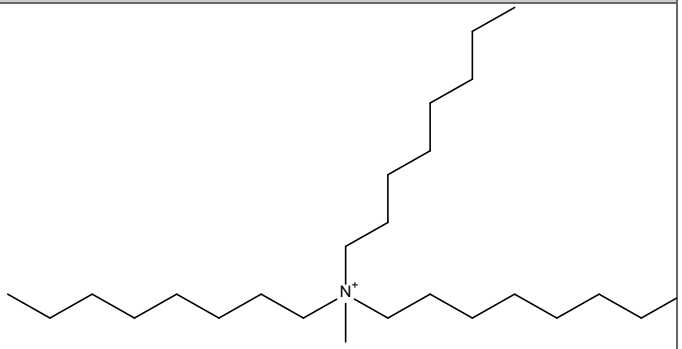
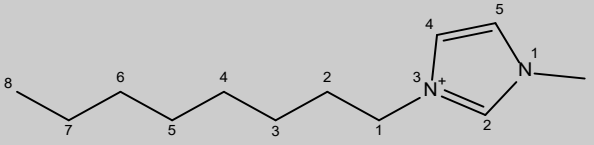
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[E3S]^+$	Triethylsulfonium	$[Et3S]^+$	
$[EMIM]^+$	1-Ethyl-3-methylimidazolium; 1-Methyl-3-ethylimidazolium	$[MEIm]^+$	
$[EMMIm]^+$	1-Ethyl-2,3-dimethylimidazolium		
$[EMpy]^+$	1-Ethyl-3-Methylpyridinium		
$[ENH3]^+$	Ethylammonium		
$[EPMPyr]^+$	N-(2',3'-Epoxypropyl)-N-methyl-2-oxopyrrolidinium; 1-Methyl-1-(oxiran-2-ylmethyl)-2-oxopyrrolidin-1-ium		
$[EtOHM2iPAm]^+$	2-Hydroxyethyl(dimethyl)isopropylammonium		

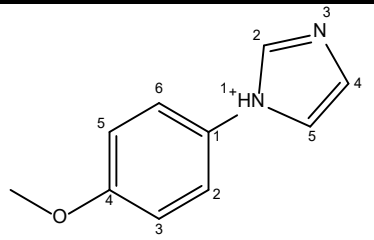
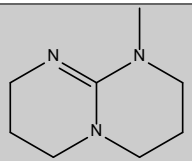
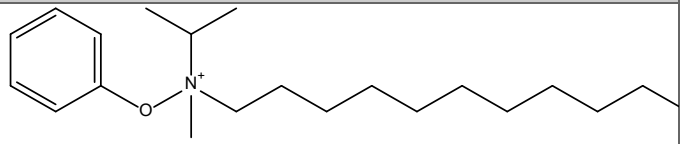
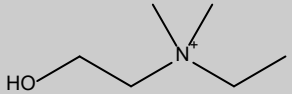
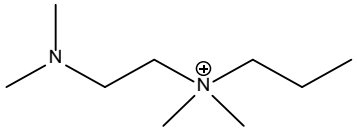
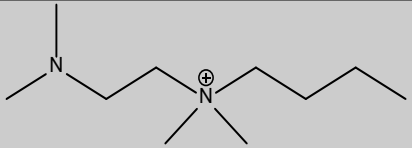
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[EtOHMIm]^+$	1-(2-Hydroxyethyl)-1-methylimidazolium;1-Ethanol-3-methylimidazolium	$[C2OHmim]^+$	
$[HexdMIm]^+$	1-Hexadecyl-3-methylimidazolium		
$[HexM3Am]^+$	Hexyl(trimethyl)ammonium	$[TMHA]^+$, $[HM3Am]^+$	
$[HiQuin]^+$	N-Hexylisoquinolinium		
$[HM2iPam]^+$	Hexyl(dimethyl)isopropylammonium		
$[HMIM]^+$	1-Hexyl-3-methylimidazolium; 1-Methyl-3-hexylimidazolium	$[MHIm]^+$	
$[HMMIM]^+$	1-Hexyl-2,3-Dimethylimidazolium		

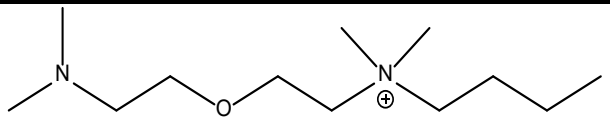
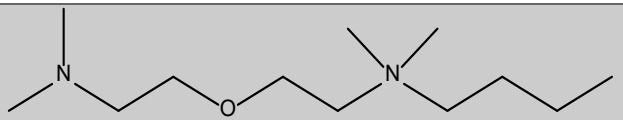
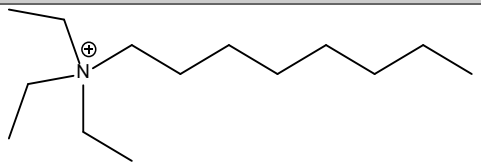
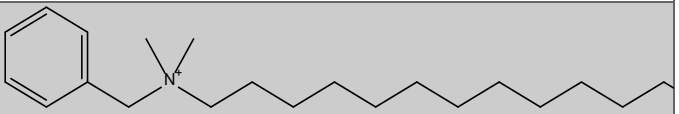
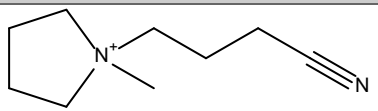
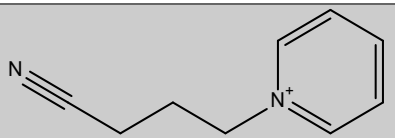
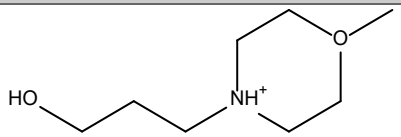
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[HMPip]^+$	1-Hexyl-1-methylpiperidinium	$[C6C1Pip]^+$	
$[HMPyrr]^+$	1-Hexyl-1-methylpyrrolidinium		
$[HOHBim]^+$	1-(6-Hydroxyhexyl)-3-butylimidazolium		
$[Hpy]^+$	N-Hexylpyridinium		
$[HxomMIm]^+$	1-Hexyloxymethyl-3-methylimidazolium	$[HexM3Im]^+$, $[HexomMIm]^+$, $[C6H13OCH2MIM]^+$	
$[M2EIm]^+$	1,2-Dimethyl-3-ethylimidazolium	$[EM2Im]^+$	
$[M2PIm]^+$	1,2-Dimethyl-3-pentylimidazolium		

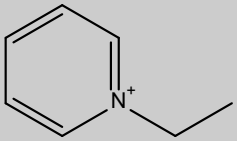
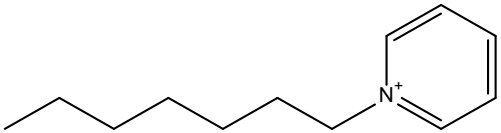
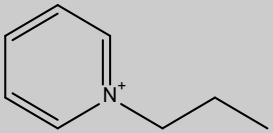
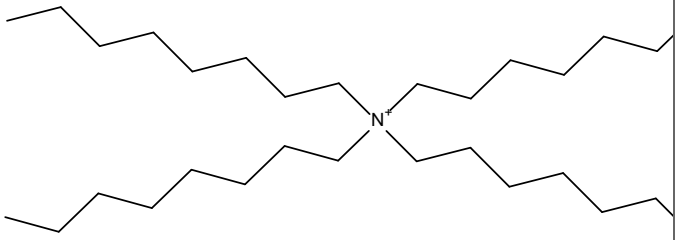
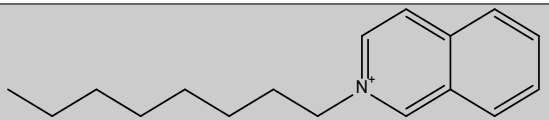
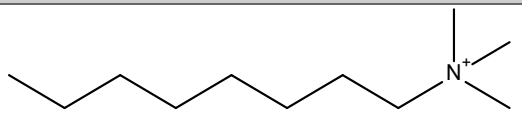
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[M3BAm]^+$	Trimethyl(butyl)ammonium	$[M3BuN]^+$	
$[MB3Am]^+$	Methyl(tributyl)ammonium		
$[MDIm]^+$	1-Methyl-3-decylimidazolium		
$[MeOCH2CH2EtIm]^+$	1-Ethyl-3-(2-methoxyethyl)imidazolium		
$[MeOCH2CH2NEt3]^+$	(2-Methoxyethyl)triethylammonium		
$[MeOCH2CH2PBu3]^+$	(2-Methoxyethyl)tributylphosphonium		

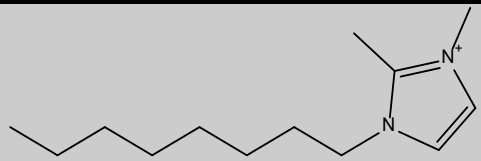
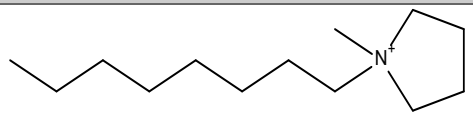
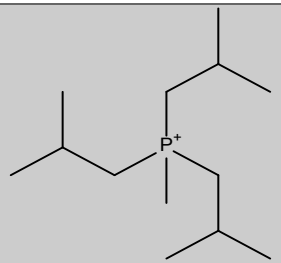
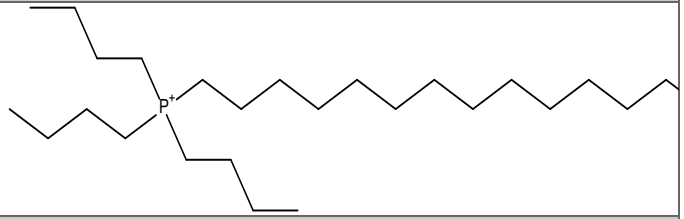
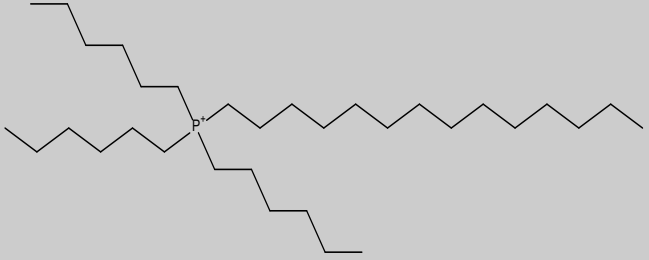
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[MeOCH2CH2PEt3]^+$	(2-Methoxyethyl)triethylphosphonium		
$[MeOCH2CH2Py]^+$	N-(2-Methoxyethyl)pyridinium		
$[MeoeM2EAm]^+$	2-Methoxyethyl(dimethyl)ethylammonium		
$[MeoeMIm]^+$	1-Methylethylether-3-methyimidazolium;1-(2-Methoxyethyl)-3-methyl-2H-1(lamda)4,3(lamda)4-imidazole	$[C2OC1mim]^+$	
$[MeoeMMorp]^+$	1-(2-Methoxyethyl)-1-methylmorpholinium		
$[MeoeMPip]^+$	1-(2-Methoxyethyl)-1-methylpiperidinium		

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[MeoeMPyrr]^+$	1-(2-Methylethyl)-1-methylpyrrolidinium		
$[MMIM]^+$	1,3-Dimethylimidazolium	$[DMIM]^+$	
$[Mo1,3CN]^+$	4-(3-Cyanopropyl)-4-methylmorpholinium		
$[Mo1,3OH]^+$	4-(3-Hydroxypropyl)-4-methylmorpholinium		
$[MO3Am]^+$	Methyl(trioctyl)ammonium		
$[MOIm]^+$	1-Methyl-3-octylimidazolium	$[mocim]^+$	

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[MPMIM]^+$	1-(4-Methoxyphenyl)imidazolium; 1-(4-Methoxyphenyl)-1H-imidazol-1-ium		
$[MTBDH]^+$	1,3,4,6,7,8-Hexahydro-1-methyl-2H-pyrimido[1,2-a]pyrimidine		
$[N1,1,12,2OPh]^+$	Dimethyldodecylphenoxyethylammonium		
$[N1122OH]^+$	Ethyl(2-hydroxyethyl)dimethyl-ammonium		
$[N112N113]^+$	N-[2-(N',N'-Dimethylamino)ethoxyethyl]N,N-(dimethyl)-1-propanaminium; N-(2-(Dimethylamino)ethyl)-N,N-dimethylpropan-1-aminium		
$[N112N114]^+$	N-(2-(N',N'-Dimethylamino)ethyl)-N,N-(dimethyl)-1-butanaminium; N-(2-(Dimethylamino)ethyl)-N,N-dimethylbutan-1-aminium		

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[N112O2N113]^+$	N-(2-(N',N'-Dimethylamino)-ethoxyethyl)-N,N-(dimethyl)-1-propanaminium; N-(2-(2-(Dimethylamino)ethoxy)ethyl)-N,N-dimethylbutan-1-aminium		
$[N112O2N114]^+$	N-(2-(N',N'-Dimethylamino)-ethoxyethyl)-N,N-(dimethyl)-1-butanaminium; 2-(2-(Butyldimethyl-l4-azaneyl)ethoxy)-N,N-dimethylethan-1-amine		
$[N2,2,2,8]^+$	N-Triethyl(octyl)ammonium		
$[NBz,1,1,14]^+$	N-Benzyl-N,N-dimethyl-N-tetradecylammonium		
$[N\text{-}C3CNMPyr]^+$	(3-Cyanopropyl)methylpyrrolidinium		
$[N\text{-}C3CNPy]^+$	(3-Cyanopropyl)pyridinium		
$[N\text{-}C3OHmMOR]^+$	4-(3-Hydroxy)-4-methylmorpholinium;(3-Hydroxypropyl)-1-methylmorpholinium		

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[NEP]^+$	N-Ethylpyridinium	$[C5H5NC2H5]^+$, $[NePy]^+$, $[Epy]^+$, $[C2PY]^+$	
$[NHP]^+$	N-Heptylpyridinium	$[C5PY]^+$	
$[NPP]^+$	N-Propylpyridinium	$[C4PY]^+$	
$[O4Am]^+$	Tetraoctylammonium		
$[OiQu]^+$	N-Octylisoquinolinium	$[C8iQuin]^+$	
$[OM3Am]^+$	Octyl(trimethyl)ammonium		

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[OMMIM]^+$	1-Octyl-2,3-dimethylimidazolium		
$[OMPyrr]^+$	1-Octyl-1-methylpyrrolidinium		
$[P1,4,4,4]^+$	Methyl(triisobutyl)phosphonium; Tri-iso-butylmethylphosphonium	$[MiB3P]^+$	
$[P14,4,4,4]^+$	Tributyltetradecylphosphonium		
$[P14,6,6,6]^+$	Trihexyl(tetradecyl)phosphonium	$[thtd\text{-}Ph]^+$, $[P6,6,6,14]^+$, $[3C6C14P]^+$, $[H3TdP]^+$	

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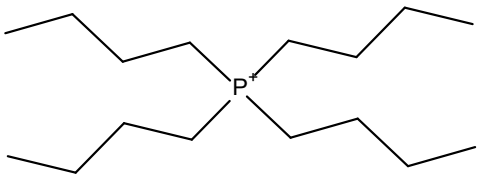
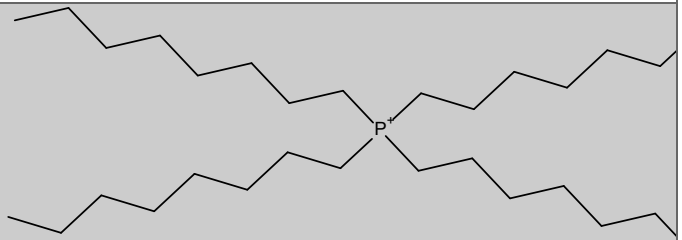
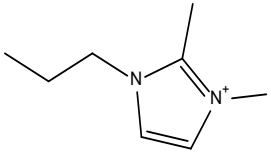
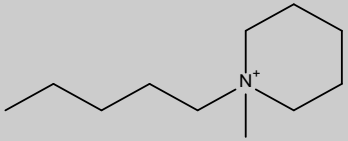
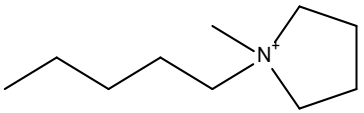
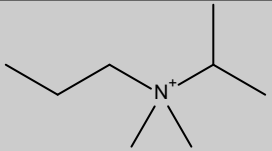
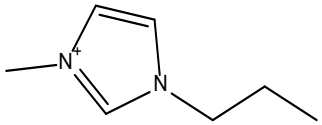
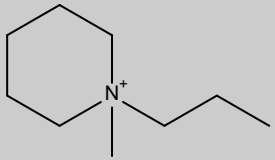
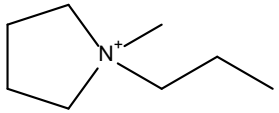
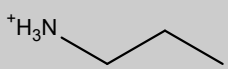
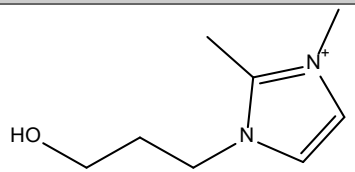
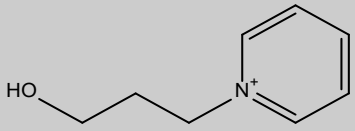
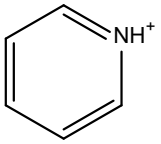
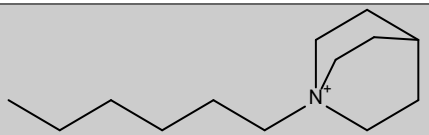
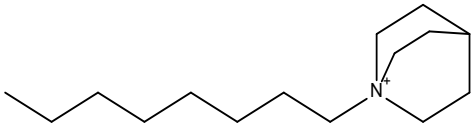
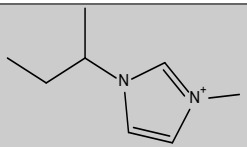
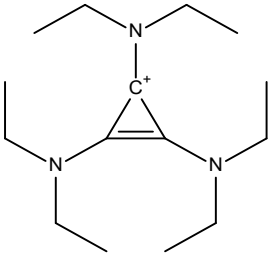
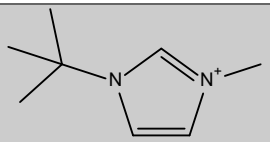
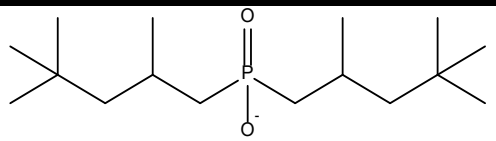
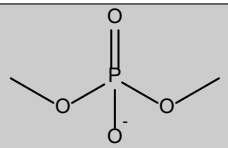
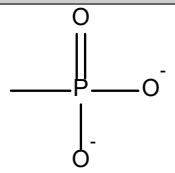
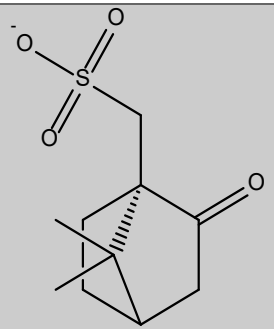
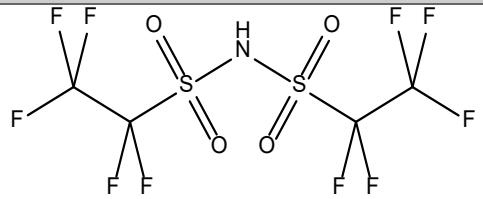
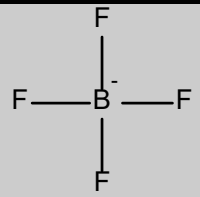
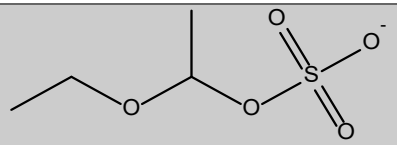
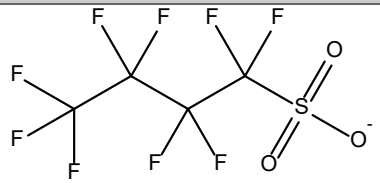
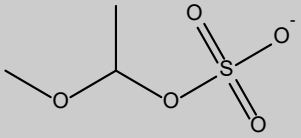
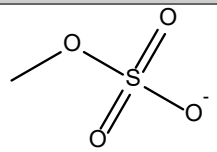
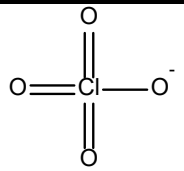
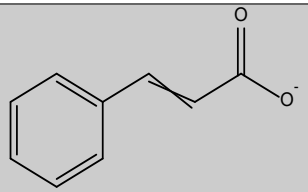
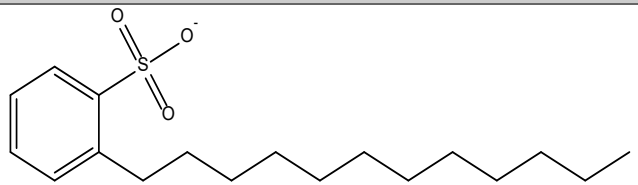
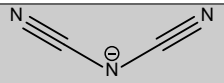
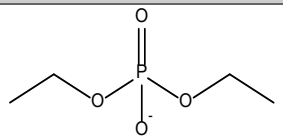
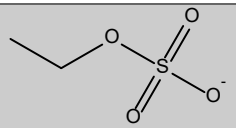
$[P4,4,4,4]^+$	Tetrabutylphosphonium		
$[P8,8,8,8]^+$	Tetraoctylphosphonium		
$[PDMIM]^+$	1-Propyl-2,3-dimethylimidazolium	$[PM2Im]^+$, $[PMMIm]^+$	
$[PeMPip]^+$	1-Pentyl-1-methylpiperidinium	$[C5C1Pip]^+$	
$[PeMPyrr]^+$	1-Pentyl-1-methylpyrrolidinium		
$[PM2iPAm]^+$	Propyl(dimethyl)isopropylammonium		

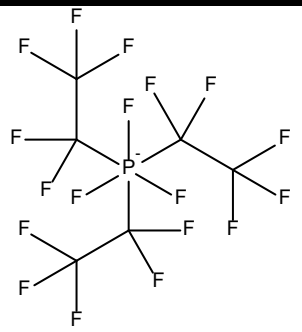
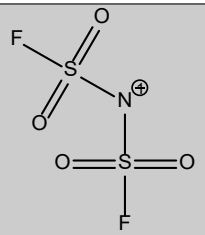
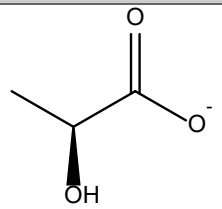
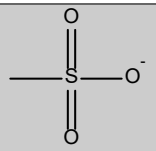
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[PMIM]^+$	1-Propyl-3-methylimidazolium		
$[PMPip]^+$	1-Propyl-1-methylpiperidinium; 1-Methyl-1-propylpiperidinium	$[MPrPip]^+$	
$[PMPyrr]^+$	1-Propyl-1-methylpyrrolidinium; 1-Methyl-1-propylpyrrolidinium; N-Propyl-N-methylpyrroldinium	$[PrMPyr]^+$	
$[PrNH3]^+$	N-Propylammonium		
$[PrOHM2Im]^+$	1-(3-Hydroxypropyl)-2,3-dimethylimidazolium		
$[PrOHPy]^+$	1-(3-Hydroxypropyl)pyridinium	$[1\text{-}PrOHPy]^+$, $[N\text{-}C3OHPY]^+$	

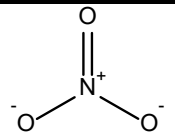
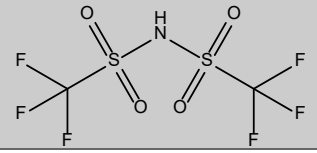
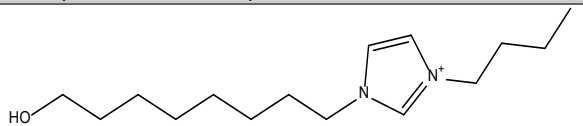
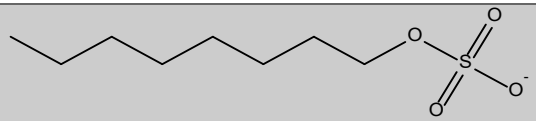
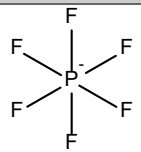
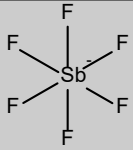
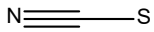
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[PY]^+$	Pyridinium	$[C5H5NH]^+$	
$[QUIN6]^+$	1-Hexylquinuclidinium		
$[QUIN8]^+$	1-Octylquinuclidinium		
$[sec\text{-}BMIM]^+$	1-sec-Butyl-3-methylimidazolium		
$[TDC]^+$	1,2,3-Tris(diethylamino)cyclopropenylium		
$[tert\text{-}BMIM]^+$	1-tert-Butyl-3-methylimidazolium		

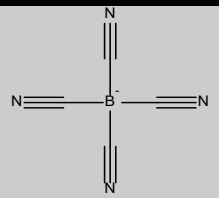
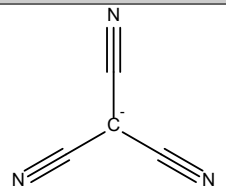
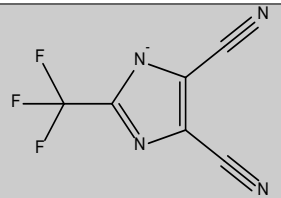
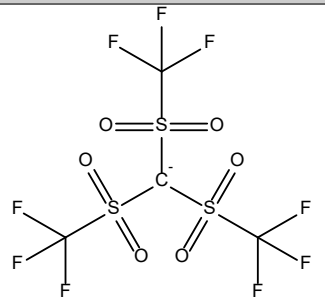
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[(C8H17)2PO2]^-$	Bis-(2,4,4-trimethylpentyl)-phosphinate		
$[(CH3)2PO4]^-$	Dimethylphosphate	$[DMPO4]^-$, $[DMP]^-$	
$[(MeO)(H)PO2]^-$	Methylphosphonate		
$[+CS]^-$	(1S)-(+)-10-Camphorsulfonate		
$[BETI]^-$	Bis(pentafluoroethylsulfonyl)imide		

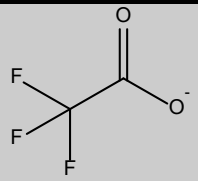
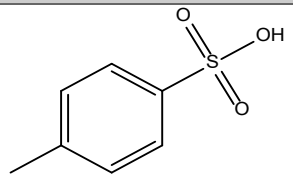
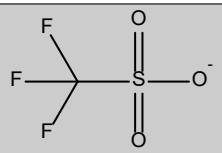
IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[BF4]^-$	Tetrafluoroborate		
$[Br]^-$	Bromide		Br^-
$[C2H5OC2H4OSO3]^-$	Ethoxyethylsulfate		
$[C4F9SO3]^-$	Nonafluoro-1-butanesulfonate		
$[CH3OC2H4SO4]^-$	Methoxyethylsulfate		
$[CH3SO4]^-$	Methylsulfate		
$[Cl]^-$	Chloride		Cl^-

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[ClO4]^-$	Perchlorate		
$[Cyn]^-$	Cinnamate		
$[DBS]^-$	Dodecylbenzenesulfonate		
$[DCA]^-$	Dicyanamide	$[N(CN)2]^-$,	
$[DEP]^-$	Diethylphosphate	$[DEPO4]^-$, $[E2PO4]^-$	
$[EtSO4]^-$	Ethylsulfate	$[ESO4]^-$	

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[FAP]^-$	Tris(pentafluoroethyl)trifluorophosphate	$[(C2F5)3PF3]^-$	
$[FSI]^-$	Bis(fluorosulfonyl)imide		
$[L\text{-}Lact]^-$	L-Lactate		
$[MeSO3]^-$	Methanesulfonate	$[CH3SO3]^-$	

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[NO3]^-$	Nitrate		
$[NTf2]^-$	Bis(trifluoromethylsulfonyl)imide; Bis(trifluoromethanesulfonyl)imide	$[Tf2N]^-$, $[CF3SO2)2N]^-$, $[BTI]^-$	
$[OOHBIm]^-$	1-(8-hydroxyoctyl)-3-Butylimidazolium		
$[OS]^-$	Octylsulfate	$[OtSO4]^-$	
$[PF6]^-$	Hexafluorophosphate		
$[SbF6]^-$	Hexafluoroantimonate		
$[SCN]^-$	Thiocyanate		

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[TCB]^-$	Tetracyanoborate	$[B(CN)4]^-$	
$[TCM]^-$	Tricyanomethanide	$[C(CN)3]^-$	
$[TDI]^-$	4,5-Dicyano-2-(trifluoromethyl)imidazolide		
$[Tf3C]^-$	Tris(trifluoromethylsulfonyl)methanide		

IL Ion Abbreviation	IL Ion Name(s)	Other Abr.	Chemical Structure
$[TFA]^-$	Trifluoroacetate	$[F3Ac]^-$, $[AcF3]^-$	
$[Tos]^-$	Tosylate		
$[Trif]^-$	Trifluoromethanesulfonate (triflate)	$[CF3SO3]^-$	

APPENDIX B

SUPPLEMENTAL INFORMATION FOR CHAPTER 3

Table B.1: Logarithm of gas-to-IL partition coefficients, log K, and logarithm of water-to-IL partition coefficients, log P, for solutes dissolved in anhydrous $[N_{112}N_{113}]^+[NTf_2]^-$ at 298.15 K

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.464	3.284
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.439	3.279
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.811	3.771
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	1.794	3.914
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.157	4.267
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.511	4.661
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.865	5.185
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	3.200	5.580
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	3.526	6.056
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.826	2.726
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	2.024	3.274
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.339	2.919
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.764	2.134
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.154	2.504
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.448	2.868
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.534	2.924
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.525	2.935
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	3.683	3.023
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.614	2.774
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	1.985	3.205
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.356	3.766
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.195	2.405
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.555	2.995
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.735	-0.055
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.050	0.330
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.345	0.765
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.350	0.850
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.699	0.149
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.323	-0.387
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.471	-1.269

Solute	E	S	A	B	L	V	log *K*	log *P*
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.678	-0.992
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.045	-0.515
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.748	-0.732
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.231	-0.069
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.421	-0.039
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.654	0.484
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.867	0.817
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.570	1.780
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.203	1.243
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.325	2.385
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.048	0.198
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.424	3.363	0.413
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.887	1.847
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.840	0.680
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.896	-1.794

Table B.2: Logarithm of gas-to-IL partition coefficients, log K, and logarithm of water-to-IL partition coefficients, log P, for solutes dissolved in anhydrous $[N_{112}N_{114}]^+[NTf_2]^-$ at 298.15 K

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.324	3.144
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.380	3.220
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.779	3.739
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	1.774	3.894
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.178	4.288
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.522	4.672
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.888	5.208
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	3.244	5.624
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	3.594	6.124
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	1.650	2.820
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.791	2.691
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	2.007	3.257

Solute	E	S	A	B	L	V	log *K*	log *P*
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.335	2.915
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.735	2.105
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.135	2.485
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.413	2.833
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.530	2.920
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.498	2.908
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.551	2.711
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	2.156	2.366
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.516	2.956
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.767	-0.023
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.085	0.365
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.375	0.795
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.374	0.874
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.343	-0.367
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.476	-1.264
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.690	-0.980
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.045	-0.515
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.756	-0.724
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.238	-0.062
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.438	-0.022
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.625	0.455
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.844	0.794
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.519	1.729
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.155	1.195
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.262	2.322
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.054	0.204
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.424	3.354	0.404
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.054	2.163	-0.197
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.843	1.803
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.878	0.718
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.757	-1.933

Table B.3: Logarithm of gas-to-IL partition coefficients, log K, and logarithm of water-to-IL partition coefficients, log P, for solutes dissolved in anhydrous $[N_{112}O_2N_{113}]^+[NTf_2]^-$ at 298.15 K

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.046	2.866
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	1.017	2.857
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	1.372	3.332
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	1.369	3.489
Octane	0.000	0.000	0.000	0.000	3.677	1.236	1.693	3.803
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.020	4.170
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.325	4.645
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	2.660	5.040
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	2.979	5.509
Tridecane	0.000	0.000	0.000	0.000	6.200	1.940	3.339	
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	1.327	2.497
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.482	2.382
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	1.631	2.881
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	1.954	2.534
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.630	2.000
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	2.981	2.331
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.238	2.658
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.334	2.724
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.307	2.717
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	1.275	2.435
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	1.616	2.836
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	1.932	3.342
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	1.928	2.138
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.250	2.690
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.755	-0.035
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.011	0.261
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.265	0.685
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.252	0.752
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.621	0.071
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.346	-0.364

Solute	E	S	A	B	L	V	log *K*	log *P*
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.643	-1.097
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.781	-0.889
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.089	-0.471
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.768	-0.712
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.237	-0.063
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.433	-0.027
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.484	0.314
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.590	0.540
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.394	1.604
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	2.080	1.120
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	2.040	2.100
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.115	0.265
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.785	1.745

Table B.4: Logarithm of gas-to-IL partition coefficients, log K, and logarithm of water-to-IL partition coefficients, log P, for solutes dissolved in anhydrous $[N_{112}O_2N_{114}]^+[Tf_2N]^-$ at 298.15 K

Solute	E	S	A	B	L	V	log *K*	log *P*
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	0.572	2.392
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	0.665	2.505
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	0.930	2.890
Octane	0.000	0.000	0.000	0.000	3.677	1.236	1.522	3.632
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	1.881	4.031
Decane	0.000	0.000	0.000	0.000	4.686	1.518	2.302	4.622
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	2.615	4.995
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	3.101	5.631
Tridecane	0.000	0.000	0.000	0.000	6.200	1.940	3.406	
Tetradecane	0.000	0.000	0.000	0.000	6.705	2.081	3.744	
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	1.136	2.306
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	1.270	2.170
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	1.516	2.766
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	1.805	2.385

Solute	E	S	A	B	L	V	log *K*	log *P*
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.578	1.948
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	2.925	2.275
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.181	2.601
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.246	2.636
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.212	2.622
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	3.416	2.756
1-Hexene	0.080	0.080	0.000	0.070	2.572	0.911	0.858	2.018
1-Hexyne	0.166	0.220	0.100	0.120	2.510	0.868	1.674	1.884
1-Heptyne	0.160	0.230	0.090	0.100	3.000	1.009	2.115	2.555
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.813	0.023
2-Butanone	0.166	0.700	0.000	0.510	2.287	0.688	3.070	0.350
2-Pentanone	0.143	0.680	0.000	0.510	2.755	0.829	3.307	0.727
3-Pentanone	0.154	0.660	0.000	0.510	2.811	0.829	3.295	0.795
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.694	0.144
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	3.370	-0.340
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.652	-1.088
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.825	-0.845
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.124	-0.436
2-Propanol	0.212	0.360	0.330	0.560	1.764	0.590	2.830	-0.650
2-Methyl-1-propanol	0.217	0.390	0.370	0.480	2.413	0.731	3.243	-0.057
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.454	-0.006
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.368	0.198
Diisopropyl ether	-0.063	0.170	0.000	0.570	2.501	1.013	1.367	0.317
Chloroform	0.425	0.490	0.150	0.020	2.480	0.617	2.234	1.444
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	1.999	1.039
Carbon tetrachloride	0.458	0.380	0.000	0.000	2.823	0.739	1.874	1.934
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	3.170	0.320
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.424	3.423	0.473
1-Nitropropane	0.242	0.950	0.000	0.310	2.894	0.706	3.786	1.336
Pyridine	0.631	0.840	0.000	0.520	3.022	0.675	3.963	0.523
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.724	1.684
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	2.815	0.655

Solute	E	S	A	B	L	V	log *K*	log *P*
Water	0.000	0.600	0.590	0.460	0.245	0.167	2.990	-1.700

APPENDIX C

SUPPLEMENTAL INFORMATION FOR CHAPTER 4

Experimental standard enthalpies of vaporization, $\Delta_{vap}H_m^0$ (in kJ mol^{-1}), of organic and organometallic and Abraham model compound descriptors used in developing the predictive $\Delta_{vap}H_m^0$ equations.

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
n-Butane	0.000	0.000	0.000	0.000	1.615	0.672	22.4
2-Methylpropane	0.000	0.000	0.000	0.000	1.409	0.672	21.6
n-Pentane	0.000	0.000	0.000	0.000	2.162	0.813	26.6
2-Methylbutane	0.000	0.000	0.000	0.000	2.013	0.813	25.0
2,2-Dimethylpropane	0.000	0.000	0.000	0.000	1.820	0.813	21.8
n-Hexane	0.000	0.000	0.000	0.000	2.668	0.954	31.6
2-Methylpentane	0.000	0.000	0.000	0.000	2.503	0.954	29.9
3-Methylpentane	0.000	0.000	0.000	0.000	2.581	0.954	30.3
2,2-Dimethylbutane	0.000	0.000	0.000	0.000	2.352	0.954	27.8
2,3-Dimethylbutane	0.000	0.000	0.000	0.000	2.495	0.954	29.2
n-Heptane	0.000	0.000	0.000	0.000	3.173	1.095	36.6
2-Methylhexane	0.000	0.000	0.000	0.000	3.001	1.095	34.9
3-Methylhexane	0.000	0.000	0.000	0.000	3.044	1.095	35.1
2,2-Dimethylpentane	0.000	0.000	0.000	0.000	2.796	1.095	32.4
2,3-Dimethylpentane	0.000	0.000	0.000	0.000	3.016	1.095	34.3
2,4-Dimethylpentane	0.000	0.000	0.000	0.000	2.809	1.095	32.7
3,3-Dimethylpentane	0.000	0.000	0.000	0.000	2.946	1.095	33.0
2,2,3-Trimethylbutane	0.000	0.000	0.000	0.000	2.918	1.095	32.0
n-Octane	0.000	0.000	0.000	0.000	3.677	1.236	41.0
2-Methylheptane	0.000	0.000	0.000	0.000	3.480	1.236	39.7
3-Methylheptane	0.000	0.000	0.000	0.000	3.510	1.236	39.8
4-Methylheptane	0.000	0.000	0.000	0.000	3.483	1.236	39.7
2,2-Dimethylhexane	0.000	0.000	0.000	0.000	3.261	1.236	37.3
2,3-Dimethylhexane	0.000	0.000	0.000	0.000	3.451	1.236	38.8
2,4-Dimethylhexane	0.000	0.000	0.000	0.000	3.319	1.236	37.8
2,5-Dimethylhexane	0.000	0.000	0.000	0.000	3.308	1.236	37.9
3,3-Dimethylhexane	0.000	0.000	0.000	0.000	3.359	1.236	37.5
3,4-Dimethylhexane	0.000	0.000	0.000	0.000	3.559	1.236	39.0
3-Ethylhexane	0.000	0.000	0.000	0.000	3.519	1.236	39.6

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
2-Methyl-3-ethylpentane	0.000	0.000	0.000	0.000	3.459	1.236	38.5
3-Methyl-3-ethylpentane	0.000	0.000	0.000	0.000	3.502	1.236	38.0
2,2,3-Trimethylpentane	0.000	0.000	0.000	0.000	3.325	1.236	37.7
2,2,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.106	1.236	35.1
2,3,4-Trimethylpentane	0.000	0.000	0.000	0.000	3.481	1.236	37.7
2,2,3,3-Tetramethylbutane	0.000	0.000	0.000	0.000	3.265	1.236	42.9
n-Nonane	0.000	0.000	0.000	0.000	4.182	1.377	46.5
2-Methyloctane	0.000	0.000	0.000	0.000	3.966	1.377	44.9
3-Methyloctane	0.000	0.000	0.000	0.000	3.998	1.377	44.9
4-Methyloctane	0.000	0.000	0.000	0.000	3.961	1.377	44.5
3-Ethylheptane	0.000	0.000	0.000	0.000	3.992	1.377	44.5
4-Ethylheptane	0.000	0.000	0.000	0.000	3.944	1.377	44.1
2,2-Dimethylheptane	0.000	0.000	0.000	0.000	3.739	1.377	42.3
2,3-Dimethylheptane	0.000	0.000	0.000	0.000	3.925	1.377	43.6
2,4-Dimethylheptane	0.000	0.000	0.000	0.000	3.758	1.377	42.9
2,5-Dimethylheptane	0.000	0.000	0.000	0.000	3.822	1.377	43.3
2,6-Dimethylheptane	0.000	0.000	0.000	0.000	3.780	1.377	43.3
3,3-Dimethylheptane	0.000	0.000	0.000	0.000	3.833	1.377	42.6
3,4-Dimethylheptane	0.000	0.000	0.000	0.000	3.935	1.377	43.6
3,5-Dimethylheptane	0.000	0.000	0.000	0.000	3.826	1.377	43.3
4,4-Dimethylheptane	0.000	0.000	0.000	0.000	3.770	1.377	42.2
2-Methyl-3-ethylhexane	0.000	0.000	0.000	0.000	3.850	1.377	43.2
2-Methyl-4-ethylhexane	0.000	0.000	0.000	0.000	3.760	1.377	42.9
3-Methyl-3-ethylhexane	0.000	0.000	0.000	0.000	3.890	1.377	42.9
3-Methyl-4-ethylhexane	0.000	0.000	0.000	0.000	3.900	1.377	43.6
2,2,3-Trimethylhexane	0.000	0.000	0.000	0.000	3.762	1.377	41.7
2,2,4-Trimethylhexane	0.000	0.000	0.000	0.000	3.605	1.377	40.7
2,2,5-Trimethylhexane	0.000	0.000	0.000	0.000	3.567	1.377	40.2
2,2,3,3-Tetramethylpentane	0.000	0.000	0.000	0.000	3.880	1.377	41.2
2,2,3,4-Tetramethylpentane	0.000	0.000	0.000	0.000	3.738	1.377	40.8
2,2,4,4-Tetramethylpentane	0.000	0.000	0.000	0.000	3.512	1.377	38.5
2,3,3,4-Tetramethylpentane	0.000	0.000	0.000	0.000	3.910	1.377	41.8

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
3,3-Diethylpentane	0.000	0.000	0.000	0.000	4.013	1.377	43.6
n-Decane	0.000	0.000	0.000	0.000	4.686	1.518	51.4
2-Methylnonane	0.000	0.000	0.000	0.000	4.453	1.518	51.0
3-Methylnonane	0.000	0.000	0.000	0.000	4.486	1.518	50.2
4-Methylnonane	0.000	0.000	0.000	0.000	4.441	1.518	49.5
5-Methylnonane	0.000	0.000	0.000	0.000	4.432	1.518	49.8
2,2-Dimethyloctane	0.000	0.000	0.000	0.000	4.225	1.518	49.0
2,3-Dimethyloctane	0.000	0.000	0.000	0.000	4.401	1.518	48.1
2,6-Dimethyloctane	0.000	0.000	0.000	0.000	4.304	1.518	49.3
2,7-Dimethyloctane	0.000	0.000	0.000	0.000	4.282	1.518	47.7
3,3-Dimethyloctane	0.000	0.000	0.000	0.000	4.307	1.518	48.5
3,4-Dimethyloctane	0.000	0.000	0.000	0.000	4.324	1.518	48.1
3,5-Dimethyloctane	0.000	0.000	0.000	0.000	4.259	1.518	48.5
3,6-Dimethyloctane	0.000	0.000	0.000	0.000	4.331	1.518	47.3
4,4-Dimethyloctane	0.000	0.000	0.000	0.000	4.236	1.518	48.1
3-Ethyloctane	0.000	0.000	0.000	0.000	4.467	1.518	49.0
4-Ethyloctane	0.000	0.000	0.000	0.000	4.409	1.518	48.1
3-Ethyl-2-methylheptane	0.000	0.000	0.000	0.000	4.337	1.518	48.1
3-Methyl-3-ethylheptane	0.000	0.000	0.000	0.000	4.368	1.518	47.7
3,4,5-Trimethylheptane	0.000	0.000	0.000	0.000	4.361	1.518	47.3
Undecane	0.000	0.000	0.000	0.000	5.191	1.659	56.4
Dodecane	0.000	0.000	0.000	0.000	5.696	1.799	60.4
Tridecane	0.000	0.000	0.000	0.000	6.200	1.940	66.5
Tetradecane	0.000	0.000	0.000	0.000	6.705	2.081	71.8
Pentadecane	0.000	0.000	0.000	0.000	7.209	2.222	75.4
Hexadecane	0.000	0.000	0.000	0.000	7.714	2.363	81.4
Heptadecane	0.000	0.000	0.000	0.000	8.218	2.504	86.0
Octadecane	0.000	0.000	0.000	0.000	8.722	2.645	90.8
Nonadecane	0.000	0.000	0.000	0.000	9.226	2.786	95.8
Cyclopropane	0.410	0.230	0.000	0.000	1.314	0.423	17.0
Cyclopentane	0.260	0.100	0.000	0.000	2.477	0.705	28.5
Methylcyclopentane	0.225	0.100	0.000	0.000	2.907	0.845	31.6

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Ethylcyclopentane	0.227	0.100	0.000	0.000	3.324	0.986	36.5
Propylcyclopentane	0.225	0.100	0.000	0.000	3.803	1.127	41.1
Pentylcyclopentane	0.220	0.080	0.000	0.000	4.600	1.409	51.0
1,1-Dimethylcyclopentane	0.205	0.100	0.000	0.000	3.029	0.986	33.8
cis-1,2-Dimethylcyclopentane	0.247	0.100	0.000	0.000	3.273	0.986	35.8
trans-1,2-Dimethylcyclopentane	0.193	0.100	0.000	0.000	3.099	0.986	34.6
cis-1,3-Dimethylcyclopentane	0.169	0.100	0.000	0.000	3.065	0.986	34.3
trans-1,3-Dimethylcyclopentane	0.156	0.100	0.000	0.000	3.075	0.986	34.5
Cyclohexane	0.310	0.100	0.000	0.000	2.964	0.845	33.0
Methylcyclohexane	0.244	0.060	0.000	0.000	3.319	0.986	35.4
1,1-Dimethylcyclohexane	0.239	0.100	0.000	0.000	3.582	1.127	38.8
cis-1,2-Dimethylcyclohexane	0.281	0.240	0.000	0.000	3.847	1.127	39.7
trans-1,2-Dimethylcyclohexane	0.227	0.200	0.000	0.000	3.728	1.127	38.4
cis-1,3-Dimethylcyclohexane	0.203	0.140	0.000	0.000	3.525	1.127	38.2
trans-1,3-Dimethylcyclohexane	0.190	0.190	0.000	0.000	3.643	1.127	39.2
cis-1,4-Dimethylcyclohexane	0.204	0.200	0.000	0.000	3.736	1.127	39.0
trans-1,4-Dimethylcyclohexane	0.191	0.170	0.000	0.000	3.639	1.127	39.9
Ethylcyclohexane	0.263	0.100	0.000	0.000	3.877	1.127	40.5
Propylcyclohexane	0.257	0.230	0.000	0.000	4.313	1.268	45.2
Butylcyclohexane	0.255	0.230	0.000	0.000	4.806	1.409	50.0
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	38.5
Cyclooctane	0.409	0.100	0.000	0.000	4.329	1.127	43.3
Cyclododecane	0.559	0.100	0.000	0.000	6.190	1.691	63.0
But-1-ene	0.100	0.080	0.000	0.070	1.529	0.629	20.1
2-Methylprop-1-ene	0.120	0.080	0.000	0.080	1.579	0.629	20.6
Pent-1-ene	0.093	0.080	0.000	0.070	2.047	0.770	25.5
cis-Pent-2-ene	0.141	0.080	0.000	0.070	2.217	0.770	26.8
trans-Pent-2-ene	0.126	0.080	0.000	0.070	2.187	0.770	26.7
3-Methylbut-1-ene	0.063	0.060	0.000	0.050	1.933	0.770	23.9
2-Methylbut-2-ene	0.159	0.090	0.000	0.080	2.229	0.770	27.1
Hex-1-ene	0.080	0.080	0.000	0.070	2.572	0.911	30.6
cis-Hex-2-ene	0.143	0.080	0.000	0.070	2.684	0.911	31.5

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
trans-Hex-2-ene	0.122	0.080	0.000	0.060	2.655	0.911	31.6
cis-Hex-3-ene	0.128	0.080	0.000	0.070	2.664	0.911	31.3
trans-Hex-3-ene	0.126	0.080	0.000	0.060	2.659	0.911	31.6
2-Methylpent-1-ene	0.090	0.080	0.000	0.080	2.591	0.911	30.5
3-Methylpent-1-ene	0.076	0.080	0.000	0.060	2.425	0.911	28.6
4-Methylpent-1-ene	0.070	0.080	0.000	0.040	2.418	0.911	28.6
2-Methylpent-2-ene	0.156	0.080	0.000	0.070	2.687	0.911	31.6
cis-3-Methylpent-2-ene	0.176	0.080	0.000	0.080	2.706	0.911	31.3
trans-3-Methylpent-2-ene	0.162	0.080	0.000	0.080	2.760	0.911	32.1
cis-4-Methylpent-2-ene	0.095	0.080	0.000	0.080	2.444	0.911	29.5
trans-4-Methylpent-2-ene	0.100	0.080	0.000	0.080	2.465	0.911	30.0
2-Ethylbut-1-ene	0.139	0.080	0.000	0.080	2.624	0.911	31.0
2,3-Dimethylbut-1-ene	0.152	0.070	0.000	0.130	2.455	0.911	29.2
2,3-Dimethylbut-2-ene	0.213	0.090	0.000	0.130	2.797	0.911	32.5
3,3-Dimethylbut-1-ene	0.037	0.040	0.000	0.130	2.201	0.911	26.6
Hept-1-ene	0.092	0.080	0.000	0.070	3.063	1.052	37.7
cis-Hept-2-ene	0.136	0.080	0.000	0.070	3.210	1.052	38.6
trans-Hept-2-ene	0.119	0.080	0.000	0.070	3.180	1.052	36.0
cis-Hept-3-ene	0.130	0.080	0.000	0.070	3.143	1.052	35.6
trans-Hept-3-ene	0.121	0.080	0.000	0.070	3.125	1.052	35.6
2-Methylhex-1-ene	0.040	0.100	0.000	0.080	3.044	1.052	35.1
3-Methylhex-1-ene	0.085	0.070	0.000	0.070	2.897	1.052	34.3
4-Methylhex-1-ene	0.097	0.070	0.000	0.080	2.968	1.052	34.7
5-Methylhex-1-ene	0.080	0.080	0.000	0.070	2.919	1.052	34.3
2-Methylhex-2-ene	0.137	0.100	0.000	0.090	3.133	1.052	35.6
cis-3-Methylhex-2-ene	0.137	0.100	0.000	0.090	3.138	1.052	35.6
cis-4-Methylhex-2-ene	0.137	0.080	0.000	0.070	2.954	1.052	34.7
trans-4-Methylhex-2-ene	0.137	0.070	0.000	0.080	2.984	1.052	34.7
cis-3-Methylhex-3-ene	0.137	0.070	0.000	0.070	2.913	1.052	36.4
2,3-Dimethylpent-1-ene	0.115	0.090	0.000	0.110	2.930	1.052	34.3
2,4-Dimethylpent-1-ene	0.089	0.080	0.000	0.110	2.930	1.052	33.1
3,3-Dimethylpent-1-ene	0.088	0.060	0.000	0.100	2.792	1.052	33.5

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
3,4-Dimethylpent-1-ene	0.094	0.080	0.000	0.110	2.852	1.052	33.9
4,4-Dimethylpent-1-ene	0.049	0.070	0.000	0.110	2.685	1.052	31.2
2,3-Dimethylpent-2-ene	0.140	0.100	0.000	0.120	3.195	1.052	35.6
cis-3,4-Dimethylpent-2-ene	0.158	0.100	0.000	0.120	3.029	1.052	34.7
trans-3,4-Dimethylpent-2-ene	0.158	0.100	0.000	0.120	3.069	1.052	35.1
cis-4,4-Dimethylpent-2-ene	0.085	0.080	0.000	0.120	2.849	1.052	32.6
trans-4,4-Dimethypent-2-ene	0.085	0.070	0.000	0.120	2.737	1.052	32.8
2,3,3-Trimethylbut-1-ene	0.113	0.090	0.000	0.150	2.815	1.052	34.3
2-Ethylpent-1-ene	0.125	0.070	0.000	0.090	3.105	1.052	35.1
3-Ethylpent-1-ene	0.085	0.080	0.000	0.080	2.901	1.052	34.3
3-Ethylpent-2-ene	0.125	0.090	0.000	0.080	3.165	1.052	35.6
Oct-1-ene	0.090	0.080	0.000	0.070	3.568	1.193	40.3
cis-Oct-2-ene	0.135	0.080	0.000	0.070	3.683	1.193	40.2
trans-Oct-2-ene	0.123	0.070	0.000	0.070	3.668	1.193	40.2
cis-Oct-3-ene	0.125	0.060	0.000	0.070	3.663	1.193	39.7
trans-Oct-3-ene	0.119	0.060	0.000	0.060	3.647	1.193	40.2
cis-Oct-4-ene	0.133	0.080	0.000	0.070	3.607	1.193	39.7
trans-Oct-4-ene	0.114	0.080	0.000	0.070	3.593	1.193	42.9
2-Ethylhex-1-ene	0.139	0.080	0.000	0.070	3.510	1.193	39.7
2,4,4-Trimethylpent-1-ene	0.090	0.070	0.000	0.070	3.289	1.193	35.7
2,4,4-Trimethylpent-2-ene	0.141	0.080	0.000	0.070	3.249	1.193	39.3
2,3-Dimethylhex-1-ene	0.110	0.080	0.000	0.120	3.373	1.193	38.5
2,3-Dimethylhex-2-ene	0.140	0.110	0.000	0.120	3.629	1.193	39.7
2,5-Dimethylhex-2-ene	0.125	0.100	0.000	0.120	3.431	1.193	38.9
cis-2,3-Dimethylhex-3-ene	0.130	0.100	0.000	0.120	3.269	1.193	38.9
Non-1-ene	0.090	0.080	0.000	0.070	4.073	1.334	44.5
Dec-1-ene	0.093	0.080	0.000	0.070	4.533	1.475	50.5
Undec-1-ene	0.091	0.080	0.000	0.070	5.023	1.616	54.3
Dodec-1-ene	0.089	0.080	0.000	0.070	5.515	1.756	60.8
Tridec-1-ene	0.093	0.060	0.000	0.070	6.046	1.897	65.3
Tetradec-1-ene	0.090	0.060	0.000	0.070	6.536	2.038	70.2
Pentadec-1-ene	0.083	0.060	0.000	0.070	7.008	2.179	75.1

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Hexadec-1-ene	0.081	0.080	0.000	0.070	7.586	2.320	80.3
Octadec-1-ene	0.079	0.080	0.000	0.070	8.476	2.602	90.0
Buta-1,3-diene	0.320	0.230	0.000	0.100	1.543	0.586	21.1
2-Methylbuta-1,3-diene	0.313	0.230	0.000	0.100	2.101	0.727	26.4
Penta-1,2-diene	0.310	0.230	0.000	0.110	2.273	0.727	28.7
cis-Penta-1,3-diene	0.345	0.230	0.000	0.100	2.256	0.727	28.3
trans-Penta-1,3-diene	0.345	0.230	0.000	0.100	2.296	0.727	27.8
Penta-1,4-diene	0.185	0.140	0.000	0.100	1.998	0.727	25.2
Cyclohexene	0.395	0.280	0.000	0.090	2.952	0.802	33.5
1-Methyl-1-cyclohexene	0.391	0.180	0.000	0.100	3.483	0.943	37.5
Cyclohepta-1,3,5-triene	0.764	0.460	0.000	0.200	3.442	0.857	38.7
But-1-yne	0.178	0.250	0.120	0.100	1.520	0.586	23.7
But-2-yne	0.261	0.230	0.000	0.210	1.856	0.586	26.7
Pent-1-yne	0.172	0.230	0.120	0.120	2.010	0.727	28.4
Hex-1-yne	0.166	0.220	0.100	0.120	2.510	0.868	33.6
Hex-2-yne	0.236	0.300	0.000	0.150	2.765	0.868	35.9
Hex-3-yne	0.224	0.300	0.000	0.150	2.659	0.868	36.0
Oct-1-yne	0.155	0.220	0.090	0.100	3.521	1.150	42.3
Oct-2-yne	0.225	0.300	0.000	0.150	3.850	1.150	44.5
Oct-4-yne	0.208	0.300	0.000	0.150	3.609	1.150	42.7
Fluorocyclohexane	0.241	0.420	0.000	0.090	3.215	0.863	37.5
Chloromethane	0.250	0.430	0.000	0.080	1.163	0.372	20.0
Dichloromethane	0.390	0.570	0.100	0.050	2.019	0.494	28.8
Trichloromethane	0.430	0.490	0.150	0.020	2.480	0.617	31.1
Tetrachloromethane	0.460	0.380	0.000	0.000	2.823	0.739	32.4
1,1-Dichloroethane	0.320	0.490	0.100	0.100	2.316	0.635	30.6
1,2-Dichloroethane	0.420	0.640	0.100	0.110	2.573	0.635	35.1
1,1,1-Trichloroethane	0.370	0.410	0.000	0.090	2.733	0.758	32.5
1,1,2-Trichloroethane	0.500	0.680	0.130	0.130	3.290	0.758	40.3
1,1,2,2-Tetrachloroethane	0.600	0.760	0.160	0.120	3.803	0.880	45.8
1,1,1,2-Tetrachloroethane	0.540	0.630	0.100	0.080	3.641	0.880	41.1
1-Chloropropane	0.216	0.400	0.000	0.100	2.202	0.654	28.5

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
2-Chloropropane	0.177	0.350	0.000	0.120	1.970	0.654	27.6
1,2-Dichloropropane	0.370	0.630	0.000	0.170	2.836	0.776	36.2
1,3-Dichloropropane	0.408	0.800	0.050	0.120	3.106	0.776	40.6
1,2,3-Trichloropropane	0.547	0.650	0.030	0.310	3.582	0.899	47.8
1-Chlorobutane	0.210	0.400	0.000	0.100	2.722	0.795	33.5
2-Chlorobutane	0.189	0.350	0.000	0.120	2.540	0.795	31.5
2-Chloro-2-methylpropane	0.142	0.300	0.000	0.030	2.273	0.795	29.0
1-Chloropentane	0.210	0.380	0.000	0.090	3.223	0.936	38.2
1-Chlorohexane	0.201	0.390	0.000	0.090	3.708	1.076	42.8
1-Chloroheptane	0.194	0.400	0.000	0.090	4.208	1.217	47.7
1-Chlorooctane	0.191	0.400	0.000	0.090	4.708	1.358	52.4
1-Chlorononane	0.188	0.400	0.000	0.090	5.208	1.499	55.9
1-Chlorodecane	0.185	0.400	0.000	0.090	5.717	1.640	64.0
1-Chloroundecane	0.183	0.400	0.000	0.090	6.208	1.781	70.2
1-Chlorododecane	0.181	0.400	0.000	0.100	6.708	1.922	71.9
1-Chlorotridecane	0.179	0.400	0.000	0.100	7.236	2.063	81.3
1-Chlorotetradecane	0.176	0.410	0.000	0.100	7.724	2.204	86.6
1-Chloropentadecane	0.175	0.420	0.000	0.100	8.247	2.345	92.6
1-Chlorohexadecane	0.173	0.420	0.000	0.100	8.785	2.485	91.6
1-Chloroheptadecane	0.172	0.430	0.000	0.100	9.257	2.626	103.6
1-Chlorooctadecane	0.170	0.430	0.000	0.100	9.791	2.767	108.8
Chlorocyclohexane	0.448	0.480	0.000	0.100	3.832	0.968	42.9
1,4-Dichlorobutane	0.413	0.950	0.000	0.170	3.501	0.917	46.4
1,5-Dichloropentane	0.421	0.960	0.000	0.170	4.251	1.058	50.7
1,6-Dichlorohexane	0.397	0.960	0.000	0.170	4.723	1.199	56.3
1,8-Dichlorooctane	0.380	0.950	0.000	0.180	5.720	1.481	65.6
Trichloroethene	0.520	0.370	0.080	0.030	2.997	0.715	34.5
Tetrachloroethene	0.640	0.440	0.000	0.000	3.584	0.837	39.7
Allyl chloride	0.327	0.560	0.000	0.050	2.109	0.611	29.9
Dibromomethane	0.710	0.690	0.110	0.070	2.886	0.600	37.0
Tribromomethane	0.970	0.680	0.150	0.060	3.784	0.775	46.1
1,2-Dibromoethane	0.747	0.760	0.100	0.170	3.382	0.740	41.7

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
1-Bromopropane	0.366	0.400	0.000	0.120	2.620	0.706	31.9
2-Bromopropane	0.332	0.350	0.000	0.140	2.390	0.706	30.2
1,2-Dibromopropane	0.747	0.760	0.100	0.170	3.382	0.881	42.2
1,3-Dibromopropane	0.723	0.800	0.000	0.270	3.872	0.881	47.6
1-Bromobutane	0.360	0.400	0.000	0.120	3.105	0.847	36.6
1-Bromo-2-methylpropane	0.337	0.370	0.000	0.120	2.960	0.847	34.9
2-Bromo-2-methylpropane	0.305	0.290	0.000	0.070	2.609	0.847	31.8
1-Bromopentane	0.356	0.400	0.000	0.120	3.611	0.988	41.4
1-Bromohexane	0.349	0.400	0.000	0.120	4.130	1.129	46.1
1-Bromoheptane	0.343	0.400	0.000	0.120	4.663	1.270	50.8
1-Bromooctane	0.339	0.400	0.000	0.120	5.143	1.411	55.8
Bromocyclohexane	0.615	0.540	0.000	0.160	4.395	1.020	45.3
1,4-Dibromobutane	0.733	0.800	0.000	0.270	4.353	1.022	52.6
Iodomethane	0.676	0.430	0.000	0.120	2.106	0.508	27.2
1-Iodopropane	0.634	0.400	0.000	0.140	3.130	0.790	36.3
2-Iodopropane	0.622	0.350	0.000	0.170	2.900	0.790	34.1
1-Iodobutane	0.628	0.400	0.000	0.140	3.628	0.930	40.6
2-Iodobutane	0.610	0.350	0.000	0.170	3.390	0.930	38.8
2-Iodo-2-methylpropane	0.589	0.350	0.000	0.190	3.439	0.930	37.0
1-Iodopentane	0.621	0.400	0.000	0.140	4.130	1.071	45.3
1-Iodo-3-methylbutane	0.610	0.370	0.000	0.190	3.980	1.071	42.2
1-Iodohexane	0.615	0.400	0.000	0.140	4.620	1.212	49.8
1-Iodoheptane	0.608	0.400	0.000	0.140	5.100	1.353	55.0
1-Iodooctane	0.606	0.400	0.000	0.150	5.727	1.494	59.7
1-Iodononane	0.598	0.400	0.000	0.150	6.269	1.635	64.5
1-Iododecane	0.593	0.400	0.000	0.150	6.971	1.776	69.8
Iodocyclohexane	0.904	0.600	0.000	0.120	4.785	1.104	49.6
Dimethyl ether	0.000	0.270	0.000	0.410	1.285	0.449	18.5
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	27.1
Di-n-propyl ether	0.008	0.250	0.000	0.450	2.954	1.013	35.7
Di-isopropyl ether	-0.060	0.160	0.000	0.580	2.530	1.013	32.1
Di-n-butyl ether	0.000	0.250	0.000	0.450	3.924	1.295	45.0

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Di-isobutyl ether	0.000	0.190	0.000	0.450	3.485	1.295	41.2
Methyl propyl ether	0.060	0.250	0.000	0.430	2.090	0.731	27.6
Methyl isopropyl ether	0.059	0.220	0.000	0.540	1.800	0.731	26.4
Methyl butyl ether	0.045	0.250	0.000	0.440	2.658	0.872	32.4
Methyl tert-butyl ether	0.024	0.220	0.000	0.590	2.380	0.872	29.8
Methyl tert-pentyl ether	0.050	0.210	0.000	0.600	2.916	1.013	35.5
Ethyl propyl ether	0.000	0.250	0.000	0.450	2.493	0.872	31.4
Ethyl isopropyl ether	0.037	0.220	0.000	0.550	2.240	0.872	30.0
Ethyl butyl ether	0.013	0.250	0.000	0.450	2.989	1.013	36.3
Ethyl tert-butyl ether	-0.020	0.180	0.000	0.590	2.699	1.013	33.1
Ethyl tert-pentyl ether	-0.100	0.190	0.000	0.600	3.074	1.154	38.2
Dimethoxymethane	0.099	0.460	0.000	0.520	1.894	0.649	28.9
Diethoxymethane	0.010	0.490	0.000	0.540	2.789	0.931	35.7
1,2-Dimethoxyethane	0.116	0.670	0.000	0.680	2.654	0.790	36.8
Ethylene oxide	0.250	0.740	0.070	0.320	1.371	0.341	25.9
1,2-Propylene oxide	0.243	0.740	0.070	0.350	1.775	0.481	27.9
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	32.0
2-Methyltetrahydrofuran	0.241	0.480	0.000	0.530	2.820	0.763	33.7
2,5-Dimethyltetrahydrofuran	0.204	0.380	0.000	0.580	2.980	0.904	35.4
Tetrahydropyran	0.296	0.490	0.000	0.480	3.013	0.763	38.2
1,4-Dioxane	0.329	0.750	0.000	0.640	2.892	0.681	38.6
12-Crown-4	0.420	0.990	0.000	1.390	5.287	1.362	65.6
15-Crown-5	0.411	1.200	0.000	1.750	6.779	1.703	79.6
18-Crown-6	0.400	1.470	0.000	2.100	8.228	2.043	98.2
Benzo-15-crown-5	1.055	1.940	0.000	1.590	9.403	2.029	98.9
Propanal	0.196	0.650	0.000	0.450	1.815	0.547	29.7
Butanal	0.187	0.650	0.000	0.450	2.270	0.688	33.7
Isobutanal	0.144	0.620	0.000	0.450	2.120	0.688	32.3
Pentanal	0.163	0.650	0.000	0.450	2.851	0.829	38.6
Hexanal	0.146	0.650	0.000	0.450	3.357	0.970	42.5
Heptanal	0.140	0.650	0.000	0.450	3.865	1.111	48.0
Octanal	0.160	0.650	0.000	0.450	4.361	1.252	51.0

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Nonanal	0.150	0.650	0.000	0.450	4.834	1.392	55.3
Decanal	0.128	0.650	0.000	0.450	5.369	1.533	60.5
Undecanal	0.122	0.650	0.000	0.450	5.902	1.674	64.6
Dodecanal	0.116	0.650	0.000	0.450	6.419	1.815	70.2
Tridecanal	0.110	0.650	0.000	0.450	6.930	1.956	73.3
Tetradecanal	0.104	0.650	0.000	0.450	7.265	2.097	80.2
Hexadecanal	0.095	0.650	0.000	0.450	8.340	2.379	89.7
Propanone	0.179	0.700	0.040	0.490	1.696	0.547	30.5
Butanone	0.166	0.700	0.000	0.510	2.287	0.688	34.8
Pentan-2-one	0.143	0.680	0.000	0.510	2.755	0.829	38.5
Pentan-3-one	0.154	0.660	0.000	0.510	2.811	0.829	38.6
3-Methylbutan-2-one	0.134	0.650	0.000	0.510	2.692	0.829	36.8
Hexan-2-one	0.136	0.680	0.000	0.510	3.286	0.970	43.1
Hexan-3-one	0.136	0.660	0.000	0.510	3.271	0.970	41.9
4-Methylpentan-2-one	0.111	0.650	0.000	0.510	3.089	0.970	42.5
3-Methylpentan-2-one	0.110	0.650	0.000	0.510	3.163	0.970	41.5
2-Methylpentan-3-one	0.117	0.630	0.000	0.510	3.011	0.970	39.8
3,3-Dimethylbutan-2-one	0.106	0.620	0.000	0.510	2.928	0.970	40.4
Heptan-2-one	0.123	0.680	0.000	0.510	3.760	1.111	46.1
Heptan-4-one	0.113	0.640	0.000	0.510	3.705	1.111	46.7
2,4-Dimethylpentan-3-one	0.072	0.600	0.000	0.510	3.403	1.111	43.4
Octan-2-one	0.108	0.680	0.000	0.510	4.257	1.252	52.6
Nonan-2-one	0.113	0.680	0.000	0.510	4.735	1.392	56.4
Nonan-5-one	0.103	0.660	0.000	0.510	4.698	1.392	53.3
2,6-Dimethylheptan-4-one	0.051	0.600	0.000	0.510	4.244	1.392	50.9
Decan-2-one	0.108	0.680	0.000	0.510	5.245	1.533	60.9
Undecan-2-one	0.101	0.680	0.000	0.510	5.732	1.674	67.0
Dodecan-2-one	0.103	0.680	0.000	0.510	6.184	1.815	71.8
Cyclopentanone	0.373	0.860	0.000	0.520	3.221	0.720	42.7
Cyclohexanone	0.403	0.860	0.000	0.560	3.792	0.861	45.1
Methyl formate	0.192	0.680	0.000	0.380	1.285	0.465	28.5
Ethyl formate	0.146	0.660	0.000	0.380	1.845	0.606	31.5

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Propyl formate	0.132	0.630	0.000	0.380	2.433	0.747	32.5
Butyl formate	0.121	0.630	0.000	0.380	2.958	0.888	41.3
Pentyl formate	0.101	0.630	0.000	0.380	3.488	1.028	45.2
Hexyl formate	0.090	0.630	0.000	0.380	3.970	1.169	50.0
Methyl acetate	0.142	0.640	0.000	0.450	1.911	0.606	32.2
Ethyl acetate	0.106	0.620	0.000	0.450	2.314	0.747	35.1
Propyl acetate	0.092	0.600	0.000	0.450	2.819	0.888	39.8
Isopropyl acetate	0.055	0.570	0.000	0.470	2.546	0.888	37.2
Butyl acetate	0.071	0.600	0.000	0.450	3.353	1.028	43.6
s-Butylacetate	0.044	0.570	0.000	0.470	3.054	1.028	40.7
tert-Butyl acetate	0.025	0.540	0.000	0.470	2.802	1.028	38.0
Pentyl acetate	0.067	0.600	0.000	0.450	3.844	1.169	48.0
Isoamyl acetate	0.051	0.570	0.000	0.470	3.740	1.169	46.4
Hexyl acetate	0.056	0.600	0.000	0.450	4.290	1.310	51.9
Heptyl acetate	0.050	0.600	0.000	0.450	4.796	1.451	57.1
Octyl acetate	0.046	0.600	0.000	0.450	5.270	1.592	61.7
Nonyl acetate	0.043	0.600	0.000	0.450	5.768	1.733	66.8
Decyl acetate	0.041	0.600	0.000	0.450	6.240	1.874	71.6
Undecyl acetate	0.039	0.600	0.000	0.450	6.730	2.015	75.1
Dodecyl acetate	0.038	0.600	0.000	0.450	7.219	2.156	81.8
Tridecyl acetate	0.036	0.600	0.000	0.450	7.706	2.297	87.2
Tetradecyl acetate	0.034	0.600	0.000	0.450	8.192	2.437	89.9
Methyl propanoate	0.128	0.600	0.000	0.450	2.431	0.747	36.0
Ethyl propanoate	0.087	0.580	0.000	0.450	2.807	0.888	39.3
Propyl propanoate	0.070	0.560	0.000	0.450	3.338	1.028	43.2
Butyl propanoate	0.058	0.560	0.000	0.470	3.833	1.169	48.5
Pentyl propanoate	0.050	0.560	0.000	0.450	4.331	1.310	52.2
Hexyl propanoate	0.074	0.560	0.000	0.450	4.796	1.451	57.1
Methyl butanoate	0.106	0.600	0.000	0.450	2.893	0.888	40.1
Ethyl butanoate	0.068	0.580	0.000	0.450	3.271	1.028	42.7
Methyl pentanoate	0.108	0.600	0.000	0.450	3.392	1.028	43.1
Ethyl pentanoate	0.049	0.580	0.000	0.450	3.769	1.169	47.0

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Methyl hexanoate	0.080	0.600	0.000	0.450	3.874	1.169	48.0
Ethyl hexanoate	0.043	0.580	0.000	0.450	4.251	1.310	51.7
Methyl heptanoate	0.079	0.600	0.000	0.450	4.356	1.310	53.2
Methyl octanoate	0.065	0.600	0.000	0.450	4.838	1.451	56.9
Ethyl octanoate	0.024	0.580	0.000	0.450	5.215	1.592	62.0
Ethyl decanoate	0.013	0.580	0.000	0.450	6.180	1.874	70.5
Methyl dodecanoate	0.037	0.600	0.000	0.450	6.767	2.015	76.5
Ethyl dodecanoate	0.002	0.580	0.000	0.450	7.144	2.156	80.0
Methyl tridecanoate	0.042	0.640	0.000	0.450	7.271	2.156	82.7
Ethyl 2-methylbutanoate	0.026	0.550	0.000	0.470	3.565	1.169	44.7
Methyl acrylate	0.254	0.660	0.000	0.420	2.360	0.704	35.8
Butyl acrylate	0.177	0.620	0.000	0.420	3.790	1.126	43.7
Diethyl succinate	0.108	1.000	0.000	0.840	4.940	1.385	65.1
Dibutyl succinate	0.040	0.950	0.000	0.840	6.856	1.948	79.1
Dimethyl adipate	0.169	1.190	0.000	0.920	5.239	1.385	69.0
Diethyl adipate	0.087	1.100	0.000	1.010	5.930	1.666	74.0
Dipropyl adipate	0.055	1.130	0.000	1.020	7.023	1.948	81.0
Dimethyl suberate	0.147	1.260	0.000	0.990	6.175	1.666	78.1
Dimethyl sebacate	0.130	1.270	0.000	0.990	7.257	1.948	86.4
Dimethyl azelate	0.139	1.270	0.000	0.990	6.775	1.807	82.3
Dimethyl carbonate	0.142	0.590	0.000	0.530	2.240	0.664	38.0
Diethyl carbonate	0.061	0.690	0.000	0.500	3.167	0.946	43.6
Acetonitrile	0.237	0.900	0.070	0.320	1.739	0.404	33.3
Propionitrile	0.162	0.900	0.020	0.360	2.082	0.545	36.0
Butyronitrile	0.188	0.900	0.000	0.360	2.548	0.686	39.3
2-Methylproprionitrile	0.142	0.870	0.000	0.400	2.465	0.686	39.2
Pentanenitrile	0.177	0.900	0.000	0.360	3.108	0.827	43.6
Hexanenitrile	0.166	0.900	0.000	0.360	3.608	0.968	47.9
Heptanenitrile	0.159	0.900	0.000	0.360	4.089	1.109	51.9
Octanenitrile	0.162	0.900	0.000	0.360	4.585	1.250	56.8
Nonanenitrile	0.159	0.900	0.000	0.360	4.970	1.391	62.0
Decanenitrile	0.156	0.900	0.000	0.360	5.460	1.532	66.8

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Undecanenitrile	0.154	0.900	0.000	0.360	5.940	1.673	71.8
Dodecanenitrile	0.132	0.900	0.000	0.360	6.460	1.813	76.1
n-Propylamine	0.225	0.350	0.160	0.610	2.141	0.631	31.3
n-Butylamine	0.224	0.350	0.160	0.610	2.618	0.772	35.7
n-Pentylamine	0.211	0.350	0.160	0.610	3.139	0.913	40.1
n-Hexylamine	0.197	0.350	0.160	0.610	3.655	1.054	45.1
n-Heptylamine	0.197	0.350	0.160	0.610	4.153	1.195	50.0
n-Octylamine	0.187	0.350	0.160	0.610	4.600	1.336	55.1
n-Decylamine	0.182	0.350	0.160	0.610	5.606	1.617	65.3
n-Dodecylamine	0.173	0.350	0.160	0.610	6.625	1.899	75.3
Cyclopentylamine	0.409	0.560	0.190	0.570	3.003	0.804	40.2
Cyclohexylamine	0.326	0.560	0.190	0.580	3.796	0.945	42.8
Diethylamine	0.154	0.300	0.080	0.690	2.395	0.772	31.3
Di-n-propylamine	0.124	0.300	0.080	0.690	3.351	1.054	40.0
Di-isopropylamine	0.053	0.210	0.070	0.740	2.893	1.054	34.6
Di-n-butylamine	0.107	0.300	0.080	0.690	4.349	1.336	49.4
Di-n-pentylamine	0.099	0.300	0.080	0.690	5.224	1.617	61.2
Methylisopropylamine	0.132	0.270	0.080	0.690	2.293	0.772	30.7
Methylbutylamine	0.151	0.300	0.060	0.650	3.038	0.913	38.1
Ethylbutylamine	0.124	0.320	0.080	0.650	3.269	1.054	40.2
Triethylamine	0.101	0.150	0.000	0.790	3.040	1.054	34.8
2-Methoxyethylamine	0.266	0.600	0.160	0.840	2.435	0.690	38.2
Nitromethane	0.313	0.950	0.060	0.310	1.892	0.424	38.3
Nitropropane	0.242	0.950	0.000	0.310	2.894	0.706	43.9
2-Nitropropane	0.216	0.920	0.000	0.330	2.550	0.706	43.4
Nitrobutane	0.227	0.950	0.000	0.290	3.415	0.846	48.1
Nitropentane	0.212	0.950	0.000	0.290	3.938	0.987	51.0
Formamide	0.468	1.310	0.640	0.570	2.447	0.365	69.1
N-Ethylformamide	0.371	1.300	0.400	0.560	3.189	0.647	58.4
N,N-Dimethylformamide	0.367	1.310	0.000	0.740	3.173	0.647	46.7
N,N-Diethylformamide	0.305	1.250	0.000	0.740	3.995	0.929	52.6
N,N-Dipropylformamide	0.285	1.160	0.000	0.750	4.975	1.210	60.1

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
N,N-Dibutylformamide	0.232	1.090	0.000	0.760	5.618	1.492	66.7
N,N-Diethylacetamide	0.315	1.300	0.000	0.780	4.490	1.070	54.4
Formic acid	0.343	0.750	0.760	0.330	1.545	0.324	46.3
Acetic acid	0.265	0.640	0.620	0.440	1.816	0.465	51.6
Propanoic acid	0.233	0.650	0.610	0.440	2.276	0.606	55.0
Butanoic acid	0.210	0.640	0.610	0.450	2.750	0.747	58.2
Pentanoic acid	0.205	0.630	0.620	0.450	3.227	0.888	65.9
3-Methylbutanoic acid	0.178	0.600	0.610	0.460	3.151	0.888	61.2
Hexanoic acid	0.174	0.630	0.620	0.440	3.697	1.028	69.2
Heptanoic acid	0.149	0.640	0.620	0.440	4.183	1.169	72.9
Octanoic acid	0.150	0.650	0.620	0.450	4.680	1.310	81.0
Acrylic acid	0.357	0.580	0.600	0.430	2.282	0.563	53.1
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	37.4
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	42.3
Propan-1-ol	0.236	0.420	0.370	0.480	2.031	0.590	47.5
Propan-2-ol	0.212	0.360	0.330	0.560	1.764	0.590	45.3
Butan-1-ol	0.224	0.420	0.370	0.480	2.601	0.731	52.1
2-Methylpropan-1-ol	0.217	0.390	0.370	0.480	2.413	0.731	50.8
Butan-2-ol	0.217	0.360	0.330	0.560	2.338	0.731	49.7
2-Methylpropan-2-ol	0.180	0.300	0.310	0.600	1.963	0.731	46.6
Pentan-1-ol	0.219	0.420	0.370	0.480	3.106	0.872	56.9
Pentan-2-ol	0.195	0.360	0.330	0.560	2.840	0.872	53.0
Pentan-3-ol	0.218	0.360	0.330	0.560	2.860	0.872	52.9
2-Methylbutan-1-ol	0.219	0.390	0.370	0.480	3.011	0.872	54.1
3-Methylbutan-1-ol	0.192	0.390	0.370	0.480	3.011	0.872	54.3
2-Methylbutan-2-ol	0.194	0.300	0.310	0.600	2.630	0.872	50.1
Hexan-1-ol	0.210	0.420	0.370	0.480	3.610	1.013	61.6
Hexan-2-ol	0.187	0.360	0.330	0.560	3.340	1.013	58.3
Hexan-3-ol	0.200	0.360	0.330	0.560	3.343	1.013	58.6
2-Methylpentan-1-ol	0.211	0.390	0.310	0.560	3.471	1.013	59.4
3-Methylpentan-1-ol	0.211	0.390	0.310	0.560	3.493	1.013	61.7
2-Methyl-pentan-2-ol	0.169	0.300	0.310	0.600	3.081	1.013	54.7

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
4-Methyl-pentan-2-ol	0.167	0.330	0.330	0.560	3.179	1.013	57.3
2-Methyl-pentan-3-ol	0.207	0.330	0.330	0.560	3.240	1.013	56.0
3-Methyl-pentan-3-ol	0.210	0.300	0.310	0.600	3.277	1.013	55.7
2,3-Dimethylbutan-2-ol	0.208	0.270	0.310	0.650	3.223	1.013	54.0
3,3-Dimethylbutan-2-ol	0.193	0.300	0.330	0.560	3.090	1.013	53.8
Heptan-1-ol	0.211	0.420	0.370	0.480	4.115	1.154	66.8
Heptan-2-ol	0.188	0.360	0.330	0.560	3.838	1.154	62.1
Heptan-4-ol	0.180	0.360	0.330	0.560	3.850	1.154	62.4
2-Methylhexan-2-ol	0.163	0.300	0.310	0.630	3.686	1.154	58.6
3-Ethylpentan-3-ol	0.234	0.300	0.310	0.640	3.838	1.154	57.3
Octan-1-ol	0.199	0.420	0.370	0.480	4.619	1.295	71.0
Octan-2-ol	0.158	0.360	0.330	0.560	4.339	1.295	67.9
Octan-3-ol	0.176	0.360	0.330	0.560	4.290	1.295	67.9
Octan-4-ol	0.160	0.360	0.330	0.560	4.300	1.295	67.9
Nonan-1-ol	0.193	0.420	0.370	0.480	5.120	1.435	76.9
Nonan-2-ol	0.168	0.360	0.330	0.560	4.817	1.435	72.9
2,6-Dimethylheptan-4-ol	0.116	0.300	0.330	0.670	4.660	1.435	65.2
Decan-1-ol	0.191	0.420	0.370	0.480	5.610	1.576	81.5
Undecan-1-ol	0.181	0.420	0.370	0.480	6.128	1.717	84.6
Dodecan-1-ol	0.175	0.420	0.370	0.480	6.620	1.858	91.8
Tridecan-1-ol	0.169	0.420	0.370	0.480	7.137	1.999	94.7
Tetradecan-1-ol	0.163	0.420	0.370	0.480	7.636	2.140	102.2
Pentadecan-1-ol	0.157	0.420	0.370	0.480	8.146	2.281	103.5
Hexadecan-1-ol	0.151	0.420	0.370	0.480	8.654	2.422	107.7
Heptadecan-1-ol	0.148	0.420	0.370	0.480	9.164	2.563	112.5
Octadecan-1-ol	0.145	0.420	0.370	0.480	9.662	2.704	116.8
Eicosan-1-ol	0.140	0.420	0.370	0.480	10.667	2.985	125.9
Cyclopentanol	0.427	0.540	0.320	0.560	3.241	0.763	57.5
Cyclohexanol	0.460	0.540	0.320	0.570	3.758	0.904	62.0
Cycloheptanol	0.513	0.540	0.320	0.580	4.407	1.045	67.4
Allyl alcohol	0.342	0.460	0.380	0.480	1.951	0.547	44.8
Ethane-1,2-diol	0.404	0.900	0.580	0.780	2.661	0.508	65.6

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Propan-1,2-diol	0.373	0.900	0.580	0.800	2.918	0.649	67.5
Propan-1,3-diol	0.397	0.890	0.770	0.870	2.863	0.649	72.4
Butan-1,2-diol	0.361	0.900	0.580	0.840	3.356	0.790	73.3
Butan-1,3-diol	0.377	1.010	0.590	0.850	3.358	0.790	72.8
meso-Butan-2,3-diol	0.365	0.930	0.600	0.880	3.291	0.790	66.6
Butan-1,4-diol	0.395	0.930	0.720	0.900	3.795	0.790	79.3
Pentan-1,2-diol	0.347	0.900	0.580	0.840	3.835	0.931	74.6
Pentan-1,5-diol	0.388	0.900	0.720	0.920	4.200	0.931	86.8
Hexan-1,2-diol	0.326	0.900	0.580	0.840	4.306	1.071	78.7
Hexan-1,6-diol	0.385	0.960	0.720	0.960	4.600	1.071	90.7
Heptan-1,7-diol	0.381	0.970	0.720	0.970	4.980	1.212	96.2
Octan-1,8-diol	0.380	0.970	0.720	0.970	5.397	1.353	105.4
Nonan-1,9-diol	0.375	0.980	0.750	0.980	5.780	1.494	112.8
Decan-1,10-diol	0.370	0.960	0.750	0.970	6.180	1.635	120.4
Dodecan-1,12-diol	0.360	0.980	0.750	0.990	6.970	1.917	130.5
Glycerol	0.512	0.760	0.470	1.430	3.973	0.707	91.7
Ethanethiol	0.392	0.420	0.000	0.200	2.079	0.554	27.3
Propanethiol	0.385	0.420	0.000	0.210	2.598	0.695	31.9
Butanethiol	0.382	0.430	0.000	0.210	3.059	0.836	36.5
3-Methylbutanethiol	0.343	0.320	0.000	0.240	3.500	0.977	39.9
s-Butanethiol	0.340	0.360	0.000	0.250	2.950	0.836	34.1
Pentanethiol	0.369	0.430	0.000	0.210	3.624	0.977	41.1
Hexanethiol	0.361	0.420	0.000	0.210	4.133	1.118	44.8
Heptanethiol	0.357	0.410	0.000	0.210	4.635	1.258	50.6
Decanethiol	0.342	0.400	0.000	0.210	6.280	1.681	65.5
Ethane-1,2-dithiol	0.810	0.780	0.000	0.420	3.369	0.717	44.7
Propane-1,3-dithiol	0.784	0.840	0.000	0.480	3.860	0.858	49.7
Dimethyl sulphide	0.404	0.430	0.000	0.270	2.037	0.554	27.9
Methyl ethyl sulfide	0.390	0.360	0.000	0.300	2.372	0.695	31.5
Diethyl sulphide	0.373	0.380	0.000	0.330	3.021	0.836	35.8
Methyl propyl sulfide	0.380	0.380	0.000	0.340	3.140	0.836	36.2
Methyl isopropyl sulfide	0.366	0.360	0.000	0.410	2.881	0.836	34.1

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Methyl butyl sulfide	0.373	0.390	0.000	0.340	3.600	0.977	41.0
Methyl tert-butyl sulfide	0.340	0.270	0.000	0.480	3.150	0.977	34.2
Ethyl propyl sulfide	0.365	0.390	0.000	0.360	3.500	0.977	39.5
Ethyl isopropyl sulfide	0.351	0.340	0.000	0.420	3.260	0.977	38.5
Di-n-propyl sulfide	0.358	0.380	0.000	0.340	4.010	1.118	44.7
Di-isopropyl sulfide	0.328	0.260	0.000	0.410	3.545	1.118	39.6
Methyl pentyl sulfide	0.367	0.390	0.000	0.340	4.130	1.118	44.6
Ethyl butyl sulfide	0.358	0.370	0.000	0.360	3.527	1.118	44.6
Ethyl tert-butyl sulfide	0.325	0.300	0.000	0.470	3.520	1.118	39.3
Propyl isopropyl sulfide	0.345	0.330	0.000	0.420	3.750	1.118	41.8
Dibutyl sulfide	0.345	0.370	0.000	0.350	5.044	1.399	54.2
Dimethyl disulfide	0.696	0.600	0.000	0.220	3.052	0.717	38.5
Diethyl disulfide	0.671	0.540	0.000	0.270	4.036	0.997	45.2
Dipropyl disulfide	0.653	0.520	0.000	0.270	4.984	1.281	53.8
Diisopropyl disulfide	0.612	0.460	0.000	0.410	4.538	1.281	49.3
Dibutyl disulfide	0.638	0.520	0.000	0.270	5.908	1.563	62.3
Diisobutyl disulfide	0.600	0.400	0.000	0.380	5.558	1.563	57.2
Dipentyl disulfide	0.625	0.520	0.000	0.270	6.922	1.845	71.1
Carbon disulfide	0.876	0.260	0.000	0.030	2.370	0.491	27.5
Tetramethylsilicon	-0.057	0.080	0.000	0.030	1.812	0.918	26.0
Tetraethylsilicon	0.126	-0.120	0.000	0.000	4.348	1.482	39.0
Tetramethyltin	0.324	0.110	0.000	0.100	2.651	1.043	31.1
Tetraethyltin	0.464	0.180	0.000	0.130	4.923	1.607	50.6
Tetraethyllead	0.864	0.050	0.000	0.050	5.460	1.648	56.6
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	33.8
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	38.1
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	42.2
o-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	43.4
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	42.7
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	42.3
n-Propylbenene	0.604	0.500	0.000	0.150	4.230	1.139	46.2
Isopropylbenzene	0.602	0.490	0.000	0.160	4.084	1.139	45.1

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
1,2,3-Trimethylbenzene	0.728	0.610	0.000	0.190	4.565	1.139	49.1
1,2,4-Trimethylbenzene	0.677	0.560	0.000	0.190	4.441	1.139	47.9
1,3,5-Trimethylbenzene	0.649	0.520	0.000	0.190	4.344	1.139	47.5
2-Ethyltoluene	0.680	0.550	0.000	0.180	4.346	1.139	47.7
4-Ethyltoluene	0.630	0.510	0.000	0.180	4.289	1.139	46.6
n-Butylbenzene	0.600	0.510	0.000	0.150	4.730	1.280	46.0
Isobutylbenzene	0.580	0.470	0.000	0.150	4.500	1.280	49.5
s-Butylbenzene	0.603	0.480	0.000	0.160	4.506	1.280	49.5
tert-Butylbenzene	0.619	0.490	0.000	0.180	4.413	1.280	49.1
4-Isopropyltoluene	0.607	0.490	0.000	0.190	4.590	1.280	50.3
n-Pentylbenzene	0.594	0.510	0.000	0.150	5.230	1.421	55.1
tert-Pentylbenzene	0.620	0.490	0.000	0.160	4.909	1.421	52.3
n-Hexylbenzene	0.591	0.500	0.000	0.150	5.720	1.562	60.0
n-Heptylbenzene	0.577	0.480	0.000	0.150	6.219	1.703	64.2
n-Nonylbenzene	0.578	0.480	0.000	0.150	7.212	1.985	74.8
n-Decylbenzene	0.579	0.470	0.000	0.150	7.708	2.125	78.2
Styrene	0.849	0.650	0.000	0.160	3.856	0.955	43.5
a-Methylstyrene	0.851	0.640	0.000	0.190	4.292	1.096	48.9
Naphthalene	1.340	0.920	0.000	0.200	5.161	1.085	54.6
Fluorobenzene	0.477	0.570	0.000	0.100	2.788	0.734	34.5
1,4-Difluorobenzene	0.384	0.600	0.000	0.060	2.766	0.752	35.8
Pentafluorobenzene	0.154	0.680	0.000	0.020	2.578	0.805	36.2
Hexafluorobenzene	0.088	0.560	0.000	0.010	2.345	0.823	35.7
Trifluoromethylbenzene	0.225	0.480	0.000	0.110	2.894	0.910	37.1
Chlorobenzene	0.718	0.650	0.000	0.070	3.657	0.839	41.0
1,2-Dichlorobenzene	0.872	0.780	0.000	0.040	4.518	0.961	48.5
1,3-Dichlorobenzene	0.847	0.730	0.000	0.020	4.410	0.961	47.0
1,4-Dichlorobenzene	0.825	0.750	0.000	0.020	4.435	0.961	47.8
1,2,3-Trichlorobenzene	1.030	0.860	0.000	0.000	5.419	1.084	57.2
1,2,4-Trichlorobenzene	0.980	0.810	0.000	0.000	5.248	1.084	55.5
1,3,5-Trichlorobenzene	0.980	0.730	0.000	0.000	5.045	1.084	59.0
1,2,3,4-Tetrachlorobenzene	1.180	0.920	0.000	0.000	6.171	1.206	60.1

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
1,2,3,5-Tetrachlorobenzene	1.160	0.850	0.000	0.000	5.802	1.206	60.7
1,2,4,5-Tetrachlorobenzene	1.160	0.860	0.000	0.000	5.926	1.206	60.7
Pentachlorobenzene	1.330	0.920	0.060	0.000	6.630	1.328	67.7
2-Chlorotoluene	0.762	0.650	0.000	0.070	4.173	0.980	46.1
3-Chlorotoluene	0.736	0.670	0.000	0.070	4.179	0.980	46.1
4-Chlorotoluene	0.705	0.740	0.000	0.050	4.205	0.980	46.4
Benzyl chloride	0.821	0.860	0.000	0.140	4.353	0.980	50.1
1-Chloronaphthalene	1.417	1.000	0.000	0.140	5.856	1.208	62.0
2-Chloronaphthalene	1.450	1.000	0.000	0.140	5.834	1.208	62.3
Bromobenzene	0.882	0.730	0.000	0.090	4.041	0.891	44.5
2-Bromotoluene	0.923	0.720	0.000	0.090	4.559	1.032	47.7
3-Bromotoluene	0.896	0.750	0.000	0.090	4.577	1.032	48.4
4-Bromotoluene	0.879	0.740	0.000	0.090	4.586	1.032	47.3
Benzyl bromide	1.014	0.940	0.000	0.200	4.680	1.032	53.3
Iodobenzene	1.188	0.820	0.000	0.120	4.502	0.975	48.5
1-Chloro-4-bromobenzene	0.995	0.830	0.000	0.000	4.917	1.014	52.3
1-Bromonaphthalene	1.598	1.130	0.000	0.130	6.682	1.260	63.9
2-Bromonaphthalene	1.610	1.130	0.000	0.150	6.678	1.260	66.1
Anisole	0.708	0.750	0.000	0.290	3.890	0.916	46.8
Phenetole	0.681	0.700	0.000	0.320	4.242	1.057	51.0
1,2-Dimethoxybenzene	0.832	1.050	0.000	0.610	5.043	1.116	64.5
1,3-Dimethoxybenzene	0.816	1.010	0.000	0.450	5.022	1.116	61.5
1,4-Dimethoxybenzene	0.806	1.000	0.000	0.500	5.044	1.116	61.6
Diphenyl ether	1.216	1.080	0.000	0.200	6.287	1.383	66.1
Benzaldehyde	0.820	1.000	0.000	0.390	4.008	0.873	49.0
Acetophenone	0.818	1.010	0.000	0.480	4.501	1.014	53.4
Methyl benzoate	0.733	0.850	0.000	0.460	4.704	1.073	55.6
Phenyl acetate	0.661	1.130	0.000	0.540	4.414	1.073	53.3
Dimethyl phthalate	0.780	1.260	0.000	0.880	6.275	1.429	76.7
Diethyl phthalate	0.729	1.260	0.000	0.900	7.214	1.711	82.1
Dibutyl phthalate	0.695	1.270	0.000	0.950	8.970	2.274	95.8
Butylbenzyl phthalate	1.300	1.510	0.000	1.130	10.820	2.459	109.8

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Dimethyl isophthalate	0.780	1.480	0.000	0.670	6.519	1.429	77.2
Dimethyl terephthalate	0.780	1.430	0.000	0.640	6.453	1.429	78.6
o-Toluidine	0.966	0.920	0.230	0.450	4.442	0.957	62.7
m-Toluidine	0.946	0.980	0.230	0.450	4.680	0.957	59.6
p-Toluidine	0.923	0.950	0.230	0.450	4.452	0.957	57.8
2,6-Dimethylaniline	0.962	0.930	0.200	0.480	4.966	1.098	59.6
2-Chloroaniline	1.033	0.920	0.250	0.310	4.674	0.939	57.1
3-Chloroaniline	1.053	1.100	0.300	0.300	4.909	0.939	61.1
4-Chloroaniline	1.060	1.130	0.300	0.310	4.889	0.939	62.3
1-Naphthylamine	1.670	1.260	0.200	0.570	6.490	1.185	73.3
N-Methylaniline	0.948	0.900	0.170	0.430	4.478	0.957	58.6
N,N-Dimethylaniline	0.957	0.810	0.000	0.410	4.701	1.098	52.8
Nitrobenzene	0.871	1.110	0.000	0.280	4.557	0.891	55.0
2-Nitrotoluene	0.866	1.110	0.000	0.280	4.878	1.032	59.6
Phenol	0.805	0.890	0.600	0.300	3.766	0.775	58.8
2-Fluorophenol	0.660	0.690	0.610	0.260	3.453	0.793	52.3
3-Fluorophenol	0.667	0.980	0.680	0.170	3.842	0.793	60.1
4-Fluorophenol	0.670	0.970	0.630	0.230	3.844	0.793	60.0
2-Chlorophenol	0.853	0.880	0.320	0.310	4.178	0.898	52.3
3-Chlorophenol	0.909	1.060	0.690	0.150	4.773	0.898	63.5
4-Chlorophenol	0.915	1.080	0.670	0.200	4.775	0.898	64.4
2,3-Dichlorophenol	0.960	0.920	0.440	0.210	4.978	0.898	71.7
2,4-Dichlorophenol	0.960	0.820	0.540	0.170	4.896	0.898	59.0
2,5-Dichlorophenol	0.960	0.840	0.520	0.180	4.966	0.898	56.7
2,6-Dichlorophenol	0.900	0.860	0.360	0.240	4.777	0.898	59.6
3,4-Dichlorophenol	1.020	1.240	0.930	0.000	5.480	0.898	70.8
4-Iodophenol	1.380	1.220	0.680	0.200	5.492	1.033	73.0
2-Methoxyphenol	0.837	0.910	0.220	0.520	4.449	0.975	62.6
3-Methoxyphenol	0.879	1.170	0.590	0.390	4.803	0.975	75.9
Benzyl alcohol	0.803	0.870	0.390	0.560	4.221	0.916	65.5
2-Phenylethanol	0.811	0.860	0.310	0.650	4.628	1.057	69.7
Thiophenol	1.000	0.800	0.120	0.170	4.110	0.880	47.5

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
Phenyl methyl sulfide	1.063	0.680	0.000	0.320	4.663	1.021	50.6
Pyridine	0.631	0.840	0.000	0.520	3.022	0.675	40.2
2-Methylpyridine	0.598	0.750	0.000	0.580	3.422	0.816	42.5
3-Methylpyridine	0.631	0.810	0.000	0.540	3.631	0.816	44.6
4-Methylpyridine	0.630	0.820	0.000	0.540	3.640	0.816	44.8
2,3-Dimethylpyridine	0.657	0.770	0.000	0.620	4.045	0.957	47.7
2,4-Dimethylpyridine	0.634	0.760	0.000	0.630	4.006	0.957	47.5
2,6-Dimethylpyridine	0.607	0.700	0.000	0.630	3.760	0.957	45.3
3,4-Dimethylpyridine	0.676	0.850	0.000	0.620	4.317	0.957	50.5
3,5-Dimethylpyridine	0.659	0.790	0.000	0.600	4.214	0.957	48.5
2-Ethylpyridine	0.613	0.710	0.000	0.590	3.844	0.957	44.7
4-Ethylpyridine	0.634	0.800	0.000	0.570	4.124	0.957	46.3
4-tert-Butylpyridine	0.631	0.750	0.000	0.660	4.772	1.239	54.4
2-Chloropyridine	0.738	1.040	0.000	0.370	3.875	0.798	51.0
3-Chloropyridine	0.732	0.830	0.000	0.400	3.783	0.798	47.9
2-Bromopyridine	0.921	1.210	0.000	0.360	4.386	0.850	54.4
3-Bromopyridine	0.905	1.010	0.000	0.340	4.185	0.850	52.1
3-Acetylpyridine	0.795	1.170	0.000	0.900	4.880	0.973	66.1
4-Acetylpyridine	0.771	1.130	0.000	0.840	4.660	0.973	66.5
Quinoline	1.268	0.970	0.000	0.540	5.457	1.044	58.1
Pyrrolidine	0.406	0.950	0.240	0.420	2.877	0.663	37.6
N-Methylpyrrolidine	0.303	0.980	0.000	0.400	3.132	0.804	34.2
3-Methylpiperidine	0.374	0.370	0.060	0.740	3.233	0.945	44.4
4-Methylpiperidine	0.368	0.370	0.060	0.740	3.229	0.945	40.6
N-Ethylpiperidine	0.300	0.560	0.000	0.600	3.816	1.086	40.8
N-Propylpiperidine	0.355	0.540	0.000	0.570	4.365	1.227	44.9
Morpholine	0.434	0.790	0.060	0.910	3.289	0.722	44.5
N-Methylmorpholine	0.333	0.740	0.000	0.900	3.270	0.863	39.4
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	34.6
2-Methylthiophene	0.688	0.560	0.000	0.160	3.308	0.782	38.7
3-Methylthiophene	0.689	0.580	0.000	0.130	3.450	0.782	39.4
2-Ethylthiophene	0.685	0.580	0.000	0.130	3.870	0.923	39.7

Organic Compound	E	S	A	B	L	V	$\Delta_{vap}H_m^0$
2,5-Dimethylthiophene	0.690	0.540	0.000	0.160	3.769	0.923	40.2
Dimethyl sulfoxide	0.522	1.720	0.000	0.970	3.401	0.613	52.9

APPENDIX D

SUPPLEMENTAL INFORMATION FOR CHAPTER 10

Table D.1: Solute descriptors for log K at 298 K, log K_w, and p^0 for solutes used in Chapter 10.

Solute	CAS-RN	E	S	A	B	V	L	logK_w	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
(E)-Hept-2-ene	14686-13-6	0.120	0.080	0.000	0.070	1.052	3.180	-1.230	5.178	LSER Dataset 2017	155	161
(E)-Hex-2-enal	6728-26-3	0.400	0.800	0.000	0.450	0.927	3.400	2.700		LSER Dataset 2017	155	
(E)-Oct-2-enal	2548-87-0	0.350	0.750	0.000	0.430	1.209	4.579	2.520		LSER Dataset 2017	155	
(Z)-1,2-Dichloroethene	156-59-2	0.440	0.610	0.110	0.050	0.592	2.439	0.860	27.227	LSER Dataset 2017	155	162
(Z)-Pent-2-ene	627-20-3	0.140	0.080	0.000	0.070	0.770	2.211	-0.960	66.069	LSER Dataset 2017	155	162
1,1,1,2,3,3-Hexafluoropropane	431-63-0	-0.590	0.200	0.150	0.050	0.638	0.631	0.940	205.589	LSER Dataset 2017	155	162
1,1,1,2-Tetrachloroethane	630-20-6	0.540	0.630	0.100	0.080	0.880	3.641		1.603	LSER Dataset 2017		162
1,1,1,2-Tetrafluoroethane	811-97-2	-0.390	0.160	0.160	0.050	0.461	0.403		665.273	LSER Dataset 2017		162
1,1,1-Trichloroethane	71-55-6	0.370	0.410	0.000	0.090	0.758	2.733	0.140	16.240	LSER Dataset 2017	155	161
1,1,1-Trifluoroethane	420-46-2	-0.330	0.100	0.000	0.100	0.444	0.324		1261.828	LSER Dataset 2017		162
1,1,2,2-Tetrachloroethane	79-34-5	0.600	0.760	0.160	0.120	0.880	3.803	1.810	3.083	LSER Dataset 2017	155	162
1,1,2-Trichloroethane	79-00-5	0.500	0.680	0.130	0.080	0.758	3.290	1.460	3.234	LSER Dataset 2017	155	161
1,1,2-TrichloroTrifluoroethane	76-13-1	0.010	0.130	0.000	0.000	0.811	2.210	-1.300	44.463	LSER Dataset 2017	150	162
1,1-Dibromoethane	557-91-5	0.650	0.640	0.100	0.160	0.740	3.001		3.404	LSER Dataset 2017		162
1,1-Dichloro-1-fluoroethane	1717-00-6	0.080	0.430	0.010	0.050	0.653	1.920		78.524	LSER Dataset 2017		162
1,1-Dichloroethane	75-34-3	0.320	0.490	0.100	0.100	0.635	2.316	0.620	30.269	LSER Dataset 2017	155	162
1,1-Difluoroethane	75-37-6	-0.250	0.470	0.040	0.070	0.426	0.570		597.035	LSER Dataset 2017		162
1,1-Difluoroethylene	75-38-7	-0.100	0.000	0.000	0.050	0.383	0.240		4027.170	LSER Dataset 2017		162
1,1-Dimethylcyclohexane	590-66-9	0.240	0.100	0.000	0.000	1.127	3.582		3.020	LSER Dataset 2017		162
1,1-Dimethylcyclopentane	1638-26-2	0.210	0.100	0.000	0.000	0.986	3.029		10.139	LSER Dataset 2017		162
1,2,3,4-Tetrachlorobenzene	634-66-2	1.180	0.920	0.000	0.000	1.206	6.171	0.980	0.004	LSER Dataset 2017	155	161
1,2,3,4-Tetrahydronaphthalene	119-64-2	0.890	0.650	0.000	0.170	1.171	5.203		0.050	LSER Dataset 2017		162
1,2,3,5-Tetrachlorobenzene	634-90-2	1.160	0.850	0.000	0.000	1.206	5.922	1.190	0.007	LSER Dataset 2017	155	161
1,2,3-Trichlorobenzene	87-61-6	1.030	0.860	0.000	0.000	1.084	5.419	0.9 1	0.034	LSER Dataset 2017	155	161
1,2,3-Trimethylbenzene	526-73-8	0.730	0.610	0.000	0.190	1.139	4.565	0.890	0.216	LSER Dataset 2017	155	162
1,2,4,5-Tetrachlorobenzene	95-94-3	1.160	0.860	0.000	0.000	1.206	5.926	0.980	0.006	LSER Dataset 2017	155	161
1,2,4-Trichlorobenzene	120-82-1	0.980	0.810	0.000	0.000	1.084	5.248	0.820	0.057	LSER Dataset 2017	155	162
1,2,4-Trimethylbenzene	95-63-6	0.680	0.560	0.000	0.190	1.139	4.441	0.630	0.287	LSER Dataset 2017	155	162
1,2-Dibromoethane	106-93-4	0.750	0.760	0.100	0.170	0.740	3.382	1.710	1.778	LSER Dataset 2017	155	162
1,2-Dichlorobenzene	95-50-1	0.870	0.780	0.000	0.040	0.961	4.518	1.000	0.181	LSER Dataset 2017	155	162
1,2-Dichloroethane	107-06-2	0.420	0.640	0.100	0.110	0.635	2.573	1.310	10.641	LSER Dataset 2017	155	162
1,2-Dichloropropane	78-87-5	0.370	0.630	0.000	0.170	0.776	2.836	0.930	6.887	LSER Dataset 2017	155	162
1,2-Dichlorotetrafluoroethane	76-14-2	-0.190	0.050	0.000	0.000	0.706	1.427		214.783	LSER Dataset 2017		162
1,3,5-Trichlorobenzene	108-70-3	0.980	0.730	0.000	0.000	1.084	5.045	0.570	0.058	LSER Dataset 2017	155	161
1,3-Butadiene	106-99-0	0.320	0.230	0.000	0.100	0.586	1.543	-0.450	281.190	LSER Dataset 2017	155	162
1,3-Cyclohexadiene	592-57-4	0.520	0.380	0.000	0.120	0.759	2.859		12.972	LSER Dataset 2017		162
1,3-Dichloro-2-propanol	96-23-1	0.550	0.690	0.420	0.600	0.835	3.364	5.180	0.125	LSER Dataset 2017	150	161
1,3-Dichlorobenzene	541-73-1	0.850	0.730	0.000	0.020	0.961	4.410	0.720	0.286	LSER Dataset 2017	155	162

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
1,3-Dichloropropane	142-28-9	0.410	0.740	0.000	0.170	0.776	3.101	1.390	2.427	LSER Dataset 2017	[155]	[161]
1,3-Dimethylnaphthalene	575-41-7	1.390	0.920	0.000	0.200	1.367	6.236	1.810	0.001	LSER Dataset 2017	[155]	[161]
1,4-Dichlorobutane	110-56-5	0.410	0.950	0.000	0.170	0.917	3.501	1.700	2.662	LSER Dataset 2017	[155]	[161]
1,4-Dimethylnaphthalene	571-58-4	1.400	0.910	0.000	0.200	1.367	6.339	2.070	0.007	LSER Dataset 2017	[155]	[161]
1,4-Dioxane	123-91-1	0.330	0.750	0.000	0.640	0.681	2.892	3.710	5.093	LSER Dataset 2017	[155]	[162]
1,4-Hexadiene	592-45-0	0.240	0.200	0.000	0.100	0.868	2.675		23.281	LSER Dataset 2017		[162]
1,6-Heptadiene	3070-53-9	0.190	0.200	0.000	0.100	1.009	3.028	-0.850	6.884	LSER Dataset 2017	[150]	[161]
1-Bromo-2-methylpropane	78-77-3	0.340	0.370	0.000	0.120	0.847	2.960	0.020	8.003	LSER Dataset 2017	[155]	[161]
1-Bromobutane	109-65-9	0.360	0.400	0.000	0.120	0.847	3.105	0.290	5.051	LSER Dataset 2017	[155]	[161]
1-Bromoheptane	629-04-9	0.340	0.400	0.000	0.120	1.270	4.663	-0.250	0.169	LSER Dataset 2017	[155]	[162]
1-Bromohexane	111-25-1	0.350	0.400	0.000	0.120	1.129	4.130	-0.130	0.282	LSER Dataset 2017	[155]	[161]
1-Bromooctane	111-83-1	0.340	0.400	0.000	0.120	1.411	5.000	-0.380	0.022	LSER Dataset 2017	[155]	[161]
1-Bromopentane	110-53-2	0.360	0.400	0.000	0.120	0.988	3.611	0.070	1.134	LSER Dataset 2017	[155]	[161]
1-Bromopropane	106-94-5	0.370	0.400	0.000	0.120	0.706	2.620	0.410	18.450	LSER Dataset 2017	[155]	[162]
1-Butanol	71-36-3	0.220	0.420	0.370	0.480	0.731	2.601	3.460	0.893	LSER Dataset 2017	[155]	[162]
1-Butene	106-98-9	0.100	0.080	0.000	0.070	0.629	1.529		296.483	LSER Dataset 2017	[155]	[162]
1-Butyne	107-00-6	0.180	0.230	0.130	0.150	0.586	1.520	0.120	188.365	LSER Dataset 2017	[155]	[162]
1-Chloro-1,1-difluoroethane	75-68-3	-0.080	0.240	0.060	0.060	0.548	1.081		337.287	LSER Dataset 2017		[162]
1-Chloroanthraquinone	82-44-0	1.900	1.790	0.000	0.570	1.651	9.171	6.030		LSER Dataset 2017	[150]	
1-Chlorobutane	109-69-3	0.210	0.400	0.000	0.100	0.795	2.722	0.120	13.992	LSER Dataset 2017	[155]	[161]
1-Chloroheptane	629-06-1	0.190	0.400	0.000	0.100	1.217	4.282	-0.210	0.220	LSER Dataset 2017	[155]	[161]
1-Chlorohexane	544-10-5	0.200	0.400	0.000	0.100	1.076	3.777	0.000	0.737	LSER Dataset 2017	[155]	[161]
1-Chloropentane	543-59-9	0.210	0.400	0.000	0.100	0.936	3.223	0.050	4.365	LSER Dataset 2017	[155]	[162]
1-Chloroprop-2-ene	107-05-1	0.330	0.560	0.000	0.050	0.611	2.109	0.420		LSER Dataset 2017	[155]	
1-Cyanobutane	110-59-8	0.180	0.900	0.000	0.360	0.827	3.108	2.580	0.973	LSER Dataset 2017	[155]	[162]
1-Cyanopropane	109-74-0	0.190	0.900	0.000	0.360	0.686	2.548	2.670	2.600	LSER Dataset 2017	[155]	[162]
1-Decanol	112-30-1	0.190	0.420	0.370	0.480	1.576	5.628	2.670	0.001	LSER Dataset 2017	[155]	[162]
1-Decene	872-05-9	0.090	0.080	0.000	0.070	1.475	4.533	-1.640	0.226	LSER Dataset 2017	[163]	[162]
1-Decyne	764-93-2	0.140	0.220	0.090	0.100	1.432	4.537			LSER Dataset 2017		
1-Dodecene	112-41-4	0.090	0.080	0.000	0.070	1.756	5.515		0.026	LSER Dataset 2017		[162]
1-Ethylnaphthalene	1127-76-0	1.370	0.870	0.000	0.200	1.367	6.136	1.760	0.005	LSER Dataset 2017	[155]	[161]
1H-1,2,4-Triazole	288-88-0	0.660	1.500	0.970	0.430	0.495	3.271	8.520		LSER Dataset 2017	[150]	
1-Heptanol	111-70-6	0.210	0.420	0.370	0.480	1.154	4.115	3.090	0.027	LSER Dataset 2017	[155]	[162]
1-Heptene	592-76-7	0.090	0.080	0.000	0.070	1.052	3.063	-1.220	7.516	LSER Dataset 2017	[155]	[162]
1-Heptyne	628-71-7	0.160	0.230	0.130	0.100	1.009	3.000	-0.440	5.697	LSER Dataset 2017	[155]	[161]
1-Hexadecene	629-73-2	0.080	0.080	0.000	0.070	2.320	7.500		0.000	LSER Dataset 2017		[162]
1-Hexanol	111-27-3	0.210	0.420	0.370	0.480	1.013	3.610	3.230	0.167	LSER Dataset 2017	[155]	[161]
1-Hexene	592-41-6	0.080	0.080	0.000	0.070	0.911	2.572	-1.160	24.660	LSER Dataset 2017	[155]	[162]
1-Hexyne	693-02-7	0.170	0.230	0.130	0.100	0.868	2.510	-0.210	17.283	LSER Dataset 2017	[155]	[161]
1-Iodobutane	542-69-8	0.630	0.400	0.000	0.150	0.930	3.628	0.180	1.811	LSER Dataset 2017	[155]	[162]
1-Iodoheptane	4282-40-0	0.610	0.400	0.000	0.140	1.353	5.100	-0.200		LSER Dataset 2017	[155]	
1-Iodohexane	638-45-9	0.620	0.400	0.000	0.150	1.212	4.620	-0.060		LSER Dataset 2017	[155]	
1-Iodopentane	628-17-1	0.620	0.400	0.000	0.150	1.071	4.130	0.100		LSER Dataset 2017	[155]	
1-Iodopropane	107-08-4	0.630	0.400	0.000	0.150	0.790	3.130	0.390	5.741	LSER Dataset 2017	[155]	[162]

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
1-Methyl-3-propylbenzene	1074-43-7	0.620	0.500	0.000	0.180	1.280	4.710		0.152	LSER Dataset 2017		162
1-Methyl-4-propylbenzene	1074-55-1	0.620	0.500	0.000	0.180	1.280	4.734		0.147	LSER Dataset 2017		162
1-Methylcyclohexene	591-49-1	0.390	0.200	0.000	0.100	0.943	3.483	-0.490	3.975	LSER Dataset 2017	155	161
1-Methylnaphthalene	90-12-0	1.340	0.940	0.000	0.220	1.226	5.802	1.790	0.010	LSER Dataset 2017	155	162
1-Naphthol	90-15-3	1.520	1.050	0.610	0.370	1.144	6.130	5.630	0.000	LSER Dataset 2017	155	161
1-Naphthylamine	134-32-7	1.670	1.260	0.200	0.570	1.185	6.490	5.340	0.001	LSER Dataset 2017	155	161
1-Nitrobutane	627-05-4	0.230	0.950	0.000	0.290	0.846	3.415	2.270	1.020	LSER Dataset 2017	155	161
1-Nitropentane	628-05-7	0.210	0.950	0.000	0.290	0.987	3.938	2.070	0.142	LSER Dataset 2017	155	161
1-Nitropropane	108-03-2	0.240	0.950	0.000	0.310	0.706	2.894	2.450	1.370	LSER Dataset 2017	155	161
1-Nonanol	143-08-8	0.190	0.420	0.370	0.480	1.435	5.124	2.850	0.003	LSER Dataset 2017	155	162
1-Nonene	124-11-8	0.090	0.080	0.000	0.070	1.334	4.073	-1.510	0.719	LSER Dataset 2017	155	162
1-Nonyne	3452-09-3'	0.150	0.220	0.090	0.100	1.291	4.019		0.720	LSER Dataset 2017		164
1-Octanol	111-87-5	0.200	0.420	0.370	0.480	1.295	4.619	3.000	0.011	LSER Dataset 2017	155	162
1-Octene	111-66-0	0.090	0.080	0.000	0.070	1.193	3.568	-1.410	2.328	LSER Dataset 2017	163	162
1-Octyne	629-05-0	0.160	0.230	0.130	0.100	1.150	3.521	-0.520	1.789	LSER Dataset 2017	155	161
1-Pentadecene	13360-61-7	0.080	0.080	0.000	0.070	2.179	7.006		0.001	LSER Dataset 2017		162
1-Pentanol	71-41-0	0.220	0.420	0.370	0.480	0.872	3.106	3.350	0.332	LSER Dataset 2017	155	162
1-Pentene	109-67-1	0.090	0.080	0.000	0.070	0.770	2.047	-1.230	85.114	LSER Dataset 2017	155	162
1-Pentyne	627-19-0	0.170	0.230	0.130	0.100	0.727	2.010	-0.010	58.076	LSER Dataset 2017	155	162
1-Propanal	123-38-6	0.200	0.650	0.000	0.450	0.547	1.815	2.520	42.462	LSER Dataset 2017	155	162
1-Propanol	71-23-8	0.240	0.420	0.370	0.480	0.590	2.031	3.560	2.812	LSER Dataset 2017	155	162
1-Tetradecene	1120-36-1	0.090	0.080	0.000	0.070	2.038	6.513		0.002	LSER Dataset 2017		162
1-Tridecene	2437-56-1	0.090	0.080	0.000	0.070	1.897	6.020		0.007	LSER Dataset 2017		162
1-Undecene	821-95-4	0.090	0.080	0.000	0.070	1.616	5.023		0.067	LSER Dataset 2017		162
2,2,2-Trifluoroethanol	75-89-8	0.020	0.600	0.570	0.250	0.502	1.224	3.160	9.559	LSER Dataset 2017	155	161
2,2,3,3-Tetramethylpentane	7154-79-2	0.000	0.000	0.000	0.000	1.377	3.880		1.268	LSER Dataset 2017		162
2,2,3-Trimethylbutane	464-06-2	0.000	0.000	0.000	0.000	1.095	2.918		13.646	LSER Dataset 2017		162
2,2,3-Trimethylpentane	564-02-3	0.000	0.000	0.000	0.000	1.236	3.325		4.276	LSER Dataset 2017		162
2,2,4,4-Tetramethylpentane	1070-87-7	0.000	0.000	0.000	0.000	1.377	3.512		2.673	LSER Dataset 2017		162
2,2,4-Trimethylpentane	540-84-1	0.000	0.000	0.000	0.000	1.236	3.106	-2.120	6.577	LSER Dataset 2017	155	162
2,2,5-Trimethylhexane	3522-94-9	0.000	0.000	0.000	0.000	1.377	3.567	-2.150	2.223	LSER Dataset 2017	155	162
2,2-Dichloro-1,1,1-trifluoroethane	306-83-2	-0.160	0.400	0.220	0.000	0.688	1.746		91.411	LSER Dataset 2017		162
2,2-Dimethyl-3-ethylpentane	16747-32-3	0.000	0.000	0.000	0.000	1.377	3.740		1.503	LSER Dataset 2017		162
2,2-Dimethylbutane	75-83-2	0.000	0.000	0.000	0.000	0.954	2.352	-1.840	42.756	LSER Dataset 2017	155	162
2,2-Dimethylhexane	590-73-8	0.000	0.000	0.000	0.000	1.236	3.261		4.539	LSER Dataset 2017		162
2,2-Dimethyloctane	15869-87-1	0.000	0.000	0.000	0.000	1.518	4.225		0.485	LSER Dataset 2017		162
2,2-Dimethylpentane	590-35-2	0.000	0.000	0.000	0.000	1.095	2.796	-2.110	14.028	LSER Dataset 2017	155	162
2,2-Dimethylpropane	630-18-2	0.140	0.840	0.000	0.420	0.827	2.800	-1.840		LSER Dataset 2017	155	
2,3,3-Trimethyl-1-butene	594-56-9	0.110	0.090	0.000	0.150	1.052	2.815		14.859	LSER Dataset 2017		162
2,3,3-Trimethylpentane	560-21-4	0.000	0.000	0.000	0.000	1.236	3.428		3.597	LSER Dataset 2017		162
2,3,4-Trimethylpentane	565-75-3	0.000	0.000	0.000	0.000	1.236	3.481	-1.880	3.614	LSER Dataset 2017	155	162
2,3-Butanediol	513-85-9	0.340	0.930	0.610	0.880	0.790	3.250		0.024	LSER Dataset 2017		162

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
2,3-Dimethyl-1,3-butaDiene	513-81-5	0.350	0.230	0.000	0.140	0.868	2.690	-0.290	20.184	LSER Dataset 2017	155	162
2,3-Dimethyl-1-butene	563-78-0	0.150	0.070	0.000	0.130	0.911	2.455		33.651	LSER Dataset 2017		162
2,3-Dimethyl-1-hexene	16746-86-4	0.110	0.080	0.000	0.120	1.193	3.373		3.698	LSER Dataset 2017		162
2,3-Dimethyl-2-butene	563-79-1	0.210	0.090	0.000	0.130	0.911	2.797		16.672	LSER Dataset 2017		162
2,3-Dimethylbutane	79-29-8	0.000	0.000	0.000	0.000	0.954	2.495	-1.720	31.333	LSER Dataset 2017	155	162
2,3-Dimethylhexane	584-94-1	0.000	0.000	0.000	0.000	1.236	3.451		3.126	LSER Dataset 2017		162
2,3-Dimethylnaphthalene	581-40-8	1.430	0.950	0.000	0.200	1.367	6.291	2.040	0.002	LSER Dataset 2017	155	161
2,3-Dimethylpentane	565-59-3	0.000	0.000	0.000	0.000	1.095	3.016	-1.850	9.162	LSER Dataset 2017	155	162
2,3-Dimethylphenol	526-75-0	0.850	0.810	0.530	0.360	1.057	4.952	4.520		LSER Dataset 2017	155	
2,3-Dimethylpyridine	583-61-9	0.660	0.770	0.000	0.620	0.957	4.045	3.540	0.309	LSER Dataset 2017	155	161
2,4,4-Trimethyl-1-pentene	107-39-1	0.090	0.070	0.000	0.070	1.193	3.289		5.957	LSER Dataset 2017		162
2,4,4-Trimethyl-2-pentene	107-40-4	0.140	0.080	0.000	0.070	1.193	3.249		4.786	LSER Dataset 2017		162
2,4-Dichlorotoluene	95-73-8	0.920	0.740	0.000	0.030	1.102	4.951		0.061	LSER Dataset 2017		162
2,4-Dimethyl-3-ethylpentane	1068-87-7	0.000	0.000	0.000	0.000	1.377	3.828		1.337	LSER Dataset 2017		162
2,4-Dimethylhexane	589-43-5	0.000	0.000	0.000	0.000	1.236	3.319		4.046	LSER Dataset 2017		162
2,4-Dimethylpentan-3-one	565-80-0	0.070	0.600	0.000	0.510	1.111	3.403	2.010		LSER Dataset 2017	155	
2,4-Dimethylpentane	108-08-7	0.000	0.000	0.000	0.000	1.095	2.809	-2.080	13.122	LSER Dataset 2017	155	162
2,4-Dimethylphenol	105-67-9	0.840	0.800	0.530	0.390	1.057	4.770	4.410	0.014	LSER Dataset 2017	155	162
2,4-Dimethylpyridine	108-47-4	0.630	0.760	0.000	0.630	0.957	4.006	3.570	0.346	LSER Dataset 2017	155	161
2,5-Dimethylhexane	592-13-2	0.000	0.000	0.000	0.000	1.236	3.308	-2.020	4.036	LSER Dataset 2017	150	162
2,5-Dimethylphenol	95-87-4	0.940	0.790	0.540	0.370	1.057	4.774	4.340		LSER Dataset 2017	155	
2,5-Dimethylpyridine	589-93-5	0.630	0.740	0.000	0.620	0.957	3.986	3.460	0.377	LSER Dataset 2017	155	161
2,5-Dimethyltetrahydrofuran	1003-38-9	0.200	0.380	0.000	0.580	0.904	2.980	2.140	7.055	LSER Dataset 2017	155	161
2,6-Dimethylaniline	87-62-7	0.970	0.890	0.200	0.460	1.098	5.028	3.820	0.016	LSER Dataset 2017	155	161
2,6-Dimethylheptane	1072-05-5	0.000	0.000	0.000	0.000	1.377	3.780		1.242	LSER Dataset 2017		162
2,6-Dimethylnaphthalene	581-42-0	1.350	0.820	0.000	0.250	1.367	6.146	1.930	0.003	LSER Dataset 2017	155	161
2,6-Dimethylphenol	576-26-1	0.860	0.790	0.390	0.390	1.057	4.680	3.860		LSER Dataset 2017	155	
2,6-Dimethylpyridine	108-48-5	0.610	0.700	0.000	0.620	0.957	3.760	3.370	0.773	LSER Dataset 2017	155	162
2-Bromo-2-chloro-1,1,1-trifluoroethane	151-67-7	0.100	0.380	0.150	0.030	0.741	2.177	0.120	40.797	LSER Dataset 2017	150	161
2-Bromo-2-methylpropane	507-19-7	0.310	0.250	0.000	0.140	0.847	2.616	-0.620	17.957	LSER Dataset 2017	155	161
2-Bromopropane	75-26-3	0.330	0.350	0.000	0.140	0.706	2.390	0.350	28.840	LSER Dataset 2017	155	162
2-Butanol	78-92-2	0.220	0.360	0.330	0.560	0.731	2.338	3.390	2.415	LSER Dataset 2017	155	162
2-Butoxyethanol	111-76-2	0.200	0.500	0.300	0.830	1.071	3.806	4.590	0.067	LSER Dataset 2017	155	161
2-Chloro-1,1,1,2-Tetrafluoroethane	2837-89-0	-0.300	0.170	0.100	0.070	0.584	0.904		383.707	LSER Dataset 2017		162
2-Chloro-2-methylpropane	507-20-0	0.140	0.250	0.000	0.120	0.795	2.217	-0.800	13.521	LSER Dataset 2017	155	162
2-Chloroaniline	95-51-2	1.030	0.920	0.250	0.310	0.939	4.674	3.600		LSER Dataset 2017	155	
2-Chlorobutane	78-86-4	0.190	0.350	0.000	0.120	0.795	2.540	0.000	20.941	LSER Dataset 2017	155	162
2-Chlorophenol	95-57-8	0.850	0.880	0.320	0.310	0.898	4.178	3.340	0.337	LSER Dataset 2017	155	162
2-Chloropropane	75-29-6	0.180	0.350	0.000	0.120	0.654	1.970	0.180	69.637	LSER Dataset 2017	155	161
2-Chloropyridine	109-09-1	0.740	1.030	0.000	0.370	0.798	3.875	3.220	0.314	LSER Dataset 2017	155	161

Solute	CAS-RN	E	S	A	B	V	L	$\log K_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
2-Chlorotoluene	95-49-8	0.760	0.650	0.000	0.070	0.980	4.173	0.840	0.470	LSER Dataset 2017	155	162
2-Decanone	693-54-9	0.110	0.680	0.000	0.510	1.533	5.245	1.720	0.017	LSER Dataset 2017	155	161
2-Ethoxyethanol	110-80-5	0.240	0.500	0.300	0.830	0.790	2.815	4.920		LSER Dataset 2017	150	
2-Ethoxyethyl acetate	111-15-9	0.100	0.790	0.000	0.790	1.087	3.747		0.282	LSER Dataset 2017		162
2-Ethyl-1-butanol	97-95-0	0.230	0.390	0.370	0.480	1.013	3.523		0.204	LSER Dataset 2017		162
2-Ethyl-1-butene	760-21-4	0.140	0.080	0.000	0.080	0.911	2.624		23.388	LSER Dataset 2017		162
2-Ethyl-1-hexanol	104-76-7	0.210	0.390	0.370	0.480	1.295	4.433		0.019	LSER Dataset 2017		162
2-Ethyl-1-pentene	3404-71-5	0.130	0.070	0.000	0.090	1.052	3.105		7.621	LSER Dataset 2017		162
2-Ethyl-p-xylene	1758-88-9	0.690	0.550	0.000	0.190	1.280	4.824		0.126	LSER Dataset 2017		162
2-Ethylpyrazine	13925-00-3	0.620	0.840	0.000	0.670	0.916	3.887	4.000		LSER Dataset 2017	155	
2-Ethylpyridine	100-71-0	0.610	0.700	0.000	0.590	0.957	3.844	3.180	0.543	LSER Dataset 2017	155	161
2-Ethyltoluene	611-14-3	0.680	0.550	0.000	0.180	1.139	4.346	0.760	0.503	LSER Dataset 2017	155	161
2-Fluorophenol	367-12-4	0.660	0.690	0.610	0.260	0.793	3.453	3.880	0.340	LSER Dataset 2017	155	161
2-Heptanone	110-43-0	0.120	0.680	0.000	0.510	1.111	3.760	2.230	0.521	LSER Dataset 2017	155	162
2-Hexanone	591-78-6	0.140	0.680	0.000	0.510	0.970	3.286	2.410	1.552	LSER Dataset 2017	155	162
2-Hexyne	764-35-2	0.240	0.300	0.000	0.150	0.868	2.765		10.666	LSER Dataset 2017		162
2-Hydroxybenzoic acid	69-72-7	0.900	0.850	0.730	0.370	0.990	4.732	5.390		LSER Dataset 2017	150	
2-Iodophenol	533-58-4	1.360	1.000	0.400	0.350	1.033	4.964	4.550		LSER Dataset 2017	155	
2-Isobutylpyrazine	29460-92-2	0.620	0.870	0.000	0.650	1.198	4.900	3.700		LSER Dataset 2017	155	
2-Methoxyaniline	90-04-0	0.990	1.030	0.230	0.500	1.016	4.818	4.490		LSER Dataset 2017	155	
2-Methoxybenzoic acid	579-75-9	0.900	1.410	0.450	0.620	1.131	5.636	6.800		LSER Dataset 2017	150	
2-Methoxyethanol	109-86-4	0.270	0.500	0.300	0.840	0.649	2.490	5.080	1.128	LSER Dataset 2017	150	161
2-Methoxyphenol	90-05-1	0.840	0.910	0.220	0.520	0.975	4.449	4.090		LSER Dataset 2017	155	
2-Methyl-1-butanol	137-32-6	0.190	0.390	0.370	0.480	0.872	3.011	3.240	0.486	LSER Dataset 2017	155	162
2-Methyl-1-butene	563-46-2	0.120	0.090	0.000	0.070	0.770	2.097		81.283	LSER Dataset 2017		162
2-Methyl-1-hexene	6094-02-6	0.040	0.100	0.000	0.080	1.052	3.044		8.110	LSER Dataset 2017		162
2-Methyl-1-pentene	763-29-1	0.090	0.080	0.000	0.070	0.911	2.588	-1.080	26.062	LSER Dataset 2017	155	162
2-Methyl-2-butanol	75-85-4	0.190	0.300	0.310	0.600	0.872	2.630	3.250	2.223	LSER Dataset 2017	155	162
2-Methyl-2-butene	513-35-9	0.160	0.080	0.000	0.070	0.770	2.226	-0.960	62.517	LSER Dataset 2017	155	162
2-Methyl-2-pentene	625-27-4	0.160	0.080	0.000	0.070	0.911	2.687		21.038	LSER Dataset 2017		162
2-Methyl-3-ethylpentane	609-26-7	0.000	0.000	0.000	0.000	1.236	3.459		3.184	LSER Dataset 2017		162
2-Methylbenzoic acid	118-90-1	0.730	0.840	0.420	0.440	1.073	4.677	4.300		LSER Dataset 2017	150	
2-Methylbuta-1,3-diene	78-79-5	0.310	0.230	0.000	0.100	0.727	2.101	-0.500	73.451	LSER Dataset 2017	155	162
2-Methylbutane	78-78-4	0.000	0.000	0.000	0.000	0.813	2.013	-1.750	91.622	LSER Dataset 2017	155	162
2-Methylheptane	592-27-8	0.000	0.000	0.000	0.000	1.236	3.480		2.748	LSER Dataset 2017		162
2-Methylhexane	591-76-4	0.000	0.000	0.000	0.000	1.095	3.001	-2.150	8.770	LSER Dataset 2017	155	162
2-Methylnonane	871-83-0	0.000	0.000	0.000	0.000	1.518	4.453		0.251	LSER Dataset 2017		162
2-Methyloctane	3221-61-2	0.000	0.000	0.000	0.000	1.377	3.966		0.845	LSER Dataset 2017		162
2-Methylpentan-2-ol	590-36-3	0.170	0.300	0.310	0.600	1.013	3.081	2.880	0.604	LSER Dataset 2017	155	161
2-Methylpentan-3-ol	565-67-3	0.210	0.330	0.330	0.560	1.013	3.240	2.850	0.705	LSER Dataset 2017	155	161
2-Methylpentane	107-83-5	0.000	0.000	0.000	0.000	0.954	2.503	-1.840	28.119	LSER Dataset 2017	155	162
2-Methylpropan-1-ol	78-83-1	0.220	0.390	0.370	0.480	0.731	2.413	3.300	1.400	LSER Dataset 2017	155	162
2-Methylpropanal	78-84-2	0.140	0.620	0.000	0.450	0.688	2.120	2.100	21.086	LSER Dataset 2017	155	162
2-Methylpropane	75-28-5	0.000	0.000	0.000	0.000	0.672	1.409	-1.700	351.560	LSER Dataset 2017	155	162

Solute	CAS-RN	E	S	A	B	V	L	$\log K_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
2-Methylpyrazine	109-08-0	0.630	0.860	0.000	0.670	0.775	3.254	4.040		LSER Dataset 2017	155	
2-Methylpyridine	109-06-8	0.600	0.750	0.000	0.570	0.816	3.422	3.400	1.510	LSER Dataset 2017	155	162
2-Methyltetrahydrofuran	96-47-9	0.240	0.480	0.000	0.530	0.763	2.820	2.420	12.182	LSER Dataset 2017	155	161
2-Methylthiophene	554-14-3	0.690	0.560	0.000	0.160	0.782	3.308	1.010	3.304	LSER Dataset 2017	155	162
2-Naphthol	135-19-3	1.520	1.080	0.610	0.400	1.144	6.200	5.950	0.000	LSER Dataset 2017	155	161
2-Naphthylamine	91-59-8	1.670	1.280	0.220	0.550	1.185	6.540	5.480	0.000	LSER Dataset 2017	155	161
2-Nitroaniline	88-74-4	1.180	1.370	0.300	0.360	0.990	5.627	5.410		LSER Dataset 2017	155	
2-Nitrophenol	88-75-5	1.020	1.050	0.050	0.370	0.949	4.760	3.360		LSER Dataset 2017	155	
2-Nitropropane	79-46-9	0.220	0.920	0.000	0.320	0.706	2.550	2.300	2.302	LSER Dataset 2017	155	161
2-Nitrotoluene	88-72-2	0.870	1.110	0.000	0.280	1.032	4.878	2.630		LSER Dataset 2017	155	
2-Octanol	123-96-6	0.160	0.360	0.330	0.560	1.295	4.339		0.032	LSER Dataset 2017		162
2-Octanone	111-13-7	0.110	0.680	0.000	0.510	1.252	4.257	2.110	0.134	LSER Dataset 2017	155	161
2-Pentanol	6032-29-7	0.200	0.360	0.330	0.560	0.872	2.840	3.220	0.822	LSER Dataset 2017	155	162
2-Pentanone	107-87-9	0.140	0.680	0.000	0.510	0.829	2.755	2.580	4.742	LSER Dataset 2017	155	162
2-Phenylethanol	60-12-8	0.780	0.830	0.300	0.660	1.057	4.628	4.980	0.011	LSER Dataset 2017	155	161
2-Propoxyethanol	2807-30-9	0.210	0.500	0.300	0.830	0.931	3.310	4.700		LSER Dataset 2017	155	
3,3,5-Trimethylheptane	7154-80-5	0.000	0.000	0.000	0.000	1.518	4.254		0.557	LSER Dataset 2017		162
3,3-Diethylpentane	1067-20-5	0.000	0.230	0.000	0.000	1.377	4.065		0.973	LSER Dataset 2017		162
3,3-Dimethyl-1-butene	558-37-2	0.040	0.040	0.000	0.130	0.911	2.201		57.544	LSER Dataset 2017		162
3,3-Dimethylbutan-2-one	75-97-8	0.110	0.620	0.000	0.510	0.970	2.928	2.280	3.619	LSER Dataset 2017	155	161
3,3-Dimethylhexane	563-16-6	0.000	0.000	0.000	0.000	1.236	3.359		3.811	LSER Dataset 2017		162
3,3-Dimethylpentane	562-49-2	0.000	0.000	0.000	0.000	1.095	2.946	-1.880	11.015	LSER Dataset 2017	155	162
3,4-Dimethylhexane	583-48-2	0.000	0.000	0.000	0.000	1.236	3.559		2.891	LSER Dataset 2017		162
3,4-Dimethylphenol	95-65-8	0.830	0.860	0.560	0.390	1.057	4.980	4.770		LSER Dataset 2017	155	
3,4-Dimethylpyridine	583-58-4	0.680	0.850	0.000	0.610	0.957	4.317	3.830	0.091	LSER Dataset 2017	155	161
3,5-Dimethylphenol	108-68-9	0.820	0.840	0.570	0.360	1.057	4.856	4.600		LSER Dataset 2017	155	
3,5-Dimethylpyridine	591-22-0	0.660	0.790	0.000	0.600	0.957	4.214	3.550	0.169	LSER Dataset 2017	155	161
3,5-Dinitrobenzoic acid	99-34-3	1.250	1.630	0.700	0.590	1.280	6.984	8.300		LSER Dataset 2017	150	
3-Acetylpyridine	350-03-8	0.800	1.170	0.000	0.900	0.973	4.880	6.060		LSER Dataset 2017	155	
3-Chloroaniline	108-42-9	1.050	1.100	0.300	0.300	0.939	4.909	4.270		LSER Dataset 2017	155	
3-Chlorobenzoic acid	535-80-8	0.840	0.950	0.630	0.320	1.054	5.197	5.150		LSER Dataset 2017	150	
3-Chlorophenol	108-43-0	0.910	1.060	0.690	0.150	0.898	4.773	4.850		LSER Dataset 2017	155	
3-Chloropyridine	626-60-8	0.730	0.830	0.000	0.410	0.798	3.783	2.940		LSER Dataset 2017	155	
3-Cyanophenol	873-62-1	0.930	1.550	0.770	0.280	0.930	5.180	7.080		LSER Dataset 2017	155	
3-Cyanopyridine	100-54-9	0.750	1.260	0.000	0.620	0.830	4.164	4.950		LSER Dataset 2017	155	
3-Ethyl-1-pentene	4038-04-4'	0.090	0.080	0.000	0.080	1.052	2.901		10.839	LSER Dataset 2017		162
3-Ethylhexane	619-99-8	0.000	0.000	0.000	0.000	1.236	3.519		2.679	LSER Dataset 2017		162
3-Ethyl-*o*-xylene	933-98-2	0.740	0.610	0.000	0.190	1.280	4.946		0.083	LSER Dataset 2017		162
3-Ethylpentane	617-78-7	0.000	0.000	0.000	0.000	1.095	3.091		7.762	LSER Dataset 2017		162
3-Ethylphenol	620-17-7	0.810	0.910	0.550	0.370	1.057	4.741	4.590		LSER Dataset 2017	155	
3-Ethylpyridine	536-78-7	0.640	0.790	0.000	0.570	0.957	4.093	3.370	0.220	LSER Dataset 2017	155	161
3-Formylpyridine	500-22-1	0.820	1.160	0.000	0.760	0.832	4.258	5.210		LSER Dataset 2017	155	
3-Hexanol	623-37-0	0.200	0.360	0.330	0.560	1.013	3.343	2.980	0.666	LSER Dataset 2017	155	161
3-Hexanone	589-38-8	0.140	0.660	0.000	0.510	0.970	3.271	2.270	1.854	LSER Dataset 2017	64	162

Solute	CAS-RN	E	S	A	B	V	L	$\log K_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
3-Hydroxybenzaldehyde	100-83-4	0.990	1.380	0.730	0.400	0.932	5.060	6.970		LSER Dataset 2017	155	
3-Methoxyaniline	536-90-3	1.030	1.220	0.250	0.550	1.016	5.023	5.350		LSER Dataset 2017	155	
3-Methoxyphenol	150-19-6	0.880	1.170	0.590	0.380	0.975	4.803	5.620		LSER Dataset 2017	155	
3-Methyl-1-butanol	123-51-3	0.190	0.390	0.370	0.480	0.872	3.011	3.240	0.294	LSER Dataset 2017	155	161
3-Methyl-1-butene	563-45-1	0.060	0.080	0.000	0.070	0.770	1.910	-1.340	120.226	LSER Dataset 2017	155	162
3-Methyl-1-hexene	3404-61-3	0.090	0.070	0.000	0.070	1.052	2.897		10.990	LSER Dataset 2017		162
3-Methyl-3-ethylpentane	1067-08-9	0.000	0.000	0.000	0.000	1.236	3.502		3.062	LSER Dataset 2017		162
3-Methylbenzoic acid	99-04-7	0.730	0.890	0.600	0.400	1.073	4.819	4.980		LSER Dataset 2017	150	
3-Methylbutan-2-one	563-80-4	0.130	0.650	0.000	0.510	0.829	2.692	2.380		LSER Dataset 2017	155	
3-Methylbutanoic acid	503-74-2	0.180	0.570	0.600	0.500	0.888	3.140	4.470	0.065	LSER Dataset 2017	155	161
3-Methylheptane	589-81-1	0.000	0.000	0.000	0.000	1.236	3.510	-2.180	2.612	LSER Dataset 2017	155	162
3-Methylhexane	589-34-4	0.000	0.000	0.000	0.000	1.095	3.044	-1.990	8.185	LSER Dataset 2017	155	162
3-Methylnonane	5911-04-6'	0.000	0.000	0.000	0.000	1.518	4.486		0.264	LSER Dataset 2017		162
3-Methyloctane	2216-33-3	0.000	0.000	0.000	0.000	1.377	3.998		0.834	LSER Dataset 2017		162
3-Methylpentane	96-14-0	0.000	0.000	0.000	0.000	0.954	2.581	-1.840	25.235	LSER Dataset 2017	155	162
3-Methylpyridine	108-99-6	0.630	0.810	0.000	0.540	0.816	3.631	3.500	0.809	LSER Dataset 2017	155	162
3-Methylthiophene	616-44-4	0.690	0.580	0.000	0.130	0.782	3.450		2.944	LSER Dataset 2017		162
3-Methyl-trans-2-pentene	616-12-6	0.160	0.080	0.000	0.080	0.911	2.760		18.621	LSER Dataset 2017		162
3-Nitroaniline	99-09-2	1.200	1.710	0.400	0.350	0.990	5.880	6.490		LSER Dataset 2017	155	
3-Nitrobenzoic acid	121-92-6	0.990	1.180	0.730	0.520	1.106	5.601	6.930		LSER Dataset 2017	150	
3-Nitrophenol	554-84-7	1.050	1.570	0.790	0.230	0.949	5.692	7.060		LSER Dataset 2017	155	
3-Nitrophthalic acid	603-11-2	1.360	2.010	1.200	0.890	1.321	7.780	12.670		LSER Dataset 2017	150	
3-Nitrotoluene	99-08-1	0.870	1.100	0.000	0.280	1.032	5.097	2.530		LSER Dataset 2017	155	
3-Pentanol	584-02-1	0.220	0.360	0.330	0.560	0.872	2.860	3.190	1.183	LSER Dataset 2017	155	161
3-Pentanone	96-22-0	0.150	0.660	0.000	0.510	0.829	2.811	2.500	4.977	LSER Dataset 2017	155	162
3-Phenylpropanol	122-97-4	0.820	0.900	0.300	0.670	1.198	5.180	5.080		LSER Dataset 2017	155	
4-Acetylpyridine	1122-54-9	0.770	1.130	0.000	0.840	0.973	4.660	5.590		LSER Dataset 2017	155	
4-Bromophenol	106-41-2	1.080	1.170	0.670	0.200	0.950	5.135	5.230	0.001	LSER Dataset 2017	155	161
4-Bromotoluene	106-38-7	0.880	0.740	0.000	0.090	1.032	4.586	1.020		LSER Dataset 2017	155	
4-Chloro-3-methylphenol	59-50-7	0.920	1.020	0.650	0.230	1.038	5.290	4.980		LSER Dataset 2017	155	
4-Chloroaniline	106-47-8	1.060	1.130	0.300	0.310	0.939	4.889	4.330		LSER Dataset 2017	155	
4-Chlorobenzoic acid	74-11-3	0.840	1.020	0.630	0.270	1.054	4.947	4.800		LSER Dataset 2017	150	
4-Chlorophenol	106-48-9	0.920	1.080	0.670	0.210	0.898	4.775	5.160		LSER Dataset 2017	155	
4-Cyanophenol	767-00-0	0.940	1.630	0.790	0.300	0.930	5.420	7.460		LSER Dataset 2017	155	
4-Cyanopyridine	100-48-1	0.750	1.210	0.000	0.590	0.830	4.033	4.420		LSER Dataset 2017	155	
4-Ethyl-*m*-xylene	874-41-9	0.690	0.550	0.000	0.190	1.280	4.846		0.119	LSER Dataset 2017		162
4-Ethyl-*o*-xylene	934-80-5	0.690	0.560	0.000	0.190	1.280	4.873		0.100	LSER Dataset 2017		162
4-Ethylphenol	123-07-9	0.800	0.900	0.550	0.360	1.057	4.737	4.500		LSER Dataset 2017	155	
4-Ethylpyridine	536-75-4	0.630	0.800	0.000	0.570	0.957	4.124	3.470	0.198	LSER Dataset 2017	155	161
4-Ethyltoluene	622-96-8	0.630	0.510	0.000	0.180	1.139	4.289	0.700	0.398	LSER Dataset 2017	155	162
4-Fluorophenol	371-41-5	0.670	0.970	0.630	0.230	0.793	3.844	4.540		LSER Dataset 2017	155	
4-Formylpyridine	872-85-5	0.800	1.120	0.000	0.740	0.832	4.600	5.140		LSER Dataset 2017	155	
4-Heptanone	123-19-3	0.110	0.660	0.000	0.510	1.111	3.705	2.140		LSER Dataset 2017	155	
4-Hydroxyacetanilide	103-90-2	1.060	1.630	1.040	0.860	1.172	6.430	10.900		LSER Dataset 2017	150	

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
4-Hydroxybenzaldehyde	123-08-0	1.010	1.400	0.770	0.440	0.932	5.533	6.480		LSER Dataset 2017	155	
4-Hydroxybenzoic acid	99-96-7	0.930	0.900	0.810	0.560	0.990	4.867	6.780		LSER Dataset 2017	150	
4-Isopropyltoluene	99-87-6	0.610	0.490	0.000	0.190	1.280	4.590	0.500	0.200	LSER Dataset 2017	155	162
4-Methoxyacetophenone	100-06-1	0.920	1.580	0.000	0.530	1.214	5.935	3.230		LSER Dataset 2017	155	
4-Methoxyaniline	104-94-9	1.050	1.190	0.230	0.610	1.016	4.949	5.490		LSER Dataset 2017	155	
4-Methoxybenzoic acid	100-09-4	0.900	1.250	0.620	0.520	1.131	5.741	6.700		LSER Dataset 2017	150	
4-Methyl-1-pentene	691-37-2	0.070	0.080	0.000	0.040	0.911	2.418		36.224	LSER Dataset 2017		162
4-Methylacetophenone	122-00-9	0.840	1.000	0.000	0.520	1.155	5.080	3.450		LSER Dataset 2017	155	
4-Methylbenzaldehyde	104-87-0	0.860	1.000	0.000	0.420	1.014	4.592	3.130		LSER Dataset 2017	155	
4-Methyl-cis-2-pentene	691-38-3	0.100	0.080	0.000	0.080	0.911	2.444		32.509	LSER Dataset 2017		162
4-Methylheptane	589-53-7	0.000	0.000	0.000	0.000	1.236	3.483		2.729	LSER Dataset 2017		162
4-Methylnonane	17301-94-9	0.000	0.000	0.000	0.000	1.518	4.441		0.309	LSER Dataset 2017		162
4-Methyloctane	2216-34-4	0.000	0.000	0.000	0.000	1.377	3.961		0.910	LSER Dataset 2017		162
4-Methylpentan-2-ol	108-11-2	0.170	0.330	0.330	0.560	1.013	3.179	2.740	0.855	LSER Dataset 2017	155	161
4-Methylpentan-2-one	108-10-1	0.110	0.650	0.000	0.510	0.970	3.089	2.240	2.312	LSER Dataset 2017	155	161
4-Methylpyridine	108-89-4	0.630	0.820	0.000	0.550	0.816	3.640	3.620	0.767	LSER Dataset 2017	155	162
4-Nitroaniline	100-01-6	1.220	1.910	0.420	0.380	0.990	6.343	7.190		LSER Dataset 2017	150	
4-Nitrobenzoic acid	62-23-7	0.990	1.520	0.680	0.400	1.106	5.770	6.900		LSER Dataset 2017	150	
4-Nitrobenzyl chloride	100-14-1	0.600	0.520	0.000	0.140	1.154	3.325	3.770		LSER Dataset 2017	150	
4-Nitrophenol	100-02-7	1.070	1.720	0.820	0.260	0.949	5.876	7.810		LSER Dataset 2017	155	
4-n-Propylphenol	645-56-7	0.790	0.880	0.550	0.370	1.198	5.185	4.330		LSER Dataset 2017	155	
4-tert-Butylphenol	98-54-4	0.810	0.890	0.560	0.390	1.339	5.264	4.340	0.002	LSER Dataset 2017	155	161
5-Ethylidene-2-norbornene	16219-75-3	0.590	0.270	0.000	0.080	1.074	4.147		0.791	LSER Dataset 2017		162
5-Methyl-2-hexanone	110-12-3	0.110	0.680	0.000	0.530	1.111	3.713		0.693	LSER Dataset 2017		162
5-Methylnonane	15869-85-9	0.000	0.000	0.000	0.000	1.518	4.432		0.294	LSER Dataset 2017		162
Acenaphthene	83-32-9	1.600	1.050	0.000	0.220	1.259	6.469	2.360	0.000	LSER Dataset 2017	150	161
Acetaldehyde	75-07-0	0.210	0.670	0.000	0.450	0.406	1.230	2.570	119.064	LSER Dataset 2017	155	161
Acetic acid	64-19-7	0.270	0.650	0.610	0.450	0.465	1.750	4.910	2.080	LSER Dataset 2017	155	162
Acetonitrile	75-05-8	0.240	0.900	0.040	0.330	0.404	1.739	2.850	12.134	LSER Dataset 2017	150	162
Acetophenone	98-86-2	0.820	1.010	0.000	0.480	1.014	4.501	3.360	0.053	LSER Dataset 2017	155	162
Acetylene (ethyne)	74-86-2	0.190	0.470	0.120	0.050	0.304	0.070	0.000	4875.285	LSER Dataset 2017	150	162
Acetylsalicylic acid	50-78-2	0.780	1.690	0.710	0.670	1.288	6.279	8.500		LSER Dataset 2017	150	
Acrolein	107-02-8	0.320	0.610	0.000	0.460	0.504	1.757		36.559	LSER Dataset 2017		162
Ammonia	7664-41-7	0.140	0.350	0.140	0.620	0.208	0.680	3.150		LSER Dataset 2017	155	
Aniline	62-53-3	0.960	0.960	0.260	0.410	0.816	3.934		0.090	LSER Dataset 2017		162
Anthracene	120-12-7	2.290	1.340	0.000	0.280	1.454	7.568	3.030	183256169605.431	LSER Dataset 2017	150	161
Argon	7440-37-1	0.000	0.000	0.000	0.000	0.190	-0.688	-1.470		LSER Dataset 2017	155	
Benzaldehyde	100-52-7	0.820	1.000	0.000	0.390	0.873	4.008	2.950	0.173	LSER Dataset 2017	155	161
Benzamide	55-21-0	0.990	1.500	0.490	0.670	0.973	5.767	8.070		LSER Dataset 2017	155	
Benzene	71-43-2	0.610	0.520	0.000	0.140	0.716	2.786	0.630	12.647	LSER Dataset 2017	150	162
Benzil	134-81-6	1.450	1.590	0.000	0.620	1.637	7.611	4.870	0.000	LSER Dataset 2017	150	161
Benzoic acid	65-85-0	0.730	0.900	0.590	0.400	0.932	4.657	5.100	0.000	LSER Dataset 2017	150	161
Benzonitrile	100-47-0	0.740	1.110	0.000	0.330	0.871	4.039	3.090	0.108	LSER Dataset 2017	155	161
Benzotrifluoride	98-08-8	0.230	0.480	0.000	0.100	0.910	2.894	0.180	5.364	LSER Dataset 2017	155	161

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
Benzyl alcohol	100-51-6	0.800	0.870	0.330	0.560	0.916	4.221	4.860	0.011	LSER Dataset 2017	155	161
Benzyl chloride	100-44-7	0.820	0.860	0.000	0.140	0.980	4.353		0.174	LSER Dataset 2017		162
Benzyl ethyl ether	539-30-0	0.630	0.710	0.000	0.520	1.198	4.524		0.123	LSER Dataset 2017		162
Betulin	473-98-3	1.790	2.120	0.700	1.140	3.867	17.470	10.390		LSER Dataset 2017	150	
Bicyclohexyl	92-51-3	0.520	0.450	0.000	0.040	1.582	6.047		0.014	LSER Dataset 2017		162
Biotin	58-85-5	1.350	2.510	0.940	1.340	1.754	9.597	14.540		LSER Dataset 2017	165	
Biphenyl	92-52-4	1.360	0.990	0.000	0.260	1.324	6.014	1.950		LSER Dataset 2017	155	
Bromobenzene	108-86-1	0.880	0.730	0.000	0.090	0.891	4.041	1.070	0.568	LSER Dataset 2017	155	162
Bromoethane	74-96-4	0.370	0.400	0.000	0.120	0.565	2.120	0.540	62.951	LSER Dataset 2017	155	162
Bromomethane	74-83-9	0.400	0.430	0.000	0.100	0.425	1.630	0.600	218.273	LSER Dataset 2017	155	162
Bromotrichloromethane	75-62-7	0.640	0.460	0.000	0.000	0.792	3.294		5.200	LSER Dataset 2017		162
Bromotrifluoromethane	75-63-8	0.030	-0.020	0.000	0.010	0.478	0.829		1621.810	LSER Dataset 2017		162
But-1-en-3-yne	689-97-4	0.330	0.260	0.180	0.010	0.543	1.467	-0.030		LSER Dataset 2017	150	
Butane	106-97-8	0.000	0.000	0.000	0.000	0.672	1.615	-1.520	243.781	LSER Dataset 2017	155	162
Butanethiol	109-79-5	0.380	0.350	0.000	0.240	0.836	3.111	0.730	6.180	LSER Dataset 2017	155	162
Butanoic acid	107-92-6	0.210	0.620	0.600	0.450	0.747	2.830		0.135	LSER Dataset 2017	155	161
Butanone	78-93-3	0.170	0.700	0.000	0.510	0.688	2.287	2.720	12.303	LSER Dataset 2017	155	162
Butyl acetate	123-86-4	0.070	0.600	0.000	0.450	1.028	3.353	1.940	1.493	LSER Dataset 2017	155	162
Butyl acrylate	141-32-2	0.180	0.620	0.000	0.420	1.126	3.790		0.726	LSER Dataset 2017		162
Butyl ethyl ether	628-81-9	0.010	0.250	0.000	0.450	1.013	2.989		7.362	LSER Dataset 2017		162
Butyl formate	592-84-7	0.120	0.630	0.000	0.380	0.888	2.958		3.846	LSER Dataset 2017		162
Butylamine	109-73-9	0.220	0.350	0.160	0.610	0.772	2.618	3.110	12.388	LSER Dataset 2017	155	162
Butylbenzene	104-51-8	0.600	0.510	0.000	0.150	1.280	4.730	0.290	0.143	LSER Dataset 2017	155	162
butylcyclohexane	1678-93-9	0.260	0.230	0.000	0.000	1.409	4.806		0.175	LSER Dataset 2017		162
Butyraldehyde	123-72-8	0.190	0.650	0.000	0.450	0.688	2.270	2.330	14.962	LSER Dataset 2017	155	162
Caprolactam	105-60-2	0.590	1.720	0.380	0.750	0.961	4.914	7.980		LSER Dataset 2017	165	
Carbon dioxide	124-38-9	0.000	0.280	0.050	0.100	0.281	0.058	-0.080	26406.999	LSER Dataset 2017	155	161
Carbon monoxide	630-08-0	0.000	0.000	0.000	0.040	0.222	-0.836	-1.620	70212.273	LSER Dataset 2017	155	161
Carbon tetrachloride	56-23-5	0.460	0.380	0.000	0.000	0.739	2.823	-0.190	15.205	LSER Dataset 2017	150	162
Chlorobenzene	108-90-7	0.720	0.650	0.000	0.070	0.839	3.657	0.820	1.715	LSER Dataset 2017	155	161
Chlorodifluoromethane	75-45-6	-0.060	0.380	0.040	0.050	0.407	0.692		1037.528	LSER Dataset 2017		162
Chloroethane	75-00-3	0.230	0.400	0.000	0.100	0.513	1.678	0.460	159.956	LSER Dataset 2017	155	162
Chloroform	67-66-3	0.430	0.490	0.150	0.020	0.617	2.480	0.790	26.182	LSER Dataset 2017	155	162
Chloromethane	74-87-3	0.250	0.430	0.000	0.080	0.372	1.163	0.400	574.116	LSER Dataset 2017	155	162
Chloropentafluoroethane	76-15-3	-0.360	-0.120	0.000	0.000	0.601	0.543		907.821	LSER Dataset 2017		162
Chlorotrifluoromethane	75-72-9	-0.250	-0.050	0.000	0.000	0.425	0.209		3556.313	LSER Dataset 2017		162
cis-1,2-Dimethylcyclohexane	2207-01-4	0.280	0.100	0.000	0.000	1.127	3.795	-1.160	1.932	LSER Dataset 2017	155	162
cis-1,2-Dimethylcyclopentane	1192-18-3	0.250	0.100	0.000	0.000	0.986	3.273		6.295	LSER Dataset 2017		162
cis-1,3-Dimethylcyclohexane	638-04-0	0.200	0.100	0.000	0.000	1.127	3.533		2.864	LSER Dataset 2017		162
cis-1,3-Dimethylcyclopentane	2532-58-3	0.170	0.100	0.000	0.000	0.986	3.065		8.810	LSER Dataset 2017		162
cis-1,3-Pentadiene	1574-41-0	0.350	0.230	0.000	0.100	0.727	2.280		50.582	LSER Dataset 2017		162
cis-1,4-Dimethylcyclohexane	624-29-3	0.200	0.200	0.000	0.000	1.127	3.736		2.393	LSER Dataset 2017		162

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
cis-2-Butene	590-18-1	0.140	0.080	0.000	0.050	0.629	1.737		214.289	LSER Dataset 2017		162
cis-2-Heptene	6443-92-1	0.140	0.080	0.000	0.070	1.052	3.210		6.457	LSER Dataset 2017		162
cis-2-Hexene	7688-21-3	0.140	0.080	0.000	0.070	0.911	2.684		19.953	LSER Dataset 2017		162
cis-2-Octene	7642-04-8'	0.140	0.080	0.000	0.070	1.193	3.683		2.143	LSER Dataset 2017		162
cis-3-Heptene	7642-10-6'	0.130	0.080	0.000	0.070	1.052	3.143		7.079	LSER Dataset 2017		162
cis-3-Octene	14850-22-7	0.130	0.080	0.000	0.070	1.193	3.645		2.382	LSER Dataset 2017		162
cis-4-Octene	7642-15-1	0.130	0.080	0.000	0.070	1.193	3.607		2.404	LSER Dataset 2017		162
Cumene	98-82-8	0.600	0.490	0.000	0.160	1.139	4.084	0.220	0.608	LSER Dataset 2017	155	162
Cyclohepta-1,3,5-triene	544-25-2	0.760	0.460	0.000	0.180	0.857	3.442	0.730		LSER Dataset 2017	155	
Cycloheptane	291-64-5	0.350	0.100	0.000	0.000	0.986	3.704	-0.590	2.911	LSER Dataset 2017	45	162
Cycloheptanol	502-41-0	0.510	0.540	0.320	0.580	1.045	4.407	4.020		LSER Dataset 2017	155	
Cycloheptene	628-92-2	0.410	0.220	0.000	0.100	0.943	3.626		3.342	LSER Dataset 2017		162
Cyclohexane	110-82-7	0.310	0.100	0.000	0.000	0.845	2.964	-0.900	13.032	LSER Dataset 2017	155	162
Cyclohexanol	108-93-0	0.460	0.540	0.320	0.570	0.904	3.758	4.010	0.087	LSER Dataset 2017	155	162
Cyclohexanone	108-94-1	0.400	0.860	0.000	0.560	0.861	3.792	3.600	0.552	LSER Dataset 2017	155	162
Cyclohexene	110-83-8	0.400	0.200	0.000	0.100	0.802	3.021	-0.270	11.912	LSER Dataset 2017	155	162
Cyclohexylamine	108-91-8	0.330	0.560	0.160	0.580	0.945	3.796	3.370	1.265	LSER Dataset 2017	155	161
Cyclononane	293-55-0	0.430	0.100	0.000	0.000	1.268	4.829			LSER Dataset 2017		
Cyclooctane	292-64-8	0.410	0.100	0.000	0.000	1.127	4.329	-0.770	0.752	LSER Dataset 2017	64	162
Cyclopentane	287-92-3	0.260	0.100	0.000	0.000	0.705	2.477	-0.880	42.364	LSER Dataset 2017	155	162
Cyclopentanol	96-41-3	0.430	0.540	0.320	0.560	0.763	3.241	4.030	0.298	LSER Dataset 2017	155	161
Cyclopentanone	120-92-3	0.370	0.860	0.000	0.520	0.720	3.221	3.450	1.333	LSER Dataset 2017	155	161
Cyclopentene	142-29-0	0.340	0.200	0.000	0.100	0.662	2.402	-0.410	50.466	LSER Dataset 2017	155	162
Cyclopropane	75-19-4	0.410	0.230	0.000	0.000	0.423	1.314	-0.550	788.950	LSER Dataset 2017	155	161
Decane	124-18-5	0.000	0.000	0.000	0.000	1.518	4.686	-2.320	0.181	LSER Dataset 2017	64	162
Deuterium	7782-39-0	0.000	0.000	0.000	0.000	0.109	-1.200	-1.730		LSER Dataset 2017	155	
Dibromomethane	74-95-3	0.710	0.670	0.100	0.100	0.600	2.886	1.440	6.026	LSER Dataset 2017	155	162
DichloroDifluoromethane	75-71-8	0.040	0.040	0.000	0.040	0.530	0.998		651.628	LSER Dataset 2017		162
Dichlorofluoromethane	75-43-4	0.110	0.400	0.150	0.050	0.512	1.614		182.810	LSER Dataset 2017		162
Dichloromethane	75-09-2	0.390	0.570	0.100	0.050	0.494	2.019	0.960	58.345	LSER Dataset 2017	155	162
Diethyl disulfide	110-81-6	0.670	0.480	0.000	0.290	0.999	4.210	1.200	0.568	LSER Dataset 2017	155	162
Diethyl ether	60-29-7	0.040	0.260	0.000	0.440	0.731	2.012	1.170	71.779	LSER Dataset 2017	155	162
Diethyl sulfide	352-93-2	0.370	0.380	0.000	0.320	0.836	3.104	1.070	8.017	LSER Dataset 2017	155	162
Diethylamine	109-89-7	0.150	0.300	0.080	0.680	0.772	2.395	2.990	31.405	LSER Dataset 2017	155	162
Difluoromethane	75-10-5	-0.320	0.490	0.060	0.050	0.285	0.040		1690.441	LSER Dataset 2017		162
Diisobutyl ketone	108-83-8	0.050	0.600	0.000	0.510	1.392	4.244		0.224	LSER Dataset 2017		162
Diisopropyl ether	108-20-3	-0.060	0.200	0.000	0.540	1.013	2.517	1.050	19.815	LSER Dataset 2017	45	162
Diisopropyl sulfide	625-80-9	0.330	0.320	0.000	0.370	1.118	3.600	0.890	2.060	LSER Dataset 2017	155	161
Diisopropylamine	108-18-9	0.050	0.240	0.080	0.710	1.054	2.893	2.360		LSER Dataset 2017	155	
Dimethyl ether	115-10-6	0.000	0.270	0.000	0.410	0.449	1.285	1.400	577.142	LSER Dataset 2017	155	161
Dimethyl sulfide	75-18-3	0.400	0.430	0.000	0.270	0.554	2.037	1.180	64.565	LSER Dataset 2017	155	162
Dimethyl sulfoxide	67-68-5	0.520	1.740	0.000	0.880	0.613	3.459	7.410		LSER Dataset 2017	155	
Dimethyl Disulfide	624-92-0	0.700	0.600	0.000	0.220	0.717	3.052		3.828	LSER Dataset 2017		162
Dimethylacetylene	503-17-3	0.260	0.230	0.000	0.210	0.586	1.856		94.189	LSER Dataset 2017		162

Solute	CAS-RN	E	S	A	B	V	L	$\log K_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
Dimethylamine	124-40-3	0.190	0.300	0.080	0.660	0.490	1.600	3.150	203.236	LSER Dataset 2017	155	162
Di-n-butyl ether	142-96-1	0.000	0.250	0.000	0.450	1.295	3.924	0.690	0.573	LSER Dataset 2017	163	161
Di-n-butylamine	626-23-3	0.100	0.240	0.080	0.710	1.336	3.718	2.380	0.365	LSER Dataset 2017	155	162
Di-n-propyl ether	111-43-3	0.010	0.220	0.000	0.440	1.013	2.803	0.890	6.620	LSER Dataset 2017	64	161
Di-n-propyl sulfide	111-47-7	0.360	0.380	0.000	0.320	1.118	4.120	0.940	0.889	LSER Dataset 2017	155	162
Di-n-propylamine	142-84-7	0.120	0.300	0.080	0.680	1.054	3.351	2.680		LSER Dataset 2017	155	
Diphenyl sulfone	127-63-9	1.570	2.100	0.000	0.710	1.605	8.650	7.390		LSER Dataset 2017	150	
Diuron	330-54-1	1.280	1.600	0.570	0.700	1.599	8.060	8.000		LSER Dataset 2017	150	
Docosane	629-97-0	0.000	0.000	0.000	0.000	3.208	10.740	-3.570	0.000	LSER Dataset 2017	150	161
Dodecane	112-40-3	0.000	0.000	0.000	0.000	1.799	5.696		0.018	LSER Dataset 2017		162
Eicosane	112-95-8	0.000	0.000	0.000	0.000	2.927	9.731	-3.310	0.000	LSER Dataset 2017	150	161
Ethane	74-84-0	0.000	0.000	0.000	0.000	0.390	0.492	-1.340	4187.936	LSER Dataset 2017	155	162
Ethanethiol	75-08-1	0.390	0.420	0.000	0.200	0.554	2.079	0.840	70.307	LSER Dataset 2017	155	162
Ethanol	64-17-5	0.250	0.420	0.370	0.480	0.449	1.485	3.670	7.925	LSER Dataset 2017	155	162
Ethene	74-85-1	0.110	0.100	0.000	0.070	0.347	0.289	-0.940		LSER Dataset 2017	155	
Ethyl acetate	141-78-6	0.110	0.620	0.000	0.450	0.747	2.314	2.160	12.417	LSER Dataset 2017	155	162
Ethyl benzoate	93-89-0	0.690	0.850	0.000	0.460	1.214	5.075	2.670	0.037	LSER Dataset 2017	155	161
Ethyl formate	109-94-4	0.150	0.660	0.000	0.380	0.606	1.845	1.880	32.584	LSER Dataset 2017	155	162
Ethyl hexanoate	123-66-0	0.040	0.580	0.000	0.450	1.310	4.251	1.640	0.194	LSER Dataset 2017	155	161
Ethyl oxirane	75-21-8	0.250	0.740	0.070	0.320	0.341	1.371	2.150	174.985	LSER Dataset 2017	150	162
Ethyl pentanoate	539-82-2	0.050	0.580	0.000	0.450	1.169	3.769	1.830	0.545	LSER Dataset 2017	155	161
Ethyl tert-butyl ether	637-92-3	0.000	0.220	0.000	0.540	1.013	2.588	1.270	14.160	LSER Dataset 2017	163	161
Ethyl fluoride	353-36-6	0.050	0.350	0.000	0.100	0.408	0.576		918.333	LSER Dataset 2017		162
Ethyl iodide	75-03-6	0.640	0.400	0.000	0.150	0.649	2.573	0.540	17.947	LSER Dataset 2017	155	162
Ethyl isobutyrate	97-62-1	0.030	0.550	0.000	0.470	1.028	3.072		3.381	LSER Dataset 2017		162
Ethyl methacrylate	97-63-2	0.200	0.490	0.000	0.450	0.985	3.255		2.710	LSER Dataset 2017		162
Ethyl *n*-butyrate	105-54-4	0.070	0.580	0.000	0.450	1.028	3.271	1.830	2.234	LSER Dataset 2017	155	162
Ethyl *n*-octyl sulfide	3698-94-0	0.330	0.340	0.000	0.360	1.681	6.030		0.012	LSER Dataset 2017		162
Ethyl propionate	105-37-3	0.090	0.580	0.000	0.450	0.888	2.807	1.970	4.898	LSER Dataset 2017	155	162
Ethyl tert-butyl sulfide	14290-92-7	0.330	0.300	0.000	0.470	1.118	3.520		2.600	LSER Dataset 2017		162
Ethyl vinyl ether	109-92-2	0.160	0.370	0.000	0.380	0.688	1.823		68.707	LSER Dataset 2017		162
Ethylamine	75-04-7	0.240	0.350	0.160	0.610	0.490	1.677	3.300	136.593	LSER Dataset 2017	155	161
Ethylbenzene	100-41-4	0.610	0.510	0.000	0.150	0.998	3.778	0.580	1.279	LSER Dataset 2017	155	162
Ethylcyclohexane	1678-91-7	0.260	0.100	0.000	0.000	1.127	3.877	-1.580	1.710	LSER Dataset 2017	150	162
Ethylcyclopentane	1640-89-7	0.230	0.100	0.000	0.000	0.986	3.324		5.333	LSER Dataset 2017		162
Ethylene glycol	107-21-1	0.400	0.900	0.580	0.780	0.508	2.661		0.012	LSER Dataset 2017		162
Ethylenediamine	107-15-3	0.460	0.650	0.300	1.100	0.590	2.290		1.667	LSER Dataset 2017		162
Ethyleneimine	151-56-4	0.370	0.920	0.170	0.440	0.382	1.800		28.119	LSER Dataset 2017		162
Ferrocene	102-54-5	1.350	0.850	0.000	0.200	1.121	5.622	1.920	0.028	LSER Dataset 2017	150	161
Fluoranthene	206-44-0	2.380	1.550	0.000	0.240	1.585	8.827	3.440	0.000	LSER Dataset 2017	150	161
Fluorene	86-73-7	1.590	1.060	0.000	0.250	1.357	6.922	2.460	0.001	LSER Dataset 2017	155	161
Fluoro benzene	462-06-6	0.480	0.570	0.000	0.100	0.734	2.788	0.590	10.280	LSER Dataset 2017	155	162
Formaldehyde	50-00-0	0.220	0.700	0.000	0.330	0.265	0.730	2.020	518.800	LSER Dataset 2017	155	162
Formic acid	64-18-6	0.340	0.750	0.760	0.330	0.324	1.545		5.689	LSER Dataset 2017		162

Solute	CAS-RN	E	S	A	B	V	L	$\log K_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
Furan	110-00-9	0.370	0.510	0.000	0.130	0.536	1.913		79.983	LSER Dataset 2017		162
Haloperidol	52-86-8	1.930	1.560	0.440	1.770	2.798	13.192	11.300		LSER Dataset 2017	150	
Helium	7440-59-7	0.000	0.000	0.000	0.000	0.068	-1.741	-2.020		LSER Dataset 2017	155	
Heptanal	111-71-7	0.140	0.650	0.000	0.450	1.111	3.865	3.865		LSER Dataset 2017	155	
Heptane	142-82-5	0.000	0.000	0.000	0.000	1.095	3.173	-1.960	6.067	LSER Dataset 2017	155	162
Heptylamine	111-68-2	0.200	0.350	0.160	0.610	1.195	4.166	2.780		LSER Dataset 2017	155	
Hexa-1,5-diene	592-42-7	0.240	0.150	0.000	0.100	0.868	2.564	-0.740		LSER Dataset 2017	155	
Hexachlorobenzene	118-74-1	1.490	0.990	0.000	0.000	1.451	7.390	1.500	0.000	LSER Dataset 2017	150	161
Hexadecane	544-76-3	0.000	0.000	0.000	0.000	2.363	7.714		0.000	LSER Dataset 2017		162
Hexafluoropropylene	116-15-4	-0.500	-0.170	0.000	0.100	0.595	0.337	2.760		LSER Dataset 2017	155	
Hexanal	66-25-1	0.150	0.650	0.000	0.450	0.970	3.357	2.060	1.408	LSER Dataset 2017	155	161
Hexane	110-54-3	0.000	0.000	0.000	0.000	0.954	2.668	-1.820	20.277	LSER Dataset 2017	155	162
Hexanoic acid	142-62-1	0.170	0.600	0.600	0.450	1.028	3.920	4.560	0.006	LSER Dataset 2017	155	162
Hexyl acetate	142-92-7	0.060	0.600	0.000	0.450	1.310	4.351	1.660	0.123	LSER Dataset 2017	155	161
Hexylamine	111-26-2	0.200	0.350	0.160	0.610	1.054	3.655	2.900		LSER Dataset 2017	155	
Hexylbenzene	1077-16-3	0.590	0.500	0.000	0.150	1.562	5.720	0.030		LSER Dataset 2017	155	
Hydrogen	74-90-8	0.210	0.890	0.400	0.060	0.263	1.010	-1.720		LSER Dataset 2017	155	
Hydroquinone	123-31-9	1.060	1.270	1.060	0.570	0.834	4.827	8.820		LSER Dataset 2017	150	
Indan	496-11-7	0.830	0.620	0.000	0.170	1.031	4.590	1.070	0.207	LSER Dataset 2017	155	162
Iodobenzene	591-50-4	1.190	0.820	0.000	0.120	0.975	4.502	1.280	0.142	LSER Dataset 2017	155	162
Iodomethane	74-88-4	0.680	0.430	0.000	0.130	0.508	2.106	0.650	53.951	LSER Dataset 2017	155	162
Isoamyl acetate	4245-35-6	0.130	0.570	0.000	0.420	1.267	4.128	1.620		LSER Dataset 2017	155	
Isoamyl formate	110-45-2	0.090	0.600	0.000	0.400	1.028	3.306	1.560		LSER Dataset 2017	155	
Isobutene	115-11-7	0.120	0.080	0.000	0.080	0.629	1.579		303.389	LSER Dataset 2017		162
Isobutyl acetate	110-19-0	0.050	0.570	0.000	0.470	1.028	3.161	1.730	2.377	LSER Dataset 2017	155	162
Isobutyl formate	542-55-2	0.100	0.600	0.000	0.400	0.888	2.789	1.630	5.470	LSER Dataset 2017	155	162
Isobutyl isobutanoate	97-85-8	0.000	0.500	0.000	0.470	1.310	3.885	1.240		LSER Dataset 2017	155	
Isobutyl mercaptan	513-44-0	0.360	0.330	0.000	0.240	0.836	3.071		9.268	LSER Dataset 2017		162
Isobutylamine	78-81-9	0.200	0.320	0.160	0.630	0.772	2.469		18.578	LSER Dataset 2017		162
Isobutylbenzene	538-93-2	0.580	0.470	0.000	0.150	1.280	4.500	-0.120	0.265	LSER Dataset 2017	155	162
Isoflurane	26675-46-7	-0.240	0.500	0.100	0.100	0.801	1.576	-0.070	40.307	LSER Dataset 2017	155	161
Isopentyl acetate	123-92-2	0.050	0.570	0.000	0.470	1.169	3.740			LSER Dataset 2017		
Isophorone	78-59-1	0.510	1.120	0.000	0.530	1.241	4.740		0.058	LSER Dataset 2017		162
Isopropanol	67-63-0	0.210	0.360	0.330	0.560	0.590	1.764	3.480	6.053	LSER Dataset 2017	155	162
Isopropyl acetate	108-21-4	0.060	0.570	0.000	0.470	0.888	2.546	1.940	8.054	LSER Dataset 2017	155	162
Isopropyl formate	625-55-8	0.090	0.600	0.000	0.400	0.747	2.230	1.480	17.249	LSER Dataset 2017	155	161
Isopropyl mercaptan	75-33-2	0.340	0.350	0.000	0.250	0.695	2.417	0.780	36.898	LSER Dataset 2017	155	162
Isopropylamine	75-31-0	0.180	0.320	0.160	0.610	0.631	1.908		77.804	LSER Dataset 2017		162
Isopropylcyclopentane	3875-51-2	0.220	0.100	0.000	0.000	1.127	3.871		2.148	LSER Dataset 2017		162
Krypton	7439-90-9'	0.000	0.000	0.000	0.000	0.246	-0.211	-1.210		LSER Dataset 2017	155	
m-Cresol	108-39-4	0.820	0.880	0.570	0.340	0.916	4.310		0.018	LSER Dataset 2017		162
m-Cymene	535-77-3	0.620	0.490	0.000	0.190	1.280	4.556		0.232	LSER Dataset 2017		162
m-Diethylbenzene	141-93-5	0.640	0.500	0.000	0.180	1.280	4.686		0.160	LSER Dataset 2017		162
Mesitylene	108-67-8	0.650	0.520	0.000	0.190	1.139	4.344	0.660	0.337	LSER Dataset 2017	155	162

Solute	CAS-RN	E	S	A	B	V	L	$\log K_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
Methane	74-82-8	0.000	0.000	0.000	0.000	0.250	-0.323	-1.460	31574.571	LSER Dataset 2017	155	161
Methanol	67-56-1	0.280	0.440	0.430	0.470	0.308	0.970	3.740	16.827	LSER Dataset 2017	155	162
Methoxyflurane	76-38-0	0.110	0.670	0.170	0.050	0.870	2.864	0.820		LSER Dataset 2017	155	
Methyl 4-hydroxybenzoate	99-76-3	0.900	1.370	0.690	0.450	1.131	5.665	6.840		LSER Dataset 2017	150	
Methyl acetate	79-20-9	0.140	0.640	0.000	0.450	0.606	1.911	2.300	28.576	LSER Dataset 2017	155	162
Methyl benzoate	93-58-3	0.730	0.850	0.000	0.460	1.073	4.704	2.880	0.054	LSER Dataset 2017	155	161
Methyl butanoate	623-42-7	0.110	0.600	0.000	0.450	0.888	2.893	2.080	4.295	LSER Dataset 2017	155	162
Methyl cyclohexyl ketone	823-76-7	0.370	1.180	0.000	0.420	1.143	4.620	2.860		LSER Dataset 2017	155	
Methyl cyclopropyl ketone	765-43-5	0.320	1.170	0.000	0.380	0.720	3.137	3.380		LSER Dataset 2017	155	
Methyl ethyl sulfide	624-89-5	0.390	0.360	0.000	0.300	0.695	2.372	1.100	21.330	LSER Dataset 2017	155	162
Methyl formate	107-31-3	0.190	0.680	0.000	0.380	0.465	1.285	2.040	77.983	LSER Dataset 2017	155	162
Methyl hexanoate	106-70-7	0.080	0.600	0.000	0.450	1.169	3.874	I .83	0.473	LSER Dataset 2017	155	161
Methyl pentanoate	624-24-8	0.110	0.600	0.000	0.450	1.028	3.392	1.880	1.387	LSER Dataset 2017	155	161
Methyl phenyl ether	100-66-3	0.710	0.750	0.000	0.290	0.916	3.890	1.800	0.483	LSER Dataset 2017	155	162
Methyl propionate	554-12-1	0.130	0.600	0.000	0.450	0.747	2.431	2.150	11.350	LSER Dataset 2017	155	162
Methyl tert-butyl ether	1634-04-4	0.020	0.280	0.000	0.540	0.872	2.270	1.620	30.154	LSER Dataset 2017	155	161
Methyl trimethylacetate	598-98-1	0.050	0.540	0.000	0.450	1.028	2.932	1.760		LSER Dataset 2017	155	
Methyl acrylate	96-33-3	0.250	0.660	0.000	0.420	0.704	2.360		11.614	LSER Dataset 2017		162
Methyl fluoride	593-53-3	0.070	0.350	0.000	0.090	0.267	0.057		3819.443	LSER Dataset 2017		162
Methyl mercaptan	74-93-1	0.400	0.600	0.000	0.120	0.413	1.640		201.372	LSER Dataset 2017		162
Methyl n-butyl sulfide	628-29-5	0.370	0.390	0.000	0.340	0.977	3.600		2.080	LSER Dataset 2017		162
Methyl tert-butyl sulfide	6163-64-0	0.340	0.270	0.000	0.480	0.977	3.150		6.353	LSER Dataset 2017		162
Methyl-2-pyrrolidone	872-50-4	0.490	1.300	0.000	0.790	0.820	3.832		0.046	LSER Dataset 2017		162
Methylacetylene	74-99-7	0.190	0.250	0.130	0.150	0.445	1.025		580.764	LSER Dataset 2017		162
Methylamine	74-89-5	0.250	0.350	0.160	0.580	0.349	1.300	3.340	353.183	LSER Dataset 2017	155	162
Methylcyclohexane	108-87-2	0.240	0.100	0.000	0.000	0.986	3.323	-1.250	6.138	LSER Dataset 2017	155	162
Methylcyclopentane	96-37-7	0.230	0.100	0.000	0.000	0.845	2.816	-1.170	18.323	LSER Dataset 2017	155	162
Methylpyrrolidine	120-94-5	0.300	0.980	0.000	0.400	0.804	3.132		13.459	LSER Dataset 2017		162
m-Ethyltoluene	620-14-4	0.630	0.510	0.000	0.180	1.139	4.275		0.425	LSER Dataset 2017		162
m-Methylstyrene	100-80-1	0.870	0.650	0.000	0.180	1.096	4.375		0.253	LSER Dataset 2017		162
Monuron	150-68-5	1.140	1.500	0.470	0.780	1.477	7.180	7.630		LSER Dataset 2017	150	
Morpholine	110-91-8	0.430	0.790	0.060	0.910	0.722	3.289	5.260	1.371	LSER Dataset 2017	155	161
m-Xylene	108-38-3	0.620	0.520	0.000	0.160	0.998	3.839	0.610	1.119	LSER Dataset 2017	155	162
N,N-Dimethylaniline	121-69-7	0.960	0.840	0.000	0.420	1.098	4.701	2.530	0.097	LSER Dataset 2017	155	162
N,N-Dimethylformamide	68-12-2	0.370	1.310	0.000	0.730	0.647	3.173	5.730		LSER Dataset 2017	155	
Naphthalene	91-20-3	1.340	0.920	0.000	0.200	1.085	5.161	1.760	0.010	LSER Dataset 2017	155	161
Naproxen	22204-53-1	1.510	2.020	0.600	0.670	1.782	9.207	8.800		LSER Dataset 2017	150	
n-Butylacetamide	1119-49-9	0.320	1.290	0.400	0.720	1.070	4.582	6.830	0.004	LSER Dataset 2017	155	161
Neon	7440-01-9'	0.000	0.000	0.000	0.000	0.085	-1.575	-1.960		LSER Dataset 2017	155	
Neopentane	463-82-1	0.000	0.000	0.000	0.000	0.813	1.820		171.396	LSER Dataset 2017		162
Nitrobenzene	98-95-3	0.870	1.110	0.000	0.280	0.891	4.557	3.020	0.032	LSER Dataset 2017	155	161
Nitroethane	79-24-3	0.270	0.950	0.020	0.330	0.565	2.414	2.720	2.782	LSER Dataset 2017	155	161
Nitrogen	55-63-0	0.490	2.040	0.000	0.340	1.230	6.007	-1.800		LSER Dataset 2017	155	
Nitromethane	75-52-5	0.310	0.950	0.060	0.320	0.424	1.892	2.950	4.645	LSER Dataset 2017	155	161

Solute	CAS-RN	E	S	A	B	V	L	$\log K_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
Nitrous oxide	10024-97-2	0.070	0.350	0.000	0.100	0.281	0.164	-0.230		LSER Dataset 2017	155	
N-Methylaniline	100-61-8	0.950	0.900	0.170	0.430	0.957	4.478	3.440	0.060	LSER Dataset 2017	155	162
N-Methylmorpholine	109-02-4	0.330	0.740	0.000	0.900	0.863	3.270	4.640		LSER Dataset 2017	155	
N-Methylpiperidine	626-67-5	0.320	0.340	0.000	0.700	0.945	3.330	2.850		LSER Dataset 2017	155	
n-Octane	111-65-9	0.000	0.000	0.000	0.000	1.236	3.677	-2.110	1.871	LSER Dataset 2017	155	162
n-Octylamine	111-86-4	0.190	0.350	0.160	0.610	1.336	4.520	2.680		LSER Dataset 2017	155	
Nonadecane	629-92-5	0.000	0.000	0.000	0.000	2.786	9.226	-3.210	0.000	LSER Dataset 2017	150	161
Nonan-2-one	821-55-6	0.120	0.680	0.000	0.510	1.392	4.735	1.830		LSER Dataset 2017	155	
Nonan-5-one	502-56-7	0.100	0.660	0.000	0.510	1.392	4.698	1.940		LSER Dataset 2017	155	
Nonanal	124-19-6	0.150	0.650	0.000	0.450	1.392	4.856	1.520		LSER Dataset 2017	155	
Nonane	111-84-2	0.000	0.000	0.000	0.000	1.377	4.182	-2.150	0.581	LSER Dataset 2017	150	162
o-Cresol	95-48-7	0.840	0.860	0.520	0.310	0.916	4.218	4.310		LSER Dataset 2017	155	
Octadecane	593-45-3	0.000	0.000	0.000	0.000	2.645	8.722	-3.040	0.000	LSER Dataset 2017	150	161
Octafluorocyclobutane	115-25-3	-0.510	-0.390	0.000	0.070	0.705	0.722		313.329	LSER Dataset 2017		162
Octanal	124-13-0	0.160	0.650	0.000	0.450	1.252	4.361	1.680		LSER Dataset 2017	155	
o-Cymene	527-84-4	0.670	0.530	0.000	0.190	1.280	4.622		0.220	LSER Dataset 2017		162
o-Diethylbenzene	135-01-3	0.690	0.540	0.000	0.180	1.280	4.732		0.141	LSER Dataset 2017		162
o-Methylstyrene	611-15-4	0.920	0.650	0.000	0.180	1.096	4.352		0.247	LSER Dataset 2017		162
o-Toluidine	95-53-4	0.970	0.920	0.230	0.450	0.957	4.442	4.060		LSER Dataset 2017	155	
Oxygen	7782-44-7	0.000	0.000	0.000	0.000	0.183	-0.723	-1.510		LSER Dataset 2017	155	
o-Xylene	95-47-6	0.660	0.560	0.000	0.160	0.998	3.939	0.660	0.887	LSER Dataset 2017	64	162
Ozone	10028-15-6	0.000	0.100	0.090	0.000	0.242	0.039	-0.600		LSER Dataset 2017	150	
p-Cresol	106-44-5	0.820	0.870	0.570	0.320	0.916	4.312	4.500		LSER Dataset 2017	155	
p-Diethylbenzene	105-05-5	0.650	0.500	0.000	0.180	1.280	4.732		0.137	LSER Dataset 2017		162
p-Diisopropylbenzene	100-18-5	0.620	0.470	0.000	0.200	1.562	5.315		0.033	LSER Dataset 2017		162
Penta-1,4-diene	591-93-5	0.190	0.140	0.000	0.100	0.727	1.998	-0.680	97.949	LSER Dataset 2017	155	162
Pentachloroethane	76-01-7	0.650	0.660	0.170	0.060	1.002	4.267	1.020	0.486	LSER Dataset 2017	155	161
Pentadecane	629-62-9	0.000	0.000	0.000	0.000	2.222	7.209		0.001	LSER Dataset 2017		162
Pentafluoroethane	354-33-6	-0.510	0.000	0.110	0.060	0.479	0.100		1377.209	LSER Dataset 2017		162
Pentanal	110-62-3	0.160	0.650	0.000	0.450	0.829	2.851	2.220	4.447	LSER Dataset 2017	155	161
Pentane	109-66-0	0.000	0.000	0.000	0.000	0.813	2.162	-1.700	68.008	LSER Dataset 2017	155	161
Pentanoic acid	109-52-4	0.210	0.600	0.600	0.450	0.888	3.380	4.520	0.026	LSER Dataset 2017	155	162
Pentyl acetate	628-63-7	0.070	0.600	0.000	0.450	1.169	3.844	1.840	0.434	LSER Dataset 2017	155	161
Pentyl propanoate	624-54-4	0.050	0.560	0.000	0.450	1.310	4.331	1.550	0.162	LSER Dataset 2017	155	161
Pentyl mercaptan	110-66-7	0.370	0.430	0.000	0.210	0.977	3.624		1.841	LSER Dataset 2017		162
Pentylamine	110-58-7	0.210	0.350	0.160	0.610	0.913	3.139	3.000	3.999	LSER Dataset 2017	155	162
Pentylbenzene	538-68-1	0.590	0.510	0.000	0.150	1.421	5.230	0.170		LSER Dataset 2017	155	
Pentylcyclopentane	3741-00-2	0.220	0.080	0.000	0.000	1.409	4.600	-1.870		LSER Dataset 2017	155	
Phenanthrene	85-01-8	2.060	1.290	0.000	0.260	1.454	7.632	2.800	0.000	LSER Dataset 2017	150	161
Phenetole	103-73-1	0.680	0.700	0.000	0.320	1.057	4.242	1.630	0.206	LSER Dataset 2017	155	162
Phenol	108-95-2	0.810	0.890	0.600	0.300	0.775	3.766	4.850	0.039	LSER Dataset 2017	155	161
Phenyl methyl sulfide	100-68-5	1.070	0.920	0.000	0.260	1.021	4.659	2.000		LSER Dataset 2017	155	
Phenyl mercaptan	108-98-5	1.000	0.800	0.090	0.160	0.880	4.110	1.870	0.202	LSER Dataset 2017	155	162
Phenylhydrazine	100-63-0	1.120	1.090	0.340	0.530	0.916	4.900		0.003	LSER Dataset 2017		162

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
Piperidine	110-89-4	0.420	0.460	0.180	0.680	0.804	3.304		4.285	LSER Dataset 2017		162
p-Methylstyrene	622-97-9	0.870	0.650	0.000	0.180	1.096	4.399		0.244	LSER Dataset 2017		162
Prop-2-en-1-ol	107-18-6	0.340	0.440	0.440	0.470	0.547	1.951	3.690		LSER Dataset 2017	155	
Propane	74-98-6	0.000	0.000	0.000	0.000	0.531	1.050	-1.440	952.796	LSER Dataset 2017	155	162
Propanoic acid	79-09-4	0.230	0.650	0.600	0.450	0.606	2.290	4.740	0.495	LSER Dataset 2017	155	162
Propanone	67-64-1	0.180	0.700	0.040	0.490	0.547	1.696	2.790	30.761	LSER Dataset 2017	155	162
Propanonitrile	107-12-0	0.160	0.900	0.020	0.360	0.545	2.082	2.820	6.310	LSER Dataset 2017	155	162
Propargyl alcohol	107-19-7	0.410	0.570	0.380	0.590	0.504	2.050		2.084	LSER Dataset 2017		162
Propene	115-07-1	0.100	0.080	0.000	0.070	0.488	0.946	-0.970	1161.449	LSER Dataset 2017	155	162
Propyl acetate	109-60-4	0.090	0.600	0.000	0.450	0.888	2.819	2.050	4.457	LSER Dataset 2017	155	162
Propyl butanoate	105-66-8	0.050	0.560	0.000	0.450	1.169	3.783	1.670	0.017	LSER Dataset 2017	155	161
Propyl formate	110-74-7	0.130	0.630	0.000	0.380	0.747	2.433	1.820	10.990	LSER Dataset 2017	155	162
Propyl chloride	540-54-5	0.220	0.400	0.000	0.100	0.654	2.202	0.240	45.920	LSER Dataset 2017	155	162
Propyl mercaptan	107-03-9	0.390	0.350	0.000	0.240	0.695	2.685		20.559	LSER Dataset 2017		162
Propyl propionate	106-36-5	0.070	0.560	0.000	0.450	1.028	3.338	1.790	1.862	LSER Dataset 2017	155	162
Propylamine	107-10-8	0.230	0.350	0.160	0.610	0.631	2.141	3.220	41.305	LSER Dataset 2017	155	162
Propylbenzene	103-65-1	0.600	0.500	0.000	0.150	1.139	4.230	0.390	0.463	LSER Dataset 2017	155	162
Propylcyclohexane	1678-92-8	0.260	0.230	0.000	0.000	1.268	4.313		0.558	LSER Dataset 2017		162
Propylcyclopentane	2040-96-2	0.230	0.100	0.000	0.000	1.127	3.803	-1.560	1.648	LSER Dataset 2017	155	162
Propyne	80-46-6	0.810	0.890	0.560	0.420	1.480	6.200	0.350		LSER Dataset 2017	155	
p-Toluidine	106-49-0	0.920	0.950	0.230	0.450	0.957	4.452	4.090		LSER Dataset 2017	155	
p-Xylene	106-42-3	0.610	0.520	0.000	0.160	0.998	3.839	0.590	1.169	LSER Dataset 2017	155	162
Pyrene	129-00-0	2.810	1.710	0.000	0.280	1.585	8.833	3.500	0.000	LSER Dataset 2017	150	161
Pyridine	110-86-1	0.630	0.840	0.000	0.520	0.675	3.022	3.440	2.773	LSER Dataset 2017	155	162
Pyrimidine	289-95-2	0.610	0.930	0.000	0.670	0.634	2.881		2.249	LSER Dataset 2017		162
Pyrrole	109-97-7	0.610	0.730	0.410	0.290	0.577	2.865		1.096	LSER Dataset 2017		162
Pyrrolidine	123-75-1	0.410	0.950	0.240	0.420	0.663	2.877		8.395	LSER Dataset 2017		162
Quinoline	91-22-5	1.270	0.970	0.000	0.540	1.044	5.457	4.200	0.011	LSER Dataset 2017	155	162
Radon	10043-92-2	0.000	0.000	0.000	0.000	0.384	0.877	-0.650		LSER Dataset 2017	155	
Salicylamide	65-45-2	1.160	1.580	0.610	0.510	1.032	5.818	7.600		LSER Dataset 2017	150	
sec-Butyl mercaptan	513-53-1	0.340	0.360	0.000	0.250	0.836	2.950		10.765	LSER Dataset 2017		162
sec-Butylbenzene	135-98-8	0.600	0.480	0.000	0.160	1.280	4.506	0.330	0.224	LSER Dataset 2017	155	162
Styrene	100-42-5	0.850	0.650	0.000	0.160	0.955	3.856	0.950	0.817	LSER Dataset 2017	64	162
Sulfur dioxide	7446-09-5'	0.370	0.660	0.280	0.100	0.347	0.778	1.530		LSER Dataset 2017	150	
Sulfur hexafluoride	2551-62-4	-0.600	-0.200	0.000	0.000	0.464	-0.120	-2.230		LSER Dataset 2017	155	
Teflurane	124-72-1	-0.070	0.210	0.200	0.000	0.636	1.370	-0.370		LSER Dataset 2017	155	
tert-Amyl methyl ether	994-05-8	0.050	0.280	0.000	0.540	1.013	2.840	1.595	9.999	LSER Dataset 2017	163	166
tert-Butanol	75-65-0	0.180	0.300	0.310	0.600	0.731	1.963	3.280	5.581	LSER Dataset 2017	167	161
tert-Butyl mercaptan	75-66-1	0.280	0.300	0.000	0.270	0.836	2.550		24.155	LSER Dataset 2017		162
tert-Butylbenzene	98-06-6	0.620	0.490	0.000	0.160	1.280	4.413	0.320	0.290	LSER Dataset 2017	155	162
Tetrachloroethylene	127-18-4	0.640	0.440	0.000	0.000	0.837	3.584	-0.070	2.472	LSER Dataset 2017	155	162
Tetracosane	646-31-1	0.000	0.000	0.000	0.000	3.490	11.758	-3.840	0.000	LSER Dataset 2017	150	161
Tetradecane	629-59-4	0.000	0.000	0.000	0.000	2.081	6.705		0.002	LSER Dataset 2017		162
Tetrafluoroethylene	116-14-3	-0.310	-0.100	0.000	0.000	0.418	-0.050		3273.407	LSER Dataset 2017		162

Solute	CAS-RN	E	S	A	B	V	L	$logK_w$	p^0 at 298K, kPa	Coefficient Source	Source (K_w)	Source (p^0)
Tetrafluoromethane	75-73-0	-0.580	-0.260	0.000	0.000	0.320	-0.817	-2.290		LSER Dataset 2017	155	
Tetrahydrofuran	109-99-9	0.290	0.520	0.000	0.480	0.622	2.636	2.550	21.528	LSER Dataset 2017	155	162
Tetrahydrothiophene	110-01-0	0.620	0.660	0.000	0.260	0.727	3.061		2.443	LSER Dataset 2017		162
Thiophene	110-02-1	0.690	0.570	0.000	0.150	0.641	2.819	1.040	10.520	LSER Dataset 2017	155	162
Toluene	108-88-3	0.600	0.520	0.000	0.140	0.857	3.325	0.650	3.802	LSER Dataset 2017	155	162
trans 1,2-Dichloroethene	156-60-5	0.430	0.410	0.090	0.050	0.592	2.278	0.360		LSER Dataset 2017	150	
trans-1,2-Dimethylcyclohexane	6876-23-9	0.230	0.200	0.000	0.000	1.127	3.728		2.582	LSER Dataset 2017		162
trans-1,2-Dimethylcyclopentane	822-50-4	0.190	0.100	0.000	0.000	0.986	3.099		8.531	LSER Dataset 2017		162
trans-1,3-Dimethylcyclopentane	1759-58-6	0.160	0.100	0.000	0.000	0.986	3.075		8.590	LSER Dataset 2017		162
trans-1,3-pentadiene	2004-70-8	0.350	0.230	0.000	0.100	0.727	2.250		54.828	LSER Dataset 2017		162
trans-1,4-Dimethylcyclohexane	2207-04-7'	0.190	0.100	0.000	0.000	1.127	3.538	-1.550	3.027	LSER Dataset 2017	155	162
trans-2-butene	624-64-6	0.130	0.080	0.000	0.050	0.629	1.664		234.423	LSER Dataset 2017		162
trans-2-hexene	4050-45-7	0.120	0.080	0.000	0.060	0.911	2.655		20.701	LSER Dataset 2017		162
trans-2-octene	13389-42-9	0.120	0.070	0.000	0.070	1.193	3.668		2.183	LSER Dataset 2017		162
trans-2-pentene	646-04-8	0.130	0.080	0.000	0.070	0.770	2.187		67.453	LSER Dataset 2017		162
trans-3-octene	14919-01-8	0.120	0.080	0.000	0.070	1.193	3.645		2.307	LSER Dataset 2017		162
trans-4-octene	14850-23-8	0.110	0.080	0.000	0.070	1.193	3.593		2.371	LSER Dataset 2017		162
trans-Stilbene	103-30-0	1.450	1.040	0.000	0.340	1.563	7.525	2.780	0.000	LSER Dataset 2017	150	161
Trichloroethene	79-01-6	0.520	0.370	0.080	0.030	0.715	2.997	0.320	9.817	LSER Dataset 2017	155	162
Trichlorofluoromethane	75-69-4	0.210	0.240	0.000	0.070	0.634	1.950		106.170	LSER Dataset 2017		162
Tricosane	638-67-5	0.000	0.000	0.000	0.000	3.349	11.252	-3.720	0.000	LSER Dataset 2017	150	161
Tridecane	629-50-5	0.000	0.000	0.000	0.000	1.940	6.200		0.006	LSER Dataset 2017		162
Triethylamine	121-44-8	0.100	0.150	0.000	0.790	1.054	3.040	2.360	6.034	LSER Dataset 2017	155	161
Triethylphosphate	78-40-0	0.000	1.000	0.000	1.060	1.393	4.750	5.530	0.036	LSER Dataset 2017	155	161
Trifluoromethane	75-46-7	-0.430	0.180	0.110	0.030	0.303	-0.274		4698.941	LSER Dataset 2017		162
Trimethylamine	75-50-3	0.140	0.200	0.000	0.670	0.631	1.620	2.350	233.260	LSER Dataset 2017	155	161
Undecan-2-one	112-44-7	0.120	0.650	0.000	0.450	1.674	5.808	1.580		LSER Dataset 2017	155	
Undecane	1120-21-4	0.000	0.000	0.000	0.000	1.659	5.191		0.056	LSER Dataset 2017		162
Vinyl acetate	108-05-4	0.220	0.550	0.000	0.430	0.704	2.152	1.710	16.013	LSER Dataset 2017	64	161
Vinyl chloride	75-01-4	0.260	0.380	0.000	0.050	0.470	1.404		398.107	LSER Dataset 2017		162
Vinyl propionate	105-38-4	0.220	0.530	0.000	0.460	0.845	2.834		5.794	LSER Dataset 2017		162
Vinylacetonitrile	109-75-1	0.280	0.810	0.000	0.430	0.643	2.536		2.460	LSER Dataset 2017		162
Water	7732-18-5	0.000	0.450	0.820	0.350	0.167	0.260	4.640	3.170	LSER Dataset 2017	155	168
Xenon	7440-63-3	0.000	0.000	0.000	0.000	0.329	0.378	-0.970		LSER Dataset 2017	155	
α-Methylstyrene	98-83-9	0.850	0.640	0.000	0.190	1.096	4.292	0.960	0.398	LSER Dataset 2017	167	169

Table D.2: ILs and their ABSM values for log K at 298 K.

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*l*	N	R^2	SD	Year	Source
[(C3COOMe)MIM]+	[DCA]-	0.997	0.498	2.981	4.647	0.487	0.562	60	0.993	0.081	2020	This work
[(Hexom)2Im]+	[NTf2]-	-0.314	-0.479	2.076	2.376	0.287	0.835	34		0.050	2017	[14]
[(Meo)2Im]+	[NTf2]-	-0.762	-0.013	2.557	2.427	1.157	0.584	48	0.989	0.084	2011	[26; 27]
[1-PrOHPy]+	[DCA]-	-1.270	1.080	1.850	4.850	2.330	0.589	63	0.992	0.060	2017	[170]
[2,4,6-M3Py]+	[NTf2]-	0.000	0.280	1.610	1.400	0.590	0.420	21	0.98		2013	[171]
[2,6-M2Py]+	[NTf2]-	0.000	0.180	1.700	1.350	0.300	0.370	21	0.99		2013	[171]
[2-MPy]+	[NTf2]-	0.000	0.060	1.620	1.190	0.170	0.310	21	0.99		2013	[171]
[3,5-M2Py]+	[NTf2]-	0.000	0.160	1.550	1.110	0.280	0.370	21	0.99		2013	[171]
[3-MBPy]+	[TDI]-	-0.419	0.104	2.269	3.367	0.413	0.772	66	0.993	0.069	2014	[64]
[3-MBPy]+	[Trif]-	-0.564	0.035	2.697	3.977	-0.050	0.699	36		0.070	2017	[14]
[4-CNBPy]+	[NTf2]-	-0.768	0.086	2.810	2.685	0.553	0.691	64		0.091	2017	[14]
[AllMIm]+	[DCA]-	-0.815	0.534	2.719	4.550	0.450	0.514	65	0.993	0.084	2017	[14]
[AllMIm]+	[NTf2]-	-0.420	0.081	2.493	2.369	0.599	0.643	64	0.99	0.079	2017	[14]
[B3EP]+	[DEP]-	-0.357	-0.224	1.663	5.859	0.000	0.844	49	0.984	0.089	2017	[14]
[B4MPy]+	[DCA]-	-0.817	0.597	2.561	4.438	0.474	0.679	53	0.995	0.074	2020	This work
[BM2Im]+	[NTf2]-	-0.641	0.000	2.429	2.663	0.521	0.721	60		0.085	2017	[14]
[BMIM]+	[[(CH3)2PO4]-	-0.654	0.323	2.129	7.972	0.372	0.700	55	0.979	0.143	2020	This work
[BMIM]+	[BETI]-	-0.460	0.141	2.206	1.980	0.696	0.613	53	0.989	0.093	2011	[74]
[BMIm]+	[BF4]-	-0.600	0.356	2.534	3.312	0.284	0.604	66	0.997	0.099	2011	[26]
[BMIM]+	[CH3SO4]-	-0.506	0.262	2.169	3.138	0.052	0.499	22	0.947	0.149	2020	This work
[BMIM]+	[Cl]-	-1.199	0.56	2.95	8.251	0.101	0.644	54	0.986	0.1313749	2020	This work
[BMIM]+	[DCA]-	-0.773	0.435	2.553	4.844	0.505	0.658	67		0.082	2017	[14]
[BMIM]+	[MeSO3]-	-0.882	0.388	2.693	6.394	0.238	0.639	54	0.987	0.106	2020	This work
[BMIm]+	[NTf2]-	-0.394	0.089	1.969	2.283	0.873	0.696	104	0.994	0.111	2011	[26]
[BMIm]+	[OS]-	-0.228	-0.287	1.940	4.862	-0.302	0.880	56	0.984	0.116	2011	[26]
[BMIm]+	[PF6]-	-0.460	-0.191	2.747	2.228	0.363	0.663	91	0.994	0.154	2011	[26]
[BMIM]+	[SbF6]-	-0.715	-0.263	2.864	2.322	0.578	0.757	27	0.993	0.0596846	2020	This work
[BMIM]+	[SCN]-	-1.244	0.861	2.431	4.817	0.976	0.701	31	0.994	0.085	2020	This work
[BMIm]+	[TCM]-	-0.780	0.365	2.380	3.325	0.740	0.664	35		0.170	2017	[14]
[BMIM]+	[TDI]-	-0.432	-0.044	2.366	3.466	0.438	0.752	66	0.993	0.067	2014	[64]
[BMIm]+	[Trif]-	-0.649	0.164	2.278	3.850	0.552	0.694	52		0.105	2017	[14]

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*l*	N	R^2	SD	Year	Source
[BMMOR]+	[TCM]-	-0.774	0.371	2.762	3.707	0.452	0.643	61	0.991	0.136	2017	[14]
[BMPIP]+	[NTf2]-	-0.347	0.111	2.241	2.472	0.294	0.687	79	0.990	0.119	2012	[71]
[BMPy]+	[BF4]-	-0.611	0.487	2.484	3.190	0.558	0.606	38	0.999	0.062	2006	[172]
[BMPy]+	[NTf2]-	-0.522	-0.113	2.777	2.673	0.122	0.741	37		0.080	2017	[14]
[BMPy]+	[TCM]-	-0.768	0.086	2.810	2.685	0.553	0.691	64		0.091	2017	[14]
[BMPyrr]+	[DCA]-	-0.589	0.473	2.647	4.816	0.183	0.627	46	0.993	0.068	2020	This work
[BMPyrr]+	[FAP]-	-0.196	0.000	2.288	1.078	0.505	0.649	90	0.984	0.127	2013	[159]
[BMPyrr]+	[FSI]-	-0.543	0.241	2.556	2.550	0.356	0.682	65	0.989	0.086	2019	[12]
[BMPyrr]+	[NTf2]-	-0.522	0.000	2.388	2.446	0.381	0.711	43		0.099	2017	[14]
[BMPyrr]+	[SCN]-	-0.680	0.543	2.622	5.352	0.000	0.602	65	0.988	0.130	2011	[70]
[BMPyrr]+	[TCB]-	-0.387	0.057	2.498	2.686	0.343	0.688	81	0.992	0.093	2012	[71]
[BMPyrr]+	[TCM]-	-0.461	0.214	2.497	3.701	0.243	0.684	96	0.994	0.080	2014	[77]
[BMPyrr]+	[Trif]-	-0.681	0.177	2.553	4.092	0.283	0.677	66	0.995	0.089	2013	[159]
[Bzmim]+	[NTf2]-	-0.535	0.000	2.523	2.333	0.575	0.668	114	0.997	0.119	2017	[16]
[BzmPyrr]+	[NTf2]-	-0.652	0.154	2.371	2.285	0.531	0.691	48	0.986	0.091	2017	[16]
[BzPy]+	[NTf2]-	-0.830	0.000	2.617	2.452	0.526	0.711	48	0.983	0.103	2018	[17]
[C1,9(M2iPAm)2]2+	[NTf2]-	-0.894	0.175	2.533	2.544	0.492	0.690	47	0.988	0.086	2016	[66]
[C3CNC1Pyr]+	[SCN]-	-1.747	0.717	3.547	5.603	0.287	0.590	45	0.981	0.146	2020	This work
[C3MPyrr]+	[NTf2]-	-0.466	2.562	0.000	2.505	0.271	0.682	39	0.976	0.116	2013	[68]
[C5MPyrr]+	[NTf2]-	-0.549	0.000	2.317	2.425	0.385	0.747	42	0.982	0.097	2013	[68]
[ChxmIm]+	[NTf2]-	-0.513	-0.203	2.418	2.688	0.334	0.745	49	0.981	0.107	2017	[16]
[ChxmPyrr]+	[NTf2]-	0.545	-0.124	2.406	2.411	0.274	0.771	47	0.996	0.120	2018	[17]
[ChxPy]+	[NTf2]-	-0.556	0.000	2.370	2.496	0.412	0.755	49	0.986	0.093	2017	[16]
[CNMeM2iPam]+	[NTf2]-	-1.344	-0.140	3.283	3.118	0.819	0.735	42	0.978	0.126	2016	[66]
[CnPrM2Im]+	[NTf2]-	0.000	0.250	1.810	1.250	0.300	0.350	21			2013	[171]
[CNPrMIm]+	[DCA]-	-1.489	-0.418	3.089	4.807	0.626	0.644	45	0.987	0.121	2011	[26, 27]
[COC2mMOR]+	[NTf2]-	-0.687	0.107	2.766	2.516	0.615	0.629	62	0.993	0.076	2020	This work
[COC2N112]+	[FAP]-	-0.380	-0.100	2.720	1.440	0.630	0.650	65	0.984	0.107	2015	[173]
[D2MIM]+	[NTf2]-	-0.252	-0.269	1.603	1.946	0.354	0.856	40	0.979	0.082	2011	[74]
[DM3AM]+	[NTf2]-	-0.363	-0.339	1.986	2.144	0.422	0.809	46	0.974	0.102	2011	[45]
[DMPyrr]+	[NTf2]-	-0.395	-0.241	1.991	2.112	0.268	0.822	40	0.990	0.063	2012	[69]
[DoMIM]+	[NTf2]-	-0.290	-0.285	1.812	2.121	0.357	0.853	65	0.991	0.066	2020	This work

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*l*	N	R^2	SD	Year	Source
[E3S]+	[NTf2]-	-0.606	-0.196	2.992	2.444	0.355	0.690	31	0.995	0.055	2010	[174]
[EMIM]+	[(MeO)(H)PO2]-	-1.120	0.340	2.920	7.850	0.000	0.620	36	0.900	0.160	2015	[158]
[EMIM]+	[DCA]-	-0.990	0.379	2.880	4.789	0.421	0.617	75	0.989	0.114	2011	[26]
[EMIM]+	[DEP]-	-0.412	0.195	2.237	7.432	-0.091	0.714	38		0.135	2017	[14]
[EMIM]+	[EtSO4]-	-0.667	0.000	2.557	5.327	0.000	0.588	53	0.986	0.125	2011	[26]
[EMIM]+	[FAP]-	-0.290	0.053	2.123	1.106	0.997	0.617	69		0.150	2017	[14]
[EMIM]+	[MeSO3]-	-1.398	0.485	2.562	6.616	0.495	0.642	42	0.976	0.153	2011	[74]
[EMIM]+	[NTf2]-	-0.486	0.068	2.296	2.278	0.988	0.651	65	0.996	0.094	2011	[26]
[EMIM]+	[OS]-	-0.404	0.214	1.031	4.259	1.141	0.841	28	0.993	0.061	2020	This work
[EMIM]+	[TCB]-	-0.407	0.141	2.743	2.783	0.469	0.625	41		0.061	2017	[14]
[EMIM]+	[TFA]-	-0.810	0.000	2.694	5.462	0.734	0.669	28			2008	[175]
[EtOHM2iPAm]+	[NTf2]-	-0.934	0.200	2.361	2.695	1.532	0.641	43	0.986	0.086	2016	[66]
[EtOHMIm]+	[BF4]-	-1.350	0.000	3.030	3.640	0.763	0.500	37			2009	[176]; [3]
[EtOHMIm]+	[FAP]-	-0.400	0.000	2.494	1.340	2.272	0.542	102	0.990	0.120	2013	[83]
[EtOHMIm]+	[NTf2]-	-0.793	0.139	2.404	2.587	1.353	0.581	81	0.993	0.100	2011	[26]
[EtOHMIm]+	[PF6]-	-1.044	-0.042	3.092	3.116	1.189	0.508	37		0.125	2017	[14]
[HexM3Am]+	[NTf2]-	-0.469	-0.058	2.085	2.185	0.617	0.617	93	0.985	0.128	2011	[70]
[HM2iPam]+	[NTf2]-	-0.531	-0.124	2.232	2.297	0.344	0.736	47	0.980	0.099	2016	[66]
[HMIM]+	[FAP]-	-0.189	-0.086	2.077	1.090	0.844	0.696	84		0.122	2017	[14]
[HMIM]+	[NTf2]-	-0.348	-0.240	2.060	2.184	0.561	0.754	77	0.993	0.117	2011	[26]
[HMIM]+	[TCB]-	-0.373	-0.022	2.559	2.594	0.450	0.711	56		0.069	2017	[14]
[HMPip]+	[NTf2]-	-0.404	-0.245	2.469	2.348	0.075	0.775	43	0.992	0.066	2013	[177]
[HMPyrr]+	[NTf2]-	-0.533	-0.110	2.146	2.278	0.650	0.767	36	0.984	0.088	2012	[69]
[HxomMIm]+	[NTf2]-	-0.462	0.000	2.073	2.022	0.637	0.684	50	0.968	0.123	2011	[26]
[M2EIM]+	[NTf2]-	-0.565	0.214	2.347	2.075	0.896	0.655	38	0.996	0.071	2006	[172]
[M2PIm]+	[NTf2]-	0.000	0.010	1.670	1.210	0.120	0.310	21			2013	[171]
[M2PIm]+	[Tf2C]-	0.000	0.080	1.590	1.150	0.150	0.360	21			2013	[171]
[M3BAm]+	[NTf2]-	-0.457	0.000	2.188	2.375	0.663	0.668	58	0.990	0.120	2011	[26]
[MDIm]+	[TCB]-	-0.335	-0.176	2.388	2.421	0.372	0.772	42		0.050	2017	[14]
[MeOCH2CH2NEt3]+	[NTf2]-	-0.399	0.086	2.376	2.397	0.452	0.670	43	0.980	0.092	2020	[22]
[MeOCH2CH2PBu3]+	[NTf2]-	-0.233	-0.176	1.902	2.121	0.239	0.769	48	0.976	0.082	2020	[22]
[MeOCH2CH2PEt3]+	[NTf2]-	-0.437	0.000	2.291	2.503	0.431	0.725	50	0.984	0.082	2020	[22]

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*l*	N	R^2	SD	Year	Source
[MeoeM2EAm]+	[FAP]-	-0.321	-0.071	2.557	1.329	0.722	0.631	106		0.128	2017	[14]
[MeoeMIm]+	[NTf2]-	-0.509	0.065	2.476	2.271	0.671	0.603	52	0.981	0.108	2011	[26, 27]
[MeoeMMorp]+	[FAP]-	-0.364	0.000	2.645	1.319	0.887	0.595	99		0.140	2017	[14]
[MeoeMMorp]+	[NTf2]-	-0.648	0.142	2.748	2.475	0.594	0.614	62		0.092	2017	[14]
[MeoeMPip]+	[FAP]-	-0.177	0.000	2.311	1.249	0.542	0.655	103		0.137	2017	[14]
[MeoeMPip]+	[NTf2]-	-0.453	0.075	2.519	2.535	0.279	0.672	59		0.078	2017	[14]
[MeoeMPyrr]+	[FAP]-	-0.145	0.000	2.360	1.248	0.523	0.629	104	0.984	0.137	2013	[178]
[MMIM]+	[(MeO)(H)PO2]-	-1.640	0.000	3.220	9.640	0.000	0.730	21	0.900	0.110	2015	[158]
[MMIm]+	[M2PO4]-	-0.610	0.860	2.590	7.270	0.000	0.350	40			2009	[176, 3]
[Mo1,3CN]+	[TCM]-	-1.611	0.238	3.545	4.199	0.234	0.634	50	0.979	0.148	2020	This work
[Mo1,3OH]+	[TCM]-	-1.464	0.410	3.150	4.208	0.687	0.621	50	0.986	0.117	2020	This work
[MOIm]+	[BF4]-	-0.409	-0.049	1.562	2.911	0.803	0.778	61	0.987	0.140	2011	[26]
[MOIm]+	[Cl]-	-0.732	-0.069	1.804	4.169	0.839	0.832	15	0.999	0.023	2020	This work
[MOIm]+	[PF6]-	-0.118	-0.130	1.535	2.146	1.025	0.703	48		0.142	2017	[14]
[N112N113]+	[NTf2]-	-1.338	0.044	2.865	3.280	1.041	0.762	47	0.984	0.114	2019	[18]
[N112N114]+	[NTf2]-	-0.725	0.053	2.522	2.863	0.751	0.656	45	0.985	0.090	2019	[18]
[N112O2N113]+	[NTf2]-	-0.613	-0.225	2.440	2.608	0.420	0.748	43	0.978	0.098	2019	[18]
[N112O2N114]+	[NTf2]-	-0.436	-0.108	2.279	2.505	0.435	0.707	45	0.980	0.089	2019	[18]
[N2,2,2,8]+	[FSI]-	-0.461	0.084	2.276	2.395	0.168	0.778	65	0.989	0.078	2019	[12]
[N-C3CNMPyr]+	[DCA]-	-1.172	0.478	3.247	5.000	0.316	0.553	59	0.990	0.099	2020	This work
[N-C3CNPy]+	[DCA]-	-1.314	0.399	3.309	4.810	0.322	0.546	56	0.984	0.118	2020	This work
[N-C3OHmMOR]+	[NTf2]-	-0.378	-0.074	2.088	2.368	0.166	0.792	63	0.996	0.110	2017	[14]
[O4AM]+	[NTf2]-	0.000	-0.287	1.478	1.845	0.189	0.816	42	0.998	0.124	2011	[45]
[OM3AM]+	[NTf2]-	-0.426	-0.338	2.242	2.195	0.684	0.779	44	0.981	0.092	2011	[45]
[OMMIM]+	[NTf2]-	-0.682	-0.036	1.954	2.367	0.621	0.820	32	0.976	0.108	2020	This work
[Ompyrr]+	[NTf2]-	-0.587	-0.064	2.080	2.176	0.486	0.822	37	0.986	0.080	2012	[69]
[P14,6,6,6]+	[+CS]-	-0.201	-0.408	1.727	6.367	-0.241	1.035	40	0.979	0.118	2014	[13]
[P14,6,6,6]+	[BF4]-	-0.142	-1.589	3.265	1.427	-1.744	0.960	16	0.983	0.080	2020	This work
[P14,6,6,6]+	[Cl]-	0.028	-0.706	0.934	0.859	1.984	0.921	16	0.994	0.036	2020	This work
[P14,6,6,6]+	[DCA]-	-1.064	-0.253	1.341	3.579	0.105	0.882	32	0.991	0.065	2020	This work
[P14,6,6,6]+	[L-Lact]-	-0.191	-0.353	1.622	6.653	-0.332	0.907	31	0.960	0.135	2014	[13]
[P14,6,6,6]+	[NTf2]-	-0.406	-0.576	1.602	2.338	-0.009	0.959	59	0.982	0.112	2009	[67]

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*l*	N	R^2	SD	Year	Source
[P14,6,6,6]+	[OS]-	-0.181	-0.320	1.361	4.749	0.000	0.902	39		0.129	2017	[14]
[P14,6,6,6]+	[PF6]-	-0.506	0.357	0.046	0.846	2.017	0.889	29	0.991	0.067	2020	This work
[P8,8,8,8]+	[NTf2]-	-0.212	-0.337	1.522	1.705	0.074	0.880	65	0.987	0.074	2020	This work
[PDMIM]+	[BF4]-	-1.025	0.997	2.728	4.525	0.518	0.458	34		0.126	2017	[14]
[PDMIM]+	[NTf2]-	-1.220	-0.217	3.009	1.037	0.410	0.856	22	0.993	0.069	2020	This work
[PeMPip]+	[NTf2]-	-0.477	-0.186	2.639	2.450	0.103	0.761	43	0.990	0.075	2013	[177]
[PemPyrr]+	[NTf2]-	-0.549	0.000	2.317	2.425	0.385	0.747	42		0.097	2017	[14]
[PM2iPAm]+	[NTf2]-	-0.702	0.000	2.532	2.578	0.331	0.682	46	0.985	0.096	2016	[66]
[PMPip]+	[NTf2]-	-0.432	0.145	2.287	2.489	0.402	0.674	79	0.987	0.126	2011	[70]
[PMPyrr]+	[NTf2]-	-0.466	0.000	2.562	2.505	0.271	0.682	39		0.116	2017	[14]
[PrOHM2Im]+	[NTf2]-	0.000	0.210	1.500	1.250	0.660	0.340	21			2013	[171]
[PrOHPy]+	[FAP]-	-0.448	0.096	2.467	1.563	1.898	0.563	77		0.136	2017	[14]
[PrOHPy]+	[NTf2]-	-0.630	0.316	2.587	2.758	1.025	0.583	45		0.061	2017	[14]
[QUIN6]+	[NTf2]-	-0.562	-0.071	2.201	2.569	0.238	0.815	43		0.103	2017	[14]
[QUIN8]+	[NTf2]-	-0.363	-0.186	2.048	2.430	0.142	0.816	43		0.100	2017	[14]
[sec-BMIm]+	[NTf2]-	-0.558	-0.097	2.519	2.497	0.456	0.705	48	0.986	0.087	2019	[6]
[TDC]+	[DCA]-	-0.393	0.440	2.435	5.033	0.000	0.678	47	0.980	0.116	2015	[72]
[TDC]+	[NTf2]-	-0.353	0.000	2.095	2.321	0.045	0.740	44	0.987	0.073	2015	[72]
[tert-BMIm]+	[NTf2]-	-0.621	-0.118	2.603	2.689	0.410	0.693	48	0.985	0.093	2019	[6]

Table D.3: ILs and their ABSM values for log P at 298 K.

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*v*	N	R^2	SD	Year	Source
[(C3COOMe)MIM]+	[DCA]-	-0.500	0.368	1.249	1.118	-4.658	2.852	60	60.000	0.126	2020	This work
[(Hexom)2Im]+	[NTf2]-	0.107	-0.628	0.747	-1.441	-4.808	3.750	34		0.106	2017	[14]
[(Meo)2Im]+	[NTf2]-	-0.412	-0.104	0.761	-1.124	-3.776	3.055	46	0.993	0.130	2011	[26]
[3-MBPy]+	[TDI]-	-0.062	0.278	0.544	-0.833	-4.517	3.586	66	0.995	0.113	2014	[64]
[3-MBPy]+	[Trif]-	-0.088	-0.110	1.121	0.330	-5.188	3.310	36		0.121	2017	[14]
[4-CNBPy]+	[NTf2]-	-0.316	0.132	1.015	-1.040	-4.399	3.272	64		0.123	2017	[14]
[AllMIm]+	[DCA]-	-0.202	0.360	0.780	0.790	-4.475	2.621	65	0.994	0.102	2017	[14]
[AllMIm]+	[NTf2]-	0.000	0.058	0.703	-1.301	-4.343	3.159	64	0.998	0.112	2017	[14]
[B3EP]+	[DEP]-	0.120	-0.242	0.309	1.899	-5.345	3.723	49	0.994	0.128	2017	[14]
[B4MPy]+	[DCA]-	-0.422	0.539	1.016	0.898	-4.765	3.291	53	0.992	0.124	2020	This work
[BM2Im]+	[NTf2]-	-0.347	0.111	0.718	-1.195	-4.418	3.502	60		0.121	2017	[14]
[BMIM]+	[[(CH3)2PO4]-	-0.255	0.359	0.512	4.493	-4.821	3.334	55	0.987	0.159	2020	This work
[BMIM]+	[BETI]-	0.023	0.083	0.334	-1.701	-4.236	3.041	51	0.996	0.110	2011	[74]
[BMIm]+	[BF4]-	-0.082	0.454	0.541	-0.427	-4.583	2.961	66	0.992	0.132	2011	[26]
[BMIM]+	[CH3SO4]-	0.002	0.173	0.179	-0.795	-4.830	2.691	22	0.979	0.197	2020	This work
[BMIM]+	[Cl]-	-0.802	0.533	1.302	4.808	-5.075	3.173	54	2.988	0.14	2020	This work
[BMIM]+	[DCA]-	-0.272	0.448	0.722	1.103	-4.437	3.131	67		0.118	2017	[14]
[BMIM]+	[MeSO3]-	-0.494	0.343	1.050	2.972	-4.947	3.169	53	0.992	0.123	2020	This work
[BMIm]+	[NTf2]-	-0.018	0.416	0.153	-1.312	-4.187	3.347	101	0.994	0.131	2011	[26]
[BMIm]+	[OS]-	-0.050	0.198	0.179	1.146	-5.154	4.008	55	0.986	0.179	2011	[26]
[BMIm]+	[PF6]-	-0.056	0.193	0.737	-1.351	-4.526	3.109	86	0.988	0.154	2011	[26]
[BMIM]+	[SbF6]-	-0.238	-0.826	1.996	-0.65	-5.557	3.496	26	0.995	0.11	2020	This work
[BMIM]+	[SCN]-	-0.798	0.055	1.865	1.022	-4.711	3.353	31	0.992	0.116	2020	This work
[BMIm]+	[TCM]-	-0.700	0.730	2.030	1.930	1.640	2.780	33		0.120	2017	[14]
[BMIM]+	[TDI]-	-0.032	0.099	0.616	-0.254	-4.499	3.496	66	0.994	0.107	2014	[64]
[BMIm]+	[Trif]-	-0.220	0.209	0.479	0.066	-4.314	3.294	52		0.124	2017	[14]
[BMMOR]+	[TCM]-	-0.318	0.374	0.951	0.000	-4.484	3.122	61	0.994	0.114	2017	[14]
[BMPIP]+	[NTf2]-	-0.129	0.494	0.235	-1.165	-4.385	3.422	78	0.988	0.162	2012	[71]
[BMPy]+	[BF4]-	-0.032	0.489	0.466	-0.873	-4.665	2.944	38	0.992	0.141	2006	[172]
[BMPy]+	[NTf2]-	-0.192	-0.219	1.326	-1.021	-4.429	3.545	37		0.120	2017	[14]
[BMPy]+	[TCM]-	-0.800	0.910	2.100	2.350	2.070	2.990	33		0.170	2017	[14]

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*v*	N	R^2	SD	Year	Source
[BMPyrr]+	[DCA]-	-0.022	0.524	0.810	1.290	-5.041	3.029	46	0.997	0.072	2020	This work
[BMPyrr]+	[FAP]-	0.100	0.227	0.392	-2.607	-4.285	3.245	90	0.991	0.156	2013	[159]
[BMPyrr]+	[FSI]-	-0.142	0.265	0.817	-1.149	-4.592	3.287	65	0.994	0.128	2019	[12]
[BMPyrr]+	[NTf2]-	-0.269	0.000	0.747	-1.094	-4.594	3.512	43		0.133	2017	[14]
[BMPyrr]+	[SCN]-	-0.368	0.728	0.624	1.587	-4.715	3.104	64	0.983	0.177	2011	[70]
[BMPyrr]+	[TCB]-	-0.071	0.354	0.562	-1.030	-4.415	3.346	80	0.991	0.139	2012	[71]
[BMPyrr]+	[TCM]-	-0.126	0.430	0.398	0.000	-4.563	3.333	95	0.993	0.120	2014	[77]
[BMPyrr]+	[Trif]-	-0.366	0.448	0.628	0.362	-4.469	3.327	65	0.990	0.134	2013	[159]
[Bzmim]+	[NTf2]-	-0.187	0.000	0.768	-1.284	-4.378	3.310	112	0.993	0.138	2017	[16]
[BzmPyrr]+	[NTf2]-	-0.387	0.197	0.658	-1.275	-4.401	3.449	46	0.996	0.124	2017	[16]
[BzPy]+	[NTf2]-	-0.516	0.092	0.865	-1.143	-4.432	3.485	46	0.996	0.118	2018	[17]
[C1,9(M2iPAm)2]2+	[NTf2]-	-0.606	0.225	0.798	-1.034	-4.438	3.429	45	0.995	0.131	2016	[66]
[C3CNC1Pyr]+	[SCN]-	-1.388	0.588	1.949	2.232	-4.880	3.044	45	0.977	0.195	2020	This work
[C3MPyrr]+	[NTf2]-	-0.236	0.000	0.908	-1.015	-4.691	3.446	39	0.993	0.143	2013	[68]
[C5MPyrr]+	[NTf2]-	-0.303	0.000	0.727	-1.107	-4.622	3.630	42	0.995	0.132	2013	[68]
[ChxmIm]+	[NTf2]-	-0.299	-0.094	0.754	-0.851	-4.618	3.653	47	0.997	0.133	2017	[16]
[ChxmPyrr]+	[NTf2]-	-0.297	0.073	0.697	-1.157	-4.687	3.709	47	0.996	0.120	2018	[17]
[ChxPy]+	[NTf2]-	-0.344	0.146	0.703	-1.047	-4.535	3.681	47	0.996	0.123	2017	[16]
[CNMeM2iPam]+	[NTf2]-	-1.001	0.000	1.512	-0.459	-4.191	3.529	40	0.994	0.134	2016	[66]
[CNPrMIm]+	[DCA]-	-0.928	0.373	1.224	1.042	-4.307	3.046	44	0.988	0.150	2011	[26]
[COC2mMOR]+	[NTf2]-	-0.216	0.054	1.059	-1.019	-4.564	3.082	61	0.994	0.117	2020	This work
[D2MIM]+	[NTf2]-	-0.093	-0.052	0.040	-1.620	-4.667	4.034	40	0.996	0.118	2011	[74]
[DM3AM]+	[NTf2]-	-0.128	-0.131	0.329	-1.458	-4.550	3.816	46	0.996	0.132	2011	[45]
[DMPyrr]+	[NTf2]-	-0.083	-0.142	0.419	-1.467	-4.859	3.824	40	0.997	0.108	2012	[69]
[DoMIM]+	[NTf2]-	0.063	-0.055	0.275	-1.368	-4.897	3.824	46	0.997	0.108	2020	This work
[E3S]+	[NTf2]-	-0.062	-1.347	2.716	1.350	-5.274	3.242	31	0.996	0.097	2010	[174]
[EMIM]+	[(MeO)(H)PO2]-	-0.530	0.320	1.050	4.090	-4.920	2.880	33	0.980	0.170	2015	[158]
[EMIM]+	[DCA]-	-0.329	0.326	0.909	0.933	-4.540	2.904	72		0.127	2017	[14]
[EMIM]+	[DEP]-	0.022	0.289	0.434	3.796	-5.041	3.346	38		0.165	2017	[14]
[EMIM]+	[EtSO4]-	-0.079	-0.021	0.554	1.491	-4.944	2.895	53	0.992	0.147	2011	[26]
[EMIM]+	[FAP]-	0.093	0.448	0.027	-2.667	-3.673	3.082	66		0.163	2017	[14]
[EMIM]+	[MeSO3]-	-0.799	0.493	0.644	2.842	-4.440	3.007	40	0.981	0.189	2011	[74]

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*v*	N	R^2	SD	Year	Source
[EMIM]+	[NTf2]-	0.029	0.351	0.202	-1.684	-3.585	3.059	64	0.993	0.119	2011	[26]
[EMIM]+	[OS]-	0.109	0.179	-0.476	0.871	-4.308	3.695	27	0.996	0.111	2020	This work
[EMIM]+	[TCB]-	-0.151	-0.111	1.141	-0.875	-4.682	3.002	41		0.118	2017	[14]
[EMIM]+	[TFA]-	-0.129	-1.251	2.356	0.889	-4.473	3.044	28			2008	[175]
[EtOHM2iPAm]+	[NTf2]-	-0.669	0.236	0.617	-0.850	-3.356	3.270	41	0.994	0.122	2016	[66]
[EtOHMIm]+	[FAP]-	0.000	0.111	0.490	-2.383	-2.523	2.858	102	0.996	0.140	2013	[83]
[EtOHMIm]+	[NTf2]-	-0.402	0.304	0.470	-1.082	-3.510	2.977	79	0.990	0.133	2011	[26]
[EtOHMIm]+	[PF6]-	-0.541	-0.145	1.102	-0.596	-3.684	2.723	36		0.169	2017	[14]
[HexM3Am]+	[NTf2]-	-0.322	0.242	0.287	-1.383	-4.265	3.513	90	0.993	0.138	2011	[70]
[HM2iPam]+	[NTf2]-	-0.340	0.000	0.582	-1.194	-4.631	3.640	45	0.996	0.125	2016	[66]
[HMIM]+	[FAP]-	0.067	0.150	0.254	-2.530	-4.014	3.446	84		0.159	2017	[14]
[HMIM]+	[NTf2]-	-0.065	0.010	0.260	-1.476	-4.313	3.587	75	0.996	0.115	2011	[26]
[HMIM]+	[TCB]-	0.000	0.119	0.730	-1.083	-4.431	3.389	56		0.108	2017	[14]
[HMPyrr]+	[NTf2]-	-0.226	-0.083	0.560	-1.301	-4.501	3.673	36	0.994	0.123	2012	[69]
[HxomMIm]+	[NTf2]-	-0.275	0.000	0.407	-1.478	4.320	3.510	46	0.994	0.140	2011	[26]
[M2EIM]+	[NTf2]-	-0.095	0.299	0.360	-1.906	-3.805	3.177	38	0.997	0.131	2006	[172]
[M3BAm]+	[NTf2]-	0.047	-0.051	0.356	-1.262	-4.400	3.209	57		0.120	2017	[14]
[MDIm]+	[TCB]-	0.108	-0.138	0.742	-1.279	-4.667	3.526	42		0.116	2017	[14]
[MeOCH2CH2NEt3]+	[NTf2]-	-0.129	0.080	0.682	-1.084	-4.538	3.370	42	0.995	0.131	2020	[22]
[MeOCH2CH2PBu3]+	[NTf2]-	-0.045	0.041	0.218	-1.396	-4.650	3.708	48	0.996	0.121	2020	[22]
[MeOCH2CH2PEt3]+	[NTf2]-	-0.177	0.103	0.582	-1.022	-4.516	3.546	50	0.996	0.116	2020	[22]
[MeoeM2EAm]+	[FAP]-	0.034	0.119	0.628	-2.408	-4.070	3.156	105		0.149	2017	[14]
[MeoeMIm]+	[NTf2]-	-0.150	0.012	0.818	-1.289	-4.263	3.116	49		0.129	2017	[14]
[MeoeMMorp]+	[FAP]-	0.000	0.000	0.830	-2.362	-4.022	3.064	99	0.995	0.164	2017	[14]
[MeoeMMorp]+	[NTf2]-	-0.188	0.094	0.918	-1.180	-4.346	3.043	62		0.119	2017	[14]
[MeoeMPip]+	[FAP]-	0.114	0.260	0.391	-2.448	-4.245	3.281	103		0.163	2017	[14]
[MeoeMPip]+	[NTf2]-	-0.068	0.126	0.726	-1.122	-4.642	3.276	59		0.118	2017	[14]
[MeoeMPyrr]+	[FAP]-	0.130	0.168	0.477	-2.483	-4.245	3.215	102	0.989	0.158	2013	[178]
[MMIM]+	[(MeO)(H)PO2]-	0.000	0.350	0.000	4.150	-3.880	2.640	18	0.980	0.240	2015	[158]
[Mo1,3CN]+	[TCM]-	-1.175	0.167	1.914	0.695	-4.922	3.107	50	0.979	0.199	2020	This work
[Mo1,3OH]+	[TCM]-	-1.005	0.322	1.503	0.691	-4.467	3.051	50	0.985	0.164	2020	This work
[MOIm]+	[BF4]-	-0.115	0.210	0.000	-0.511	-4.338	3.617	59	0.994	0.159	2011	[26]

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*v*	N	R^2	SD	Year	Source
[MOIm]+	[Cl]-	-0.227	-1.591	2.876	-0.009	-7.594	3.743	15	0.990	0.069	2020	This work
[MOIm]+	[PF6]-	0.085	-0.123	0.000	-1.255	-4.088	3.509	47		0.156	2017	[14]
[N112N113]+	[NTf2]-	-1.042	0.143	1.160	-0.335	-3.910	3.643	45	0.993	0.138	2019	[18]
[N112N114]+	[NTf2]-	-0.397	0.000	0.779	0.712	-4.181	3.291	44	0.995	0.128	2019	[18]
[N112O2N113]+	[NTf2]-	-0.339	-0.149	0.748	-0.945	-4.542	3.605	43	0.996	0.125	2019	[18]
[N112O2N114]+	[NTf2]-	-0.205	-0.053	0.584	-1.037	-4.475	3.508	45	0.996	0.124	2019	[18]
[N2,2,2,8]+	[FSI]-	-0.109	0.231	0.596	-1.301	-4.798	3.604	65	0.995	0.126	2019	[12]
[N-C3CNMPyr]+	[DCA]-	-0.715	0.328	1.532	1.529	-4.842	2.865	59	0.990	0.132	2020	This work
[N-C3CNPy]+	[DCA]-	-0.784	0.252	1.549	1.285	-4.836	2.784	56	0.986	0.152	2020	This work
[O3Am]+	[NTf2]-	-0.044	0.111	0.398	-1.298	-4.815	3.667	63	0.996	0.110	2017	[14]
[O4AM]+	[NTf2]-	0.226	0.000	-0.212	-1.756	-4.739	3.825	42	0.993	0.164	2011	[45]
[OM3AM]+	[NTf2]-	-0.165	-0.181	0.569	-1.419	-4.677	3.711	44	0.996	0.123	2011	[45]
[OMMIM]+	[NTf2]-	-0.354	0.200	0.130	-1.444	-4.224	3.826	32	0.996	0.115	2020	This work
[Ompyrr]+	[NTf2]-	-0.253	0.000	0.520	-1.460	-4.696	3.815	37	0.997	0.102	2012	[69]
[P14,6,6,6]+	[+CS]-	0.000	0.000	0.229	2.749	-5.343	4.555	40	0.999	0.125	2014	[13]
[P14,6,6,6]+	[BF4]-	0.391	-2.129	2.779	-2.053	-7.759	4.019	16	0.999	0.078	2020	This work
[P14,6,6,6]+	[Cl]-	0.616	-1.402	0.561	-2.669	-4.091	3.585	16	0.997	0.097	2020	This work
[P14,6,6,6]+	[DCA]-	-0.693	0.110	-0.455	-0.172	-4.774	3.914	32	0.997	0.103	2020	This work
[P14,6,6,6]+	[L-Lact]-	0.000	0.000	0.000	3.241	-5.329	4.158	31	0.998	0.158	2014	[13]
[P14,6,6,6]+	[NTf2]-	-0.155	-0.163	-0.029	-1.271	-5.042	4.246	59	0.996	0.136	2011	[26]
[P14,6,6,6]+	[OS]-	0.138	-0.077	-0.248	1.073	-5.028	4.037	38		0.149	2017	[14]
[P14,6,6,6]+	[PF6]-	-0.159	0.094	-0.934	-2.155	-3.931	3.997	28	0.996	0.132	2020	This work
[P8,8,8,8]+	[NTf2]-	0.153	-0.069	-0.011	-1.800	-5.186	3.888	65	0.997	0.116	2020	This work
[PDMIM]+	[BF4]-	-0.603	0.799	0.824	0.883	-4.417	2.636	34		0.130	2017	[14]
[PDMIM]+	[NTf2]-	-0.875	0.119	1.046	-2.252	-4.334	3.929	22	0.996	0.087	2020	This work
[PeMPyrr]+	[NTf2]-	-0.303	0.000	0.727	-1.107	-4.622	3.630	42		0.132	2017	[14]
[PM2iPAm]+	[NTf2]-	-0.378	0.115	0.723	-1.061	-4.594	3.388	44	0.996	0.113	2016	[66]
[PMPip]+	[NTf2]-	-0.231	0.453	0.352	-1.263	-4.290	3.401	78	0.990	0.153	2011	[70]
[PMPyrr]+	[NTf2]-	-0.236	0.000	0.908	-1.015	-4.691	3.446	39		0.143	2017	[14]
[PrOHPy]+	[FAP]-	-0.098	0.294	0.393	-2.160	-2.785	2.961	76		0.161	2017	[14]
[PrOHPy]+	[NTf2]-	-0.117	-0.034	1.056	-0.934	-4.147	2.922	45		0.113	2017	[14]
[QUIN6]+	[NTf2]-	-0.360	0.138	0.594	-0.936	-4.776	3.864	43		0.133	2017	[14]

Cation	Anion	Constant	*e*	*s*	*a*	*b*	*v*	N	R^2	SD	Year	Source
[QUIN8]+	[NTf2]-	-0.149	0.000	0.451	-1.080	-4.886	3.861	43		0.133	2017	[14]
[sec-BMIm]+	[NTf2]-	-0.215	0.000	0.740	-1.119	-4.496	3.436	46	0.997	0.108	2019	[6]
[TDC]+	[DCA]-	-0.176	0.436	0.823	1.599	-5.051	3.452	45	0.994	0.131	2015	[72]
[TDC]+	[NTf2]-	-0.169	0.152	0.447	-1.199	-4.905	3.638	43	0.997	0.107	2015	[72]
[tert-BMIm]+	[NTf2]-	-0.275	0.000	0.796	-0.926	-4.526	3.395	46	0.996	0.112	2019	[6]

Table D.4: Cation log K ABSM values at 298 K.

Cation	*c*	*e*	*s*	*a*	*b*	*l*	N	Year	Source
[(Hexom)2Im]+	-0.314	-0.479	2.076	2.376	0.287	0.835	34	2014	[77]
[(Hxom)2Im]+	-0.314	-0.479	2.076	2.376	0.287	0.835	34	2011	[26]
[(Meo)2Im]+	-0.762	-0.013	2.557	2.427	1.154	0.584	48	2014	[77]
[1-PrOHPy]+	-0.713	0.151	2.663	2.874	1.311	0.611	122	2014	[77]
[3-MBPy]+	-0.338	0.035	2.325	2.289	0.189	0.714	37	2014	[77]
[AllMIm]+	-0.432	0.135	2.368	2.324	0.624	0.606	129	2017	[14]
[B3EP]+	-0.450	-0.331	1.731	0.788	0.774	0.783	49	2017	[14]
[BMIm]+	-0.421	0.033	2.134	2.281	0.603	0.712	485	2014	[77]
[BMMOR]+	-0.676	0.277	2.472	2.369	0.597	0.638	61	2017	[14]
[BMPip]+	-0.364	0.134	2.271	2.467	0.327	0.679	111	2014	[77]
[BMPy]+	-0.449	0.157	2.270	2.416	0.566	0.714	109	2014	[77]
[BMPyrr]+	-0.363	0.119	2.207	2.363	0.388	0.679	474	2014	[77]
[BzmIm]+	-0.535	0.000	2.523	2.333	0.575	0.668	114	2017	[16]
[BzmPyrr]+	-0.652	0.154	2.371	2.285	0.531	0.691	48	2017	[16]
[BzPy]+	-0.830	0.000	2.617	2.452	0.526	0.711	48	2018	[17]
[C1,9(M2iPAm)2]2+	-0.894	0.175	2.533	2.544	0.492	0.690	47	2016	[66]
[C3MPyrr]+	-0.466	2.562	0.000	2.505	0.271	0.682	39	2013	[68]
[C5MPyrr]+	-0.549	0.000	2.317	2.425	0.385	0.747	42	2013	[68]
[ChxmIm]+	-0.513	-0.203	2.418	2.688	0.334	0.745	49	2017	[16]
[ChxmPyrr]+	0.545	-0.124	2.406	2.411	0.274	0.771	47	2018	[17]
[ChxPy]+	-0.556	0.000	2.370	2.496	0.412	0.755	49	2017	[16]
[CNMeM2iPam]+	-1.344	-0.140	3.283	3.118	0.819	0.735	42	2016	[66]
[CNPrMIm]+	-1.119	0.073	2.617	2.543	0.816	0.699	45	2014	[77]
[D2MIM]+	-0.252	-0.269	1.603	1.946	0.354	0.856	40	2011	[74]
[DM3AM]+	-0.363	-0.339	1.986	2.144	0.422	0.809	46	2011	[45]
[DMPyrr]+	-0.395	-0.241	1.991	2.112	0.268	0.822	40	2012	[69]
[E3S]+	-0.606	-0.196	2.992	2.444	0.355	0.690	31	2014	[77]
[EMIM]+	-0.505	0.088	2.305	2.381	0.683	0.654	561	2014	[77]
[EtOHM2iPAm]+	-0.934	0.200	2.361	2.695	1.532	0.641	43	2016	[66]
[EtOHMIm]+	-0.843	0.095	2.462	2.694	1.331	0.580	151	2014	[77]

Cation	*c*	*e*	*s*	*a*	*b*	*l*	N	Year	Source
[H3TDp]+	-0.358	-0.466	1.498	2.283	0.281	0.904	98	2014	[77]
[HexdMim]+	0.019	-0.452	0.821	1.810	0.523	0.997	31	2011	[26]
[HexM3Am]+	-0.469	-0.056	2.083	2.176	0.620	0.689	93	2014	[77]
[HM2iPam]+	-0.531	-0.124	2.232	2.297	0.344	0.736	47	2016	[66]
[HMIM]+	-0.379	-0.103	2.081	2.298	0.533	0.751	335	2014	[77]
[HMPip]+	-0.404	-0.245	2.469	2.348	0.075	0.775	42	2014	[77]
[HMPyrr]+	-0.533	-0.110	2.146	2.278	0.650	0.767	36	2014	[77]
[HxomMIm]+	-0.463	-0.394	2.478	2.428	0.337	0.786	34	2014	[77]
[M2EIm]+	-0.611	0.188	2.380	2.101	0.899	0.667	39	2011	[26]
[M3BAm]+	-0.457	-0.005	2.188	2.375	0.663	0.668	58	2011	[26]
[MB3Am]+	-0.506	-0.169	2.103	2.298	0.412	0.777	44	2014	[77]
[MDIm]+	-0.391	-0.162	2.036	2.054	0.524	0.786	43	2014	[77]
[MeoeMim]+	-0.507	-0.015	2.644	2.378	0.413	0.602	52	2011	[26]
[MeoeMMorp]+	-0.675	0.021	2.823	2.588	0.542	0.644	160	2014	[77]
[MeoeMPip]+	-0.440	0.065	2.484	2.537	0.241	0.688	162	2014	[77]
[MeoeMPyrr]+	-0.380	0.018	2.497	2.534	0.162	0.671	104	2014	[77]
[MO3Am]+	-0.387	-0.130	1.460	2.327	0.501	0.927	32	2011	[26]
[MOIm]+	-0.197	-0.216	1.301	2.021	0.994	0.837	160	2014	[77]
[N112N113]+	-1.338	0.044	2.865	3.280	1.041	0.762	47	2019	[18]
[N112N114]+	-0.725	0.053	2.522	2.863	0.751	0.656	45	2019	[18]
[N112O2N113]+	-0.613	-0.225	2.440	2.608	0.420	0.748	43	2019	[18]
[N112O2N114]+	-0.436	-0.108	2.279	2.505	0.435	0.707	45	2019	[18]
[N2,2,2,8]+	-0.347	-0.063	2.034	2.317	0.179	0.787	193	2019	[12]
[NEP]+	-0.668	0.246	2.399	2.403	0.936	0.672	31	2014	[77]
[O3Am]+	-0.378	-0.074	2.088	2.368	0.166	0.792	63	2017	[14]
[O4AM]+	0.000	-0.287	1.478	1.845	0.189	0.816	42	2011	[45]
[OiQu]+	-0.338	-0.417	2.502	2.364	-0.229	0.811	36	2014	[77]
[OM3AM]+	-0.426	-0.338	2.242	2.195	0.684	0.779	44	2011	[45]
[Ompyrr]+	-0.587	-0.064	2.080	2.176	0.486	0.822	37	2014	[77]
[PDMIM]+	-0.822	0.780	2.357	3.432	0.926	0.526	34	2011	[26]
[PEMPip]+	-0.477	-0.186	2.639	2.450	0.103	0.761	41	2014	[77]
[PeMPyrr]+	-0.549	0.000	2.317	2.425	0.385	0.747	42	2014	[77]

Cation	*c*	*e*	*s*	*a*	*b*	*l*	N	Year	Source
[PM2iPAm]+	-0.702	0.000	2.532	2.578	0.331	0.682	46	2016	[66]
[PMPip]+	-0.435	0.149	2.281	2.476	0.410	0.675	79	2014	[77]
[PMPyrr]+	-0.466	0.000	2.562	2.505	0.271	0.682	39	2014	[77]
[sec-BMIm]+	-0.558	-0.097	2.519	2.497	0.456	0.705	48	2019	[6]
[tert-BMIm]+	-0.621	-0.118	2.603	2.689	0.410	0.693	48	2019	[6]

Table D.5: Cation log P ABSM values at 298 K.

Cation	*c*	*e*	*s*	*a*	*b*	*v*	N	Year	Source
[(Hexom)2Im]+	0.074	-0.541	0.642	-1.419	-4.748	3.787	34	2014	[77]
[(Hxom)2Im]+	0.107	-0.628	0.747	-1.441	-4.808	3.750	34	2011	[26]
[(Meo)2Im]+	-0.414	-0.103	0.764	-1.120	-3.781	3.056	48	2014	[77]
[1-PrOHPy]+	-0.302	-0.299	1.476	-0.503	-3.760	3.125	38	2011	[26]
[3-MBPy]+	0.040	0.087	0.657	-1.197	-4.970	3.435	36	2014	[77]
[AllMIm]+	0.028	0.127	0.519	-1.365	-4.282	3.102	129	2017	[14]
[B3EP]+	0.049	-0.315	0.303	-3.190	-4.153	3.539	49	2017	[14]
[BMIm]+	-0.048	0.328	0.296	-1.382	-4.337	3.390	509	2014	[77]
[BMMOR]+	-0.239	0.318	0.675	-1.223	-4.414	3.130	61	2017	[14]
[BMPip]+	-0.115	0.448	0.322	-1.108	-4.452	3.390	110	2014	[77]
[BMPy]+	-0.090	0.238	0.549	-1.246	-4.417	3.433	71	2014	[77]
[BMPyrr]+	-0.340	0.380	0.308	-1.276	-4.474	3.330	466	2014	[77]
[BzmIm]+	-0.187	0.000	0.768	-1.284	-4.378	3.310	112	2017	[16]
[BzmPyrr]+	-0.387	0.197	0.658	-1.275	-4.401	3.449	46	2017	[16]
[BzPy]+	-0.516	0.092	0.865	-1.143	-4.432	3.485	46	2018	[17]
[C1,9(M2iPAm)2]2+	-0.606	0.225	0.798	-1.034	-4.438	3.429	45	2016	[66]
[C3MPyrr]+	-0.236	0.000	0.908	-1.015	-4.691	3.446	39	2013	[68]
[C5MPyrr]+	-0.303	0.000	0.727	-1.107	-4.622	3.630	42	2013	[68]
[ChxmIm]+	-0.299	-0.094	0.754	-0.851	-4.618	3.653	47	2017	[16]
[ChxmIm]+	-0.299	-0.094	0.754	-0.851	-4.618	3.653	47	2017	[16]
[ChxmPyrr]+	-0.297	0.073	0.697	-1.157	-4.687	3.709	47	2018	[17]
[ChxPy]+	-0.344	0.146	0.703	-1.047	-4.535	3.681	47	2017	[16]
[CNMeM2iPam]+	-1.001	0.000	1.512	-0.459	-4.191	3.529	40	2016	[66]

Cation	*c*	*e*	*s*	*a*	*b*	*v*	N	Year	Source
[CNPrMIm]+	-0.680	0.206	0.782	-1.167	-4.055	3.301	45	2014	[77]
[D2MIM]+	-0.093	-0.052	0.040	-1.620	-4.667	4.034	40	2014	[77]
[DM3AM]+	-0.128	-0.131	0.329	-1.458	-4.550	3.816	46	2011	[45]
[DMPyrr]+	-0.083	-0.142	0.419	-1.467	-4.859	3.824	40	2012	[69]
[E3S]+	-0.062	-1.347	2.716	-1.550	-5.274	3.242	31	2011	[26]
[EMIM]+	-0.049	0.215	0.428	-1.294	-4.209	3.163	552	2014	[77]
[EtOHM2iPAm]+	-0.669	0.236	0.617	-0.850	-3.356	3.270	41	2016	[66]
[EtOHMIm]+	-0.404	0.229	0.517	-1.026	-3.493	2.931	148	2011	[26]
[H3Tdp]+	-0.049	-0.166	-0.134	-1.356	-4.775	4.045	97	2014	[77]
[HexdMIm]+	0.167	-0.218	-0.448	-1.884	-4.597	4.461	31	2011	[26]
[HexM3Am]+	-0.404	0.344	0.945	0.987	-4.526	2.957	70	2010	[45]
[HM2iPam]+	-0.340	0.000	0.582	-1.194	-4.631	3.640	45	2016	[66]
[HMIM]+	-0.083	0.098	0.348	-1.275	-4.426	3.585	335	2014	[77]
[HMPyrr]+	-0.226	-0.083	0.560	-1.301	-4.501	3.673	36	2014	[77]
[HxomMIm]+	-0.071	-0.558	1.080	-1.351	-4.718	3.646	34	2014	[77]
[M2EIm]+	-0.095	0.292	0.443	-1.681	-4.024	3.174	39	2011	[26]
[M3BAm]+	0.047	-0.021	0.356	-1.262	-4.400	3.209	57	2011	[26]
[MB3Am]+	-0.233	0.000	0.404	-1.313	-4.542	3.687	44	2014	[77]
[MDIm]+	0.036	-0.064	0.395	-1.611	-4.546	3.587	42	2014	[77]
[MeoeMim]+	-0.150	0.012	0.653	-1.289	-4.263	3.116	52	2014	[77]
[MeoeMMorp]+	-0.264	0.067	0.995	-1.058	-4.381	3.168	162	2014	[77]
[MeoeMPip]+	-0.102	0.191	0.660	-1.094	-4.665	3.360	166	2014	[77]
[MeoeMPyrr]+	-0.068	0.119	0.691	-1.140	-4.694	3.324	106	2014	[77]
[MO3Am]+	-0.092	0.000	-0.146	-1.129	-4.609	4.114	32	2011	[26]
[MOIm]+	-0.011	0.009	-0.150	-1.641	-3.980	3.872	112	2011	[26]
[N112N113]+	-1.042	0.143	1.160	-0.335	-3.910	3.643	45	2019	[18]
[N112N114]+	-0.397	0.000	0.779	0.712	-4.181	3.291	44	2019	[18]
[N112O2N113]+	-0.339	-0.149	0.748	-0.945	-4.542	3.605	43	2019	[18]
[N112O2N114]+	-0.205	-0.053	0.584	-1.037	-4.475	3.508	45	2019	[18]
[N2,2,2,8]+	-0.003	0.192	0.294	-1.339	-4.769	3.663	193	2019	[12]
[NEP]+	-0.322	0.323	0.552	-1.234	-3.951	3.370	37	2014	[77]
[O3Am]+	-0.044	0.111	0.398	-1.298	-4.815	3.667	63	2017	[14]

Cation	*c*	*e*	*s*	*a*	*b*	*v*	N	Year	Source
[O4AM]+	0.226	0.000	-0.212	-1.756	-4.739	3.825	42	2011	[45]
[OiQu]+	0.065	-0.422	0.969	-1.247	-5.404	3.701	35	2014	[77]
[OM3AM]+	-0.165	-0.181	0.569	-1.419	-4.677	3.711	44	2011	[45]
[Ompyrr]+	-0.253	0.000	0.520	-1.460	-4.696	3.815	39	2014	[77]
[P1,4,4,4]+	-0.817	0.253	1.069	2.631	0.904	0.830	32	2014	[77]
[PDMIM]+	-0.499	0.685	0.568	-0.238	-4.006	2.907	34	2011	[26]
[PeMPyrr]+	-0.303	0.000	0.727	-1.107	-4.622	3.630	42	2014	[77]
[PM2iPAm]+	-0.378	0.115	0.723	-1.061	-4.594	3.388	44	2016	[66]
[PMPip]+	-0.230	0.458	0.342	-1.259	-4.296	3.409	81	2014	[77]
[PMPyrr]+	-0.236	0.000	0.908	-1.015	-4.691	3.446	39	2014	[77]
[sec-BMIm]+	-0.215	0.000	0.740	-1.119	-4.496	3.436	46	2019	[6]
[tert-BMIm]+	-0.275	0.000	0.796	-0.926	-4.526	3.395	46	2019	[6]

Table D.6: Anion log K ABSM values at 298 K.

Anion	*c*	*e*	*s*	*a*	*b*	*l*	N	Year	Source
[+CS]-	0.157	0.058	0.229	4.084	-0.522	0.131	40	2014	[13]
[BETI]-	0.068	-0.334	0.217	-0.196	-0.238	-0.279	53	2011	[74]
[BF4]-	-0.192	0.227	0.343	0.978	-0.287	-0.075	310	2014	[77]
[DCA]-	-0.372	0.345	0.476	2.270	-0.198	-0.055	150	2014	[77]
[DEP]-	0.093	0.107	-0.068	5.071	-0.774	0.061	38	2014	[77]
[EtSO4]-	-0.173	-0.072	0.239	2.931	-0.668	-0.066	53	2014	[77]
[FAP]-	0.229	-0.049	-0.114	-1.277	0.341	-0.039	630	2014	[77]
[FSI]-	-0.147	0.134	0.295	0.133	-0.021	0.003	193	2019	[12]
[L-Lact]-	0.197	0.113	0.124	4.370	-0.613	0.003	31	2014	[13]
[MeSO3]-	-0.827	0.463	0.417	4.083	-0.280	-0.023	51	2014	[77]
[NO3]-	-0.220	0.398	0.580	2.881	-0.699	-0.108	97	2014	[77]
[NTf2]	0.000	0.000	0.000	0.000	0.000	0.000	860	2011	[26]
[OS]-	0.057	-0.126	-0.077	2.575	-0.587	0.108	97	2014	[77]
[PF6]-	-0.016	-0.158	0.529	0.035	-0.149	-0.096	206	2014	[77]
[SCN]-	-0.566	0.431	0.534	2.806	-0.272	-0.040	223	2014	[77]
[TCB]-	0.048	-0.009	0.345	0.371	-0.143	-0.012	245	2014	[77]

Anion	*c*	*e*	*s*	*a*	*b*	*l*	N	Year	Source
[TCM]-	-0.098	0.094	0.290	1.338	-0.145	0.005	96	2014	[77]
[TDI]-	-0.046	0.013	0.088	1.132	0.013	0.049	132	2014	[64]
[TFA]-	-0.295	-0.186	0.545	3.113	-0.078	0.014	32	2014	[77]
[Trif]-	-0.275	0.035	0.323	1.709	-0.175	-0.002	199	2014	[77]

Table D.7: Anion log P ABSM values at 298 K.

Anion	*c*	*e*	*s*	*a*	*b*	*v*	N	Year	Source
[+Cs]-	-0.049	-0.166	0.363	5.498	-0.568	0.510	40	2014	[13]
[BETI]-	0.071	-0.245	0.038	-0.318	0.101	-0.349	51	2014	[77]
[BF4]-	-0.084	0.129	0.240	1.108	-0.401	-0.296	305	2011	[26]
[DCA]-	-0.257	0.164	0.446	2.217	-0.256	-0.243	136	2014	[77]
[DEP]-	0.071	0.073	0.006	5.089	-0.832	0.184	38	2014	[77]
[EtSO4]-	-0.029	-0.245	0.129	2.792	-0.745	-0.264	53	2014	[77]
[FAP]-	0.198	0.049	-0.214	-1.344	0.449	-0.109	620	2014	[77]
[FSI]-	-0.092	-0.038	0.406	0.082	-0.074	-0.051	193	2019	[12]
[L-Lact]-	-0.049	-0.166	-0.134	1.885	-0.554	0.113	31	2014	[13]
[MeSO3]-	-0.646	0.347	0.315	3.997	-0.336	-0.242	49	2014	[77]
[NO3]-	-0.068	0.203	0.425	2.793	-0.681	-0.411	97	2014	[77]
[NTf2]-	0.000	0.000	0.000	0.000	0.000	0.000	843	2011	[26]
[OS]-	-0.040	-0.043	0.002	2.583	-0.577	0.424	95	2014	[77]
[PF6]-	0.007	-0.230	0.417	0.131	-0.120	-0.297	201	2014	[77]
[SCN]-	-0.534	0.187	0.644	2.801	-0.315	-0.130	220	2014	[77]
[TCB]-	0.072	-0.075	0.347	0.312	-0.121	0.061	244	2014	[77]
[TCM]-	-0.079	0.056	0.276	1.223	-0.070	-0.008	95	2014	[77]
[TDI]-	-0.043	-0.019	0.104	0.996	0.146	0.128	132	2014	[64]
[TFA]-	-0.286	-0.697	0.859	2.284	0.475	0.056	32	2014	[77]
[Trif]-	-0.228	-0.088	0.367	1.560	-0.091	-0.047	161	2014	[77]

Table D.8: Cation and anion ABSM parameters for log K values from method 1.

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[(C3COOMe)MIM]+	1	1.370	0.137	0.057	0.204	2.724	0.293	2.211	0.560	0.604	0.351	0.646	0.036
[(Hexom)2Im]+	1	-0.314	0.121	-0.479	0.180	2.076	0.258	2.376	0.494	0.287	0.310	0.835	0.032
[(Meo)2Im]+	1	-0.762	0.121	-0.013	0.180	2.557	0.258	2.427	0.494	1.157	0.310	0.584	0.032
[1-PrOHPy]+	1	-0.897	0.137	0.639	0.204	1.593	0.293	2.414	0.560	2.447	0.351	0.673	0.036
[2,4,6-M3Py]+	1	0.000	0.121	0.280	0.180	1.610	0.258	1.400	0.494	0.590	0.310	0.420	0.032
[2,6-M2Py]+	1	0.000	0.121	0.180	0.180	1.700	0.258	1.350	0.494	0.300	0.310	0.370	0.032
[2-MPy]+	1	0.000	0.121	0.060	0.180	1.620	0.258	1.190	0.494	0.170	0.310	0.310	0.032
[3,5-M2Py]+	1	0.000	0.121	0.160	0.180	1.550	0.258	1.110	0.494	0.280	0.310	0.370	0.032
[3-MBPy]+	2	-0.408	0.123	-0.033	0.183	2.502	0.263	2.594	0.503	0.045	0.315	0.745	0.032
[4-CNBPy]+	1	-0.768	0.121	0.086	0.180	2.810	0.258	2.685	0.494	0.553	0.310	0.691	0.032
[AllMIm]+	2	-0.431	0.092	0.087	0.136	2.477	0.195	2.242	0.374	0.583	0.234	0.620	0.024
[B3EP]+	1	-0.543	0.183	-0.372	0.272	1.664	0.390	0.693	0.746	0.865	0.468	0.826	0.048
[B4MPy]+	1	-0.444	0.137	0.156	0.204	2.304	0.293	2.002	0.560	0.591	0.351	0.763	0.036
[BM2Im]+	1	-0.641	0.121	0.000	0.180	2.429	0.258	2.663	0.494	0.521	0.310	0.721	0.032
[BMIM]+	15	-0.512	0.058	-0.017	0.086	2.384	0.124	2.651	0.237	0.383	0.148	0.735	0.015
[BMMOR]+	1	-0.580	0.148	0.141	0.220	2.625	0.316	2.961	0.604	0.296	0.379	0.690	0.039
[BMPIP]+	1	-0.347	0.121	0.111	0.180	2.241	0.258	2.472	0.494	0.294	0.310	0.687	0.032
[BMPy]+	3	-0.543	0.081	0.018	0.120	2.512	0.173	2.231	0.330	0.514	0.207	0.734	0.021
[BMPyrr]+	8	-0.372	0.062	-0.025	0.092	2.381	0.132	2.590	0.253	0.172	0.158	0.711	0.016
[BzmIm]+	1	-0.535	0.121	0.000	0.180	2.523	0.258	2.333	0.494	0.575	0.310	0.668	0.032
[BzmPyrr]+	1	-0.652	0.121	0.154	0.180	2.371	0.258	2.285	0.494	0.531	0.310	0.691	0.032
[BzPy]+	1	-0.830	0.121	0.000	0.180	2.617	0.258	2.452	0.494	0.526	0.310	0.711	0.032
[C1,9(M2iPAm)2]2+	1	-0.894	0.121	0.175	0.180	2.533	0.258	2.544	0.494	0.492	0.310	0.690	0.032
[C3CNC1Pyr]+	1	-1.227	0.157	-0.006	0.233	3.403	0.334	3.139	0.639	0.076	0.401	0.662	0.041
[C3MPyrr]+	1	-0.466	0.121	2.562	0.180	0.000	0.258	2.505	0.494	0.271	0.310	0.682	0.032
[C5MPyrr]+	1	-0.549	0.121	0.000	0.180	2.317	0.258	2.425	0.494	0.385	0.310	0.747	0.032
[ChxmIm]+	1	-0.513	0.121	-0.203	0.180	2.418	0.258	2.688	0.494	0.334	0.310	0.745	0.032
[ChxmPyrr]+	1	0.545	0.121	-0.124	0.180	2.406	0.258	2.411	0.494	0.274	0.310	0.771	0.032
[ChxPy]+	1	-0.556	0.121	0.000	0.180	2.370	0.258	2.496	0.494	0.412	0.310	0.755	0.032
[CNMeM2iPam]+	1	-1.344	0.121	-0.140	0.180	3.283	0.258	3.118	0.494	0.819	0.310	0.735	0.032
[CnPrM2Im]+	1	0.000	0.121	0.250	0.180	1.810	0.258	1.250	0.494	0.300	0.310	0.350	0.032

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[CNPrMIm]+	1	-1.116	0.137	-0.859	0.204	2.832	0.293	2.371	0.560	0.743	0.351	0.728	0.036
[COC2mMOR]+	1	-0.687	0.121	0.107	0.180	2.766	0.258	2.516	0.494	0.615	0.310	0.629	0.032
[COC2N112]+	1	-0.678	0.136	-0.094	0.201	2.855	0.289	2.717	0.553	0.151	0.346	0.702	0.035
[D2MIM]+	1	-0.252	0.121	-0.269	0.180	1.603	0.258	1.946	0.494	0.354	0.310	0.856	0.032
[DM3AM]+	1	-0.363	0.121	-0.339	0.180	1.986	0.258	2.144	0.494	0.422	0.310	0.809	0.032
[DMPyrr]+	1	-0.395	0.121	-0.241	0.180	1.991	0.258	2.112	0.494	0.268	0.310	0.822	0.032
[DoMIM]+	1	-0.290	0.121	-0.285	0.180	1.812	0.258	2.121	0.494	0.357	0.310	0.853	0.032
[E3S]+	1	-0.606	0.121	-0.196	0.180	2.992	0.258	2.444	0.494	0.355	0.310	0.690	0.032
[EMIM]+	10	-0.598	0.064	0.047	0.095	2.238	0.137	2.266	0.262	0.774	0.164	0.696	0.017
[EtOHM2iPAm]+	1	-0.934	0.121	0.200	0.180	2.361	0.258	2.695	0.494	1.532	0.310	0.641	0.032
[EtOHMIm]+	4	-0.946	0.071	-0.091	0.106	2.728	0.152	2.686	0.290	1.276	0.182	0.600	0.019
[HexM3Am]+	1	-0.469	0.121	-0.058	0.180	2.085	0.258	2.185	0.494	0.617	0.310	0.617	0.032
[HM2iPam]+	1	-0.531	0.121	-0.124	0.180	2.232	0.258	2.297	0.494	0.344	0.310	0.736	0.032
[HMIM]+	3	-0.428	0.080	-0.147	0.119	2.164	0.171	2.279	0.327	0.476	0.205	0.753	0.021
[HMPip]+	1	-0.404	0.121	-0.245	0.180	2.469	0.258	2.348	0.494	0.075	0.310	0.775	0.032
[HMPyrr]+	1	-0.533	0.121	-0.110	0.180	2.146	0.258	2.278	0.494	0.650	0.310	0.767	0.032
[HxomMIm]+	1	-0.462	0.121	0.000	0.180	2.073	0.258	2.022	0.494	0.637	0.310	0.684	0.032
[M2EIM]+	1	-0.565	0.121	0.214	0.180	2.347	0.258	2.075	0.494	0.896	0.310	0.655	0.032
[M2PIm]+	2	0.000	0.121	0.010	0.180	1.670	0.258	1.210	0.494	0.120	0.310	0.310	0.032
[M3BAm]+	1	-0.457	0.121	0.000	0.180	2.188	0.258	2.375	0.494	0.663	0.310	0.668	0.032
[MDIm]+	1	-0.412	0.148	-0.277	0.220	2.049	0.316	2.111	0.604	0.425	0.379	0.817	0.039
[MeOCH2CH2NEt3]+	1	-0.399	0.121	0.086	0.180	2.376	0.258	2.397	0.494	0.452	0.310	0.670	0.032
[MeOCH2CH2PBu3]+	1	-0.233	0.121	-0.176	0.180	1.902	0.258	2.121	0.494	0.239	0.310	0.769	0.032
[MeOCH2CH2PEt3]+	1	-0.437	0.121	0.000	0.180	2.291	0.258	2.503	0.494	0.431	0.310	0.725	0.032
[MeoeM2EAm]+	1	-0.619	0.136	-0.065	0.201	2.692	0.289	2.606	0.553	0.243	0.346	0.683	0.035
[MeoeMIm]+	1	-0.509	0.121	0.065	0.180	2.476	0.258	2.271	0.494	0.671	0.310	0.603	0.032
[MeoeMMorp]+	2	-0.655	0.091	0.074	0.135	2.764	0.194	2.536	0.371	0.501	0.232	0.630	0.024
[MeoeMPip]+	2	-0.464	0.091	0.041	0.135	2.483	0.194	2.531	0.371	0.171	0.232	0.689	0.024
[MeoeMPyrr]+	1	-0.443	0.136	0.006	0.201	2.495	0.289	2.525	0.553	0.044	0.346	0.681	0.035
[MMIm]+	2	-1.118	0.183	-0.293	0.272	2.538	0.390	4.056	0.746	0.774	0.468	0.806	0.048
[Mo1,3CN]+	1	-1.417	0.148	0.008	0.220	3.408	0.316	3.453	0.604	0.078	0.379	0.681	0.039
[Mo1,3OH]+	1	-1.270	0.148	0.180	0.220	3.013	0.316	3.462	0.604	0.531	0.379	0.668	0.039

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[MOIm]+	3	-0.297	0.092	-0.335	0.137	1.511	0.197	1.773	0.377	0.732	0.236	0.862	0.024
[N112N113]+	1	-1.338	0.121	0.044	0.180	2.865	0.258	3.280	0.494	1.041	0.310	0.762	0.032
[N112N114]+	1	-0.725	0.121	0.053	0.180	2.522	0.258	2.863	0.494	0.751	0.310	0.656	0.032
[N112O2N113]+	1	-0.613	0.121	-0.225	0.180	2.440	0.258	2.608	0.494	0.420	0.310	0.748	0.032
[N112O2N114]+	1	-0.436	0.121	-0.108	0.180	2.279	0.258	2.505	0.494	0.435	0.310	0.707	0.032
[N2,2,2,8]+	1	-0.290	0.182	-0.182	0.271	2.101	0.389	2.435	0.743	-0.016	0.466	0.807	0.047
[N-C3CNMPyr]+	1	-0.799	0.137	0.037	0.204	2.990	0.293	2.564	0.560	0.433	0.351	0.637	0.036
[N-C3CNPy]+	1	-0.941	0.137	-0.042	0.204	3.052	0.293	2.374	0.560	0.439	0.351	0.630	0.036
[N-C3OHmMOR]+	1	-0.378	0.121	-0.074	0.180	2.088	0.258	2.368	0.494	0.166	0.310	0.792	0.032
[O4AM]+	1	0.000	0.121	-0.287	0.180	1.478	0.258	1.845	0.494	0.189	0.310	0.816	0.032
[OM3AM]+	1	-0.426	0.121	-0.338	0.180	2.242	0.258	2.195	0.494	0.684	0.310	0.779	0.032
[OMMIM]+	1	-0.682	0.121	-0.036	0.180	1.954	0.258	2.367	0.494	0.621	0.310	0.820	0.032
[Ompyrr]+	1	-0.587	0.121	-0.064	0.180	2.080	0.258	2.176	0.494	0.486	0.310	0.822	0.032
[P14,6,6,6]+	8	-0.287	0.065	-0.732	0.097	1.415	0.140	0.789	0.267	0.371	0.167	0.966	0.017
[P8,8,8,8]+	1	-0.212	0.121	-0.337	0.180	1.522	0.258	1.705	0.494	0.074	0.310	0.880	0.032
[PDMIM]+	2	-1.083	0.092	0.302	0.137	2.670	0.196	2.227	0.376	0.697	0.235	0.716	0.024
[PEMPip]+	1	-0.477	0.121	-0.186	0.180	2.639	0.258	2.450	0.494	0.103	0.310	0.761	0.032
[PemPyrr]+	1	-0.549	0.121	0.000	0.180	2.317	0.258	2.425	0.494	0.385	0.310	0.747	0.032
[PM2iPAm]+	1	-0.702	0.121	0.000	0.180	2.532	0.258	2.578	0.494	0.331	0.310	0.682	0.032
[PMPip]+	1	-0.432	0.121	0.145	0.180	2.287	0.258	2.489	0.494	0.402	0.310	0.674	0.032
[PMPyrr]+	1	-0.466	0.121	0.000	0.180	2.562	0.258	2.505	0.494	0.271	0.310	0.682	0.032
[PrOHM2Im]+	1	0.000	0.121	0.210	0.180	1.500	0.258	1.250	0.494	0.660	0.310	0.340	0.032
[PrOHPy]+	2	-0.688	0.091	0.209	0.135	2.595	0.194	2.799	0.371	1.222	0.232	0.599	0.024
[QUIN6]+	1	-0.562	0.121	-0.071	0.180	2.201	0.258	2.569	0.494	0.238	0.310	0.815	0.032
[QUIN8]+	1	-0.363	0.121	-0.186	0.180	2.048	0.258	2.430	0.494	0.142	0.310	0.816	0.032
[sec-BMIm]+	1	-0.558	0.121	-0.097	0.180	2.519	0.258	2.497	0.494	0.456	0.310	0.705	0.032
[TDC]+	2	-0.187	0.092	-0.001	0.136	2.136	0.195	2.459	0.374	0.081	0.234	0.751	0.024
[tert-BMIm]+	1	-0.621	0.121	-0.118	0.180	2.603	0.258	2.689	0.494	0.410	0.310	0.693	0.032
[[(CH3)2PO4]-	1	-0.142	0.134	0.340	0.199	-0.255	0.286	5.321	0.548	-0.011	0.343	-0.035	0.035
[BETI]-	1	0.052	0.134	0.158	0.199	-0.178	0.286	-0.671	0.548	0.313	0.343	-0.122	0.035
[CH3SO4]-	1	0.006	0.134	0.279	0.199	-0.215	0.286	0.487	0.548	-0.331	0.343	-0.236	0.035
[Cl]-	3	-0.269	0.090	0.290	0.133	0.126	0.191	2.689	0.366	0.479	0.229	-0.056	0.023

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[SbF6]-	1	-0.203	0.134	-0.246	0.199	0.480	0.286	-0.329	0.548	0.195	0.343	0.022	0.035
[TDI]-	2	0.035	0.116	0.055	0.172	-0.126	0.247	0.794	0.472	0.212	0.296	0.022	0.030
[Trif]-	3	-0.201	0.094	0.150	0.140	0.087	0.201	1.361	0.384	0.062	0.240	-0.040	0.024
[SCN]-	3	-0.520	0.099	0.723	0.148	0.144	0.212	2.464	0.406	0.211	0.254	-0.072	0.026
[(MeO)(H)PO2]-	2	-0.522	0.137	0.293	0.204	0.682	0.292	5.584	0.559	-0.774	0.350	-0.076	0.036
[DEP]-	2	0.186	0.137	0.148	0.204	-0.001	0.292	5.166	0.559	-0.865	0.350	0.018	0.036
[EtSO4]-	1	-0.069	0.137	-0.047	0.204	0.319	0.292	3.061	0.559	-0.774	0.350	-0.108	0.036
[MeSO3]-	2	-0.585	0.099	0.422	0.148	0.317	0.212	4.047	0.405	-0.212	0.254	-0.075	0.026
[TFA]-	1	-0.212	0.137	-0.047	0.204	0.456	0.292	3.196	0.559	-0.040	0.350	-0.027	0.036
[Tf2C]-	1	0.000	0.171	0.070	0.254	-0.080	0.365	-0.060	0.699	0.030	0.438	0.050	0.045
[TCB]-	4	0.077	0.085	0.101	0.127	0.339	0.182	0.310	0.348	-0.053	0.218	-0.045	0.022
[M2PO4]-	1	0.508	0.219	1.153	0.326	0.052	0.468	3.214	0.895	-0.774	0.561	-0.456	0.057
[TCM]-	6	-0.194	0.085	0.230	0.127	0.137	0.182	0.746	0.348	0.156	0.218	-0.047	0.022
[FSI]-	2	-0.171	0.136	0.266	0.202	0.175	0.290	-0.040	0.555	0.184	0.348	-0.029	0.035
[PF6]-	4	-0.021	0.079	0.292	0.118	-0.155	0.169	0.109	0.323	0.458	0.203	-0.100	0.021
[+CS]-	1	0.086	0.138	0.324	0.204	0.312	0.294	5.578	0.562	-0.612	0.352	0.069	0.036
[L-Lact]-	1	0.096	0.138	0.379	0.204	0.207	0.294	5.864	0.562	-0.703	0.352	-0.059	0.036
[OS]-	3	0.195	0.084	0.103	0.125	-0.568	0.180	2.722	0.344	-0.230	0.216	0.075	0.022
[BF4]-	6	-0.078	0.068	0.176	0.101	0.397	0.144	1.108	0.276	-0.465	0.173	-0.118	0.018
[FAP]-	10	0.298	0.061	-0.006	0.090	-0.135	0.130	-1.277	0.248	0.479	0.156	-0.052	0.016
[DCA]-	12	-0.373	0.065	0.441	0.096	0.257	0.138	2.436	0.264	-0.117	0.166	-0.084	0.017

Table D.9: Cation and anion ABSM parameters for log P values from method 1.

Ion	# of Ins	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[(C3COOMe)MIM]+	1	-0.301	0.139	0.090	0.255	1.048	0.390	-1.305	0.576	-4.447	0.791	3.201	0.400
[(Hexom)2Im]+	1	0.107	0.122	-0.628	0.224	0.747	0.343	-1.441	0.507	-4.808	0.696	3.750	0.352
[(Meo)2Im]+	1	-0.412	0.122	-0.104	0.224	0.761	0.343	-1.124	0.507	-3.776	0.696	3.055	0.352
[3-MBPy]+	2	-0.073	0.125	0.158	0.230	0.751	0.352	-1.241	0.520	-4.824	0.714	3.512	0.361
[4-CNBPy]+	1	-0.316	0.122	0.132	0.224	1.015	0.343	-1.040	0.507	-4.399	0.696	3.272	0.352
[AllMIm]+	2	-0.002	0.093	0.070	0.170	0.641	0.260	-1.467	0.384	-4.304	0.527	3.065	0.267
[B3EP]+	1	-0.032	0.185	-0.341	0.339	0.213	0.518	-3.416	0.766	-4.400	1.052	3.605	0.532

Ion	# of Ins	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[B4MPy]+	1	-0.223	0.139	0.261	0.255	0.815	0.390	-1.525	0.576	-4.554	0.791	3.640	0.400
[BM2Im]+	1	-0.347	0.122	0.111	0.224	0.718	0.343	-1.195	0.507	-4.418	0.696	3.502	0.352
[BMIM]+	15	-0.235	0.061	0.340	0.111	0.558	0.170	-0.937	0.252	-4.040	0.346	3.470	0.175
[BMMOR]+	1	0.008	0.154	0.125	0.281	-0.129	0.431	-2.523	0.637	-8.088	0.874	3.548	0.442
[BMPIP]+	1	-0.129	0.122	0.494	0.224	0.235	0.343	-1.165	0.507	-4.385	0.696	3.422	0.352
[BMPy]+	2	-0.378	0.112	0.671	0.205	0.523	0.315	-0.985	0.465	-2.460	0.638	3.426	0.323
[BMPyrr]+	8	-0.034	0.064	0.313	0.117	0.207	0.179	-1.365	0.264	-5.166	0.363	3.485	0.184
[BzmIm]+	1	-0.187	0.122	0.000	0.224	0.768	0.343	-1.284	0.507	-4.378	0.696	3.310	0.352
[BzmPyrr]+	1	-0.387	0.122	0.197	0.224	0.658	0.343	-1.275	0.507	-4.401	0.696	3.449	0.352
[BzPy]+	1	-0.516	0.122	0.092	0.224	0.865	0.343	-1.143	0.507	-4.432	0.696	3.485	0.352
[C1,9(M2iPAm)2]2+	1	-0.606	0.122	0.225	0.224	0.798	0.343	-1.034	0.507	-4.438	0.696	3.429	0.352
[C3CNC1Pyr]+	1	-0.939	0.159	0.523	0.291	1.087	0.446	-0.224	0.659	-4.770	0.904	3.293	0.457
[C3MPyrr]+	1	-0.236	0.122	0.000	0.224	0.908	0.343	-1.015	0.507	-4.691	0.696	3.446	0.352
[C5MPyrr]+	1	-0.303	0.122	0.000	0.224	0.727	0.343	-1.107	0.507	-4.622	0.696	3.630	0.352
[ChxmIm]+	1	-0.299	0.122	-0.094	0.224	0.754	0.343	-0.851	0.507	-4.618	0.696	3.653	0.352
[ChxmPyrr]+	1	-0.297	0.122	0.073	0.224	0.697	0.343	-1.157	0.507	-4.687	0.696	3.709	0.352
[ChxPy]+	1	-0.344	0.122	0.146	0.224	0.703	0.343	-1.047	0.507	-4.535	0.696	3.681	0.352
[CNMeM2iPam]+	1	-1.001	0.122	0.000	0.224	1.512	0.343	-0.459	0.507	-4.191	0.696	3.529	0.352
[CNPrMIm]+	1	-0.729	0.139	0.095	0.255	1.023	0.390	-1.381	0.576	-4.096	0.791	3.395	0.400
[COC2mMOR]+	1	-0.216	0.122	0.054	0.224	1.059	0.343	-1.019	0.507	-4.564	0.696	3.082	0.352
[D2MIM]+	1	-0.093	0.122	-0.052	0.224	0.040	0.343	-1.620	0.507	-4.667	0.696	4.034	0.352
[DM3AM]+	1	-0.128	0.122	-0.131	0.224	0.329	0.343	-1.458	0.507	-4.550	0.696	3.816	0.352
[DMPyrr]+	1	-0.083	0.122	-0.142	0.224	0.419	0.343	-1.467	0.507	-4.859	0.696	3.824	0.352
[DoMIM]+	1	0.063	0.122	-0.055	0.224	0.275	0.343	-1.368	0.507	-4.897	0.696	3.824	0.352
[E3S]+	1	-0.062	0.122	-1.347	0.224	2.716	0.343	1.350	0.507	-5.274	0.696	3.242	0.352
[EMIM]+	10	-0.130	0.065	0.190	0.120	0.338	0.183	-1.519	0.271	-4.096	0.372	3.228	0.188
[EtOHM2iPAm]+	1	-0.669	0.122	0.236	0.224	0.617	0.343	-0.850	0.507	-3.356	0.696	3.270	0.352
[EtOHMIm]+	3	-0.394	0.080	0.023	0.146	0.845	0.224	-1.045	0.331	-3.508	0.455	3.003	0.230
[HexM3Am]+	1	-0.322	0.122	0.242	0.224	0.287	0.343	-1.383	0.507	-4.265	0.696	3.513	0.352
[HM2iPam]+	1	-0.340	0.122	0.000	0.224	0.582	0.343	-1.194	0.507	-4.631	0.696	3.640	0.352
[HMIM]+	3	-0.065	0.081	0.088	0.149	0.304	0.228	-1.440	0.336	-4.512	0.462	3.573	0.234
[HMPyrr]+	1	-0.226	0.122	-0.083	0.224	0.560	0.343	-1.301	0.507	-4.501	0.696	3.673	0.352

Ion	# of Ins	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[HxomMIm]+	1	-0.275	0.122	0.000	0.224	0.407	0.343	-1.478	0.507	4.320	0.696	3.510	0.352
[M2EIM]+	1	-0.095	0.122	0.299	0.224	0.360	0.343	-1.906	0.507	-3.805	0.696	3.177	0.352
[M3BAm]+	1	0.047	0.122	-0.051	0.224	0.356	0.343	-1.262	0.507	-4.400	0.696	3.209	0.352
[MDIm]+	1	0.106	0.150	-0.062	0.274	0.214	0.420	-1.724	0.621	-4.749	0.853	3.709	0.431
[MeOCH2CH2NEt3]+	1	-0.129	0.122	0.080	0.224	0.682	0.343	-1.084	0.507	-4.538	0.696	3.370	0.352
[MeOCH2CH2PBu3]+	1	-0.045	0.122	0.041	0.224	0.218	0.343	-1.396	0.507	-4.650	0.696	3.708	0.352
[MeOCH2CH2PEt3]+	1	-0.177	0.122	0.103	0.224	0.582	0.343	-1.022	0.507	-4.516	0.696	3.546	0.352
[MeoeM2EAm]+	1	-0.162	0.137	0.027	0.251	0.823	0.385	-1.193	0.568	-4.766	0.781	3.270	0.395
[MeoeMIm]+	1	-0.150	0.122	0.012	0.224	0.818	0.343	-1.289	0.507	-4.263	0.696	3.116	0.352
[MeoeMMorp]+	2	-0.192	0.092	0.001	0.168	0.972	0.258	-1.163	0.381	-4.532	0.523	3.110	0.264
[MeoeMPip]+	2	-0.075	0.092	0.147	0.168	0.656	0.258	-1.177	0.381	-4.792	0.523	3.335	0.264
[MeoeMPyrr]+	1	-0.066	0.137	0.076	0.251	0.672	0.385	-1.268	0.568	-4.941	0.781	3.329	0.395
[MMIm]+	1	0.400	0.185	0.220	0.339	-0.712	0.518	-1.459	0.766	-3.056	1.052	2.988	0.532
[Mo1,3CN]+	1	-0.849	0.154	-0.082	0.281	0.834	0.431	-1.828	0.637	-8.526	0.874	3.533	0.442
[Mo1,3OH]+	1	-0.679	0.154	0.073	0.281	0.423	0.431	-1.832	0.637	-8.071	0.874	3.477	0.442
[MOIm]+	3	-0.188	0.096	-0.249	0.176	0.508	0.269	-1.842	0.398	-4.551	0.546	4.030	0.276
[N112N113]+	1	-1.042	0.122	0.143	0.224	1.160	0.343	-0.335	0.507	-3.910	0.696	3.643	0.352
[N112N114]+	1	-0.397	0.122	0.000	0.224	0.779	0.343	0.712	0.507	-4.181	0.696	3.291	0.352
[N112O2N113]+	1	-0.339	0.122	-0.149	0.224	0.748	0.343	-0.945	0.507	-4.542	0.696	3.605	0.352
[N112O2N114]+	1	-0.205	0.122	-0.053	0.224	0.584	0.343	-1.037	0.507	-4.475	0.696	3.508	0.352
[N2,2,2,8]+	1	-0.001	0.184	0.279	0.338	-0.014	0.517	-1.517	0.764	-5.372	1.049	3.802	0.531
[N-C3CNMPyr]+	1	-0.516	0.139	0.050	0.255	1.331	0.390	-0.894	0.576	-4.631	0.791	3.214	0.400
[N-C3CNPy]+	1	-0.585	0.139	-0.026	0.255	1.348	0.390	-1.138	0.576	-4.625	0.791	3.133	0.400
[O4AM]+	1	0.226	0.122	0.000	0.224	-0.212	0.343	-1.756	0.507	-4.739	0.696	3.825	0.352
[OM3AM]+	1	-0.165	0.122	-0.181	0.224	0.569	0.343	-1.419	0.507	-4.677	0.696	3.711	0.352
[OMMIM]+	1	-0.354	0.122	0.200	0.224	0.130	0.343	-1.444	0.507	-4.224	0.696	3.826	0.352
[Ompyrr]+	1	-0.253	0.122	0.000	0.224	0.520	0.343	-1.460	0.507	-4.696	0.696	3.815	0.352
[P14,6,6,6]+	8	-0.028	0.068	-0.532	0.124	0.106	0.190	-2.694	0.281	-4.576	0.386	4.180	0.195
[P8,8,8,8]+	1	0.153	0.122	-0.069	0.224	-0.011	0.343	-1.800	0.507	-5.186	0.696	3.888	0.352
[PDMIM]+	2	-0.864	0.095	0.555	0.174	0.715	0.267	-1.147	0.394	-3.735	0.541	3.528	0.274
[PemPyrr]+	1	-0.303	0.122	0.000	0.224	0.727	0.343	-1.107	0.507	-4.622	0.696	3.630	0.352
[PM2iPAm]+	1	-0.378	0.122	0.115	0.224	0.723	0.343	-1.061	0.507	-4.594	0.696	3.388	0.352

Ion	# of Ins	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[PMPip]+	1	-0.231	0.122	0.453	0.224	0.352	0.343	-1.263	0.507	-4.290	0.696	3.401	0.352
[PMPyrr]+	1	-0.236	0.122	0.000	0.224	0.908	0.343	-1.015	0.507	-4.691	0.696	3.446	0.352
[PrOHPy]+	2	-0.205	0.092	0.084	0.168	0.822	0.258	-0.939	0.381	-3.814	0.523	2.998	0.264
[QUIN6]+	1	-0.360	0.122	0.138	0.224	0.594	0.343	-0.936	0.507	-4.776	0.696	3.864	0.352
[QUIN8]+	1	-0.149	0.122	0.000	0.224	0.451	0.343	-1.080	0.507	-4.886	0.696	3.861	0.352
[sec-BMIm]+	1	-0.215	0.122	0.000	0.224	0.740	0.343	-1.119	0.507	-4.496	0.696	3.436	0.352
[TDC]+	2	-0.073	0.093	0.155	0.170	0.535	0.260	-1.011	0.384	-4.873	0.527	3.720	0.267
[tert-BMIm]+	1	-0.275	0.122	0.000	0.224	0.796	0.343	-0.926	0.507	-4.526	0.696	3.395	0.352
[[(CH3)2PO4]-	1	-0.020	0.137	0.019	0.250	-0.046	0.383	5.430	0.566	-0.781	0.777	-0.136	0.393
[BETI]-	1	0.258	0.137	-0.257	0.250	-0.224	0.383	-0.764	0.566	-0.196	0.777	-0.429	0.393
[CH3SO4]-	1	0.237	0.137	-0.167	0.250	-0.379	0.383	0.142	0.566	-0.790	0.777	-0.779	0.393
[Cl]-	3	0.012	0.092	-0.673	0.169	1.189	0.258	2.534	0.382	-1.198	0.525	-0.393	0.265
[SbF6]-	1	-0.003	0.137	-1.166	0.250	1.438	0.383	0.287	0.566	-1.517	0.777	0.026	0.393
[TDI]-	2	0.107	0.118	-0.060	0.216	-0.074	0.331	0.546	0.489	-0.076	0.671	0.050	0.339
[Trif]-	3	-0.111	0.096	-0.088	0.176	0.238	0.269	1.434	0.398	0.020	0.546	-0.179	0.276
[SCN]-	3	-0.449	0.101	0.065	0.186	0.862	0.285	2.456	0.421	-0.110	0.577	-0.249	0.292
[(MeO)(H)PO2]-	2	-0.400	0.139	0.130	0.254	0.712	0.389	5.609	0.575	-0.824	0.789	-0.348	0.399
[DEP]-	2	0.152	0.139	0.099	0.254	0.096	0.389	5.315	0.575	-0.945	0.789	0.118	0.399
[EtSO4]-	1	0.051	0.139	-0.211	0.254	0.216	0.389	3.010	0.575	-0.848	0.789	-0.333	0.399
[MeSO3]-	2	-0.464	0.101	0.153	0.185	0.399	0.283	4.135	0.419	-0.626	0.575	-0.261	0.291
[TFA]-	1	0.001	0.139	-1.441	0.254	2.018	0.389	2.408	0.575	-0.377	0.789	-0.184	0.399
[TCB]-	4	0.002	0.087	-0.076	0.159	0.528	0.243	0.445	0.359	0.082	0.493	-0.183	0.249
[TCM]-	6	-0.326	0.093	0.249	0.170	1.080	0.261	2.523	0.385	3.604	0.529	-0.426	0.267
[FSI]-	2	-0.108	0.138	-0.048	0.253	0.610	0.387	0.216	0.572	0.574	0.785	-0.198	0.397
[PF6]-	4	0.043	0.081	0.109	0.149	-0.278	0.228	0.290	0.337	0.111	0.462	-0.336	0.234
[+CS]-	1	0.028	0.140	0.532	0.256	0.123	0.392	5.443	0.580	-0.767	0.796	0.375	0.402
[L-Lact]-	1	0.028	0.140	0.532	0.256	-0.106	0.392	5.935	0.580	-0.753	0.796	-0.022	0.402
[OS]-	3	0.197	0.086	0.101	0.158	-0.516	0.242	2.747	0.357	-0.593	0.490	0.287	0.248
[BF4]-	5	0.250	0.079	-0.192	0.145	0.440	0.222	0.925	0.328	-1.280	0.451	-0.491	0.228
[FAP]-	9	0.196	0.062	0.092	0.114	-0.195	0.174	-1.215	0.257	0.696	0.353	-0.114	0.179
[DCA]-	11	-0.199	0.066	0.278	0.121	0.201	0.186	2.423	0.274	-0.211	0.377	-0.349	0.190

Table D.10: Cation and anion ABSM parameters for log K values from method 2.

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[(C3COOMe)MIM]+	1	1.354	0.080	0.123	0.076	2.690	0.092	2.390	0.132	0.625	0.135	0.628	0.019
[(Hexom)2Im]+	1	-0.314	0.070	-0.479	0.067	2.076	0.081	2.376	0.116	0.287	0.118	0.835	0.017
[(Meo)2Im]+	1	-0.762	0.070	-0.013	0.067	2.557	0.081	2.427	0.116	1.157	0.118	0.584	0.017
[1-PrOHPy]+	1	-0.913	0.080	0.705	0.076	1.559	0.092	2.593	0.132	2.468	0.135	0.655	0.019
[3-MBPy]+	2	-0.328	0.072	0.004	0.069	2.346	0.083	2.325	0.119	0.233	0.122	0.741	0.017
[4-CNBPy]+	1	-0.768	0.070	0.086	0.067	2.810	0.081	2.685	0.116	0.553	0.118	0.691	0.017
[AllMIm]+	2	-0.439	0.053	0.120	0.051	2.460	0.061	2.331	0.088	0.594	0.090	0.612	0.013
[B3EP]+	1	-0.524	0.107	-0.357	0.102	1.778	0.123	0.875	0.176	0.765	0.180	0.801	0.026
[B4MPy]+	1	-0.460	0.080	0.222	0.076	2.270	0.092	2.181	0.132	0.612	0.135	0.745	0.019
[BM2Im]+	1	-0.641	0.070	0.000	0.067	2.429	0.081	2.663	0.116	0.521	0.118	0.721	0.017
[BMIM]+	13	-0.414	0.035	0.024	0.034	2.186	0.041	2.290	0.059	0.621	0.060	0.733	0.009
[BMMOR]+	1	-0.503	0.086	0.160	0.082	2.546	0.099	2.828	0.143	0.392	0.146	0.684	0.021
[BMPIP]+	1	-0.347	0.070	0.111	0.067	2.241	0.081	2.472	0.116	0.294	0.118	0.687	0.017
[BMPy]+	3	-0.446	0.048	0.004	0.046	2.524	0.056	2.235	0.080	0.501	0.082	0.727	0.012
[BMPyrr]+	8	-0.336	0.036	0.004	0.035	2.328	0.042	2.550	0.060	0.234	0.061	0.703	0.009
[BzmIm]+	1	-0.535	0.070	0.000	0.067	2.523	0.081	2.333	0.116	0.575	0.118	0.668	0.017
[BzmPyrr]+	1	-0.652	0.070	0.154	0.067	2.371	0.081	2.285	0.116	0.531	0.118	0.691	0.017
[BzPy]+	1	-0.830	0.070	0.000	0.067	2.617	0.081	2.452	0.116	0.526	0.118	0.711	0.017
[C1,9(M2iPAm)2]2+	1	-0.894	0.070	0.175	0.067	2.533	0.081	2.544	0.116	0.492	0.118	0.690	0.017
[C3CNC1Pyr]+	1	-1.160	0.091	0.029	0.087	3.277	0.105	2.938	0.151	0.227	0.154	0.656	0.022
[C3MPyrr]+	1	-0.466	0.070	2.562	0.067	0.000	0.081	2.505	0.116	0.271	0.118	0.682	0.017
[C5MPyrr]+	1	-0.549	0.070	0.000	0.067	2.317	0.081	2.425	0.116	0.385	0.118	0.747	0.017
[ChxmIm]+	1	-0.513	0.070	-0.203	0.067	2.418	0.081	2.688	0.116	0.334	0.118	0.745	0.017
[ChxmPyrr]+	1	0.545	0.070	-0.124	0.067	2.406	0.081	2.411	0.116	0.274	0.118	0.771	0.017
[ChxPy]+	1	-0.556	0.070	0.000	0.067	2.370	0.081	2.496	0.116	0.412	0.118	0.755	0.017
[CNMeM2iPam]+	1	-1.344	0.070	-0.140	0.067	3.283	0.081	3.118	0.116	0.819	0.118	0.735	0.017
[CNPrMIm]+	1	-1.132	0.080	-0.793	0.076	2.798	0.092	2.550	0.132	0.764	0.135	0.710	0.019
[COC2mMOR]+	1	-0.687	0.070	0.107	0.067	2.766	0.081	2.516	0.116	0.615	0.118	0.629	0.017
[COC2N112]+	1	-0.651	0.079	-0.068	0.075	2.843	0.090	2.754	0.130	0.170	0.133	0.693	0.019
[D2MIM]+	1	-0.252	0.070	-0.269	0.067	1.603	0.081	1.946	0.116	0.354	0.118	0.856	0.017
[DM3AM]+	1	-0.363	0.070	-0.339	0.067	1.986	0.081	2.144	0.116	0.422	0.118	0.809	0.017

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[DMPyrr]+	1	-0.395	0.070	-0.241	0.067	1.991	0.081	2.112	0.116	0.268	0.118	0.822	0.017
[DoMIM]+	1	-0.290	0.070	-0.285	0.067	1.812	0.081	2.121	0.116	0.357	0.118	0.853	0.017
[E3S]+	1	-0.606	0.070	-0.196	0.067	2.992	0.081	2.444	0.116	0.355	0.118	0.690	0.017
[EMIM]+	8	-0.579	0.039	0.062	0.038	2.352	0.045	2.448	0.065	0.674	0.066	0.671	0.010
[EtOHM2iPAm]+	1	-0.934	0.070	0.200	0.067	2.361	0.081	2.695	0.116	1.532	0.118	0.641	0.017
[EtOHMIm]+	4	-0.870	0.043	-0.011	0.041	2.596	0.050	2.715	0.072	1.415	0.073	0.593	0.010
[HexM3Am]+	1	-0.469	0.070	-0.058	0.067	2.085	0.081	2.185	0.116	0.617	0.118	0.617	0.017
[HM2iPam]+	1	-0.531	0.070	-0.124	0.067	2.232	0.081	2.297	0.116	0.344	0.118	0.736	0.017
[HMIM]+	3	-0.412	0.047	-0.133	0.045	2.167	0.054	2.310	0.077	0.479	0.079	0.745	0.011
[HMPip]+	1	-0.404	0.070	-0.245	0.067	2.469	0.081	2.348	0.116	0.075	0.118	0.775	0.017
[HMPyrr]+	1	-0.533	0.070	-0.110	0.067	2.146	0.081	2.278	0.116	0.650	0.118	0.767	0.017
[HxomMIm]+	1	-0.462	0.070	0.000	0.067	2.073	0.081	2.022	0.116	0.637	0.118	0.684	0.017
[M2EIM]+	1	-0.565	0.070	0.214	0.067	2.347	0.081	2.075	0.116	0.896	0.118	0.655	0.017
[M3BAm]+	1	-0.457	0.070	0.000	0.067	2.188	0.081	2.375	0.116	0.663	0.118	0.668	0.017
[MDIm]+	1	-0.388	0.086	-0.257	0.082	2.071	0.099	2.169	0.142	0.414	0.145	0.804	0.021
[MeOCH2CH2NEt3]+	1	-0.399	0.070	0.086	0.067	2.376	0.081	2.397	0.116	0.452	0.118	0.670	0.017
[MeOCH2CH2PBu3]+	1	-0.233	0.070	-0.176	0.067	1.902	0.081	2.121	0.116	0.239	0.118	0.769	0.017
[MeOCH2CH2PEt3]+	1	-0.437	0.070	0.000	0.067	2.291	0.081	2.503	0.116	0.431	0.118	0.725	0.017
[MeoeM2EAm]+	1	-0.592	0.079	-0.039	0.075	2.680	0.090	2.643	0.130	0.262	0.133	0.674	0.019
[MeoeMIm]+	1	-0.509	0.070	0.065	0.067	2.476	0.081	2.271	0.116	0.671	0.118	0.603	0.017
[MeoeMMorp]+	2	-0.642	0.053	0.087	0.050	2.758	0.061	2.554	0.087	0.511	0.089	0.626	0.013
[MeoeMPip]+	2	-0.451	0.053	0.053	0.050	2.477	0.061	2.549	0.087	0.181	0.089	0.685	0.013
[MeoeMPyrr]+	1	-0.416	0.079	0.032	0.075	2.483	0.090	2.562	0.130	0.063	0.133	0.672	0.019
[Mo1,3CN]+	1	-1.340	0.086	-0.056	0.082	3.424	0.099	3.624	0.143	0.063	0.146	0.677	0.021
[Mo1,3OH]+	1	-1.193	0.086	0.199	0.082	2.934	0.099	3.329	0.143	0.627	0.146	0.662	0.021
[MOIm]+	2	-0.073	0.066	-0.175	0.063	1.170	0.076	1.959	0.109	1.186	0.112	0.840	0.016
[N112N113]+	1	-1.338	0.070	0.044	0.067	2.865	0.081	3.280	0.116	1.041	0.118	0.762	0.017
[N112N114]+	1	-0.725	0.070	0.053	0.067	2.522	0.081	2.863	0.116	0.751	0.118	0.656	0.017
[N112O2N113]+	1	-0.613	0.070	-0.225	0.067	2.440	0.081	2.608	0.116	0.420	0.118	0.748	0.017
[N112O2N114]+	1	-0.436	0.070	-0.108	0.067	2.279	0.081	2.505	0.116	0.435	0.118	0.707	0.017
[N2,2,2,8]+	1	-0.254	0.106	-0.153	0.101	2.048	0.121	2.395	0.175	0.046	0.178	0.799	0.026
[N-C3CNMPyr]+	1	-0.815	0.080	0.103	0.076	2.956	0.092	2.743	0.132	0.454	0.135	0.619	0.019

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[N-C3CNPy]+	1	-0.957	0.080	0.024	0.076	3.018	0.092	2.553	0.132	0.460	0.135	0.612	0.019
[N-C3OHmMOR]+	1	-0.378	0.070	-0.074	0.067	2.088	0.081	2.368	0.116	0.166	0.118	0.792	0.017
[O4AM]+	1	0.000	0.070	-0.287	0.067	1.478	0.081	1.845	0.116	0.189	0.118	0.816	0.017
[OM3AM]+	1	-0.426	0.070	-0.338	0.067	2.242	0.081	2.195	0.116	0.684	0.118	0.779	0.017
[OMMIM]+	1	-0.682	0.070	-0.036	0.067	1.954	0.081	2.367	0.116	0.621	0.118	0.820	0.017
[Ompyrr]+	1	-0.587	0.070	-0.064	0.067	2.080	0.081	2.176	0.116	0.486	0.118	0.822	0.017
[P14,6,6,6]+	5	-0.518	0.048	-0.483	0.046	1.382	0.056	1.899	0.080	0.278	0.082	0.914	0.012
[P8,8,8,8]+	1	-0.212	0.070	-0.337	0.067	1.522	0.081	1.705	0.116	0.074	0.118	0.880	0.017
[PDMIM]+	1	-0.733	0.085	0.759	0.082	2.444	0.098	3.562	0.141	0.847	0.144	0.559	0.021
[PEMPip]+	1	-0.477	0.070	-0.186	0.067	2.639	0.081	2.450	0.116	0.103	0.118	0.761	0.017
[PemPyrr]+	1	-0.549	0.070	0.000	0.067	2.317	0.081	2.425	0.116	0.385	0.118	0.747	0.017
[PM2iPAm]+	1	-0.702	0.070	0.000	0.067	2.532	0.081	2.578	0.116	0.331	0.118	0.682	0.017
[PMPip]+	1	-0.432	0.070	0.145	0.067	2.287	0.081	2.489	0.116	0.402	0.118	0.674	0.017
[PMPyrr]+	1	-0.466	0.070	0.000	0.067	2.562	0.081	2.505	0.116	0.271	0.118	0.682	0.017
[PrOHPy]+	2	-0.675	0.053	0.222	0.050	2.589	0.061	2.818	0.087	1.232	0.089	0.594	0.013
[QUIN6]+	1	-0.562	0.070	-0.071	0.067	2.201	0.081	2.569	0.116	0.238	0.118	0.815	0.017
[QUIN8]+	1	-0.363	0.070	-0.186	0.067	2.048	0.081	2.430	0.116	0.142	0.118	0.816	0.017
[sec-BMIm]+	1	-0.558	0.070	-0.097	0.067	2.519	0.081	2.497	0.116	0.456	0.118	0.705	0.017
[TDC]+	2	-0.194	0.053	0.033	0.051	2.119	0.061	2.548	0.088	0.092	0.090	0.742	0.013
[tert-BMIm]+	1	-0.621	0.070	-0.118	0.067	2.603	0.081	2.689	0.116	0.410	0.118	0.693	0.017
[[(CH3)2PO4]-	1	-0.240	0.079	0.299	0.075	-0.057	0.090	5.682	0.130	-0.249	0.133	-0.033	0.019
[BETI]-	1	-0.046	0.079	0.117	0.075	0.020	0.090	-0.310	0.130	0.075	0.133	-0.120	0.019
[Cl]-	1	-0.785	0.079	0.536	0.075	0.764	0.090	5.961	0.130	-0.520	0.133	-0.089	0.019
[TDI]-	2	-0.054	0.068	0.016	0.065	0.052	0.078	1.109	0.112	-0.002	0.115	0.025	0.016
[Trif]-	3	-0.272	0.055	0.115	0.053	0.223	0.063	1.585	0.091	-0.101	0.093	-0.035	0.013
[SCN]-	3	-0.587	0.058	0.688	0.056	0.270	0.067	2.665	0.096	0.060	0.098	-0.066	0.014
[(MeO)(H)PO2]-	1	-0.541	0.080	0.278	0.077	0.568	0.092	5.402	0.133	-0.674	0.136	-0.051	0.019
[DEP]-	2	0.167	0.080	0.133	0.077	-0.115	0.092	4.984	0.133	-0.765	0.136	0.043	0.019
[EtSO4]-	1	-0.088	0.080	-0.062	0.077	0.205	0.092	2.879	0.133	-0.674	0.136	-0.083	0.019
[MeSO3]-	2	-0.644	0.058	0.394	0.056	0.359	0.067	4.136	0.096	-0.281	0.098	-0.061	0.014
[TCB]-	4	0.053	0.050	0.081	0.048	0.317	0.057	0.252	0.082	-0.042	0.084	-0.032	0.012
[M2PO4]-	1	-0.610	0.070	0.860	0.067	2.590	0.081	7.270	0.116	0.000	0.118	0.350	0.017

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[TCM]-	6	-0.271	0.050	0.211	0.048	0.216	0.058	0.879	0.083	0.060	0.085	-0.041	0.012
[FSI]-	2	-0.207	0.079	0.237	0.075	0.228	0.091	0.000	0.130	0.122	0.133	-0.021	0.019
[PF6]-	3	-0.088	0.055	-0.067	0.052	0.474	0.063	0.175	0.090	-0.215	0.092	-0.097	0.013
[+CS]-	1	0.317	0.085	0.075	0.081	0.345	0.098	4.468	0.141	-0.519	0.144	0.121	0.021
[L-Lact]-	1	0.327	0.085	0.130	0.081	0.240	0.098	4.754	0.141	-0.610	0.144	-0.007	0.021
[OS]-	2	0.262	0.060	-0.074	0.057	-0.133	0.069	2.711	0.099	-0.601	0.101	0.068	0.014
[BF4]-	5	-0.292	0.049	0.238	0.046	0.284	0.056	0.963	0.080	-0.329	0.082	-0.101	0.012
[FAP]-	10	0.271	0.036	-0.032	0.034	-0.123	0.041	-1.314	0.059	0.460	0.060	-0.043	0.009
[DCA]-	12	-0.357	0.038	0.375	0.036	0.291	0.044	2.257	0.063	-0.138	0.064	-0.066	0.009

Table D.11: Cation and anion ABSM parameters for log P values from method 2.

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[(C3COOMe)MIM]+	1	-0.307	0.087	0.105	0.105	1.040	0.191	-1.169	0.258	-4.535	0.694	3.159	0.386
[(Hexom)2Im]+	1	0.107	0.077	-0.628	0.093	0.747	0.168	-1.441	0.227	-4.808	0.610	3.750	0.339
[(Meo)2Im]+	1	-0.412	0.077	-0.104	0.093	0.761	0.168	-1.124	0.227	-3.776	0.610	3.055	0.339
[3-MBPy]+	2	0.033	0.079	-0.015	0.095	0.859	0.173	-1.473	0.233	-4.918	0.628	3.487	0.349
[4-CNBPy]+	1	-0.316	0.077	0.132	0.093	1.015	0.168	-1.040	0.227	-4.399	0.610	3.272	0.339
[AllMIm]+	2	-0.004	0.058	0.078	0.070	0.637	0.127	-1.399	0.172	-4.348	0.462	3.043	0.257
[B3EP]+	1	-0.019	0.117	-0.347	0.141	0.309	0.256	-3.330	0.345	-4.541	0.928	3.541	0.516
[B4MPy]+	1	-0.229	0.087	0.276	0.105	0.807	0.191	-1.389	0.258	-4.642	0.694	3.598	0.386
[BM2Im]+	1	-0.347	0.077	0.111	0.093	0.718	0.168	-1.195	0.227	-4.418	0.610	3.502	0.339
[BMIM]+	13	-0.106	0.039	0.133	0.047	0.679	0.086	-1.246	0.116	-4.126	0.312	3.442	0.173
[BMMOR]+	1	0.124	0.095	-0.163	0.114	0.137	0.207	-2.602	0.279	-8.466	0.752	3.538	0.418
[BMPIP]+	1	-0.129	0.077	0.494	0.093	0.235	0.168	-1.165	0.227	-4.385	0.610	3.422	0.339
[BMPy]+	3	-0.207	0.055	0.102	0.066	1.124	0.119	-0.878	0.161	-3.394	0.432	3.446	0.240
[BMPyrr]+	8	0.014	0.040	0.224	0.048	0.284	0.087	-1.402	0.117	-5.278	0.315	3.463	0.175
[BzmIm]+	1	-0.187	0.077	0.000	0.093	0.768	0.168	-1.284	0.227	-4.378	0.610	3.310	0.339
[BzmPyrr]+	1	-0.387	0.077	0.197	0.093	0.658	0.168	-1.275	0.227	-4.401	0.610	3.449	0.339
[BzPy]+	1	-0.516	0.077	0.092	0.093	0.865	0.168	-1.143	0.227	-4.432	0.610	3.485	0.339
[C1,9(M2iPAm)2]2+	1	-0.606	0.077	0.225	0.093	0.798	0.168	-1.034	0.227	-4.438	0.610	3.429	0.339
[C3CNC1Pyr]+	1	-0.851	0.100	0.375	0.120	1.186	0.218	-0.397	0.295	-4.869	0.793	3.268	0.441

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[C3MPyrr]+	1	-0.236	0.077	0.000	0.093	0.908	0.168	-1.015	0.227	-4.691	0.610	3.446	0.339
[C5MPyrr]+	1	-0.303	0.077	0.000	0.093	0.727	0.168	-1.107	0.227	-4.622	0.610	3.630	0.339
[ChxmIm]+	1	-0.299	0.077	-0.094	0.093	0.754	0.168	-0.851	0.227	-4.618	0.610	3.653	0.339
[ChxmPyrr]+	1	-0.297	0.077	0.073	0.093	0.697	0.168	-1.157	0.227	-4.687	0.610	3.709	0.339
[ChxPy]+	1	-0.344	0.077	0.146	0.093	0.703	0.168	-1.047	0.227	-4.535	0.610	3.681	0.339
[CNMeM2iPam]+	1	-1.001	0.077	0.000	0.093	1.512	0.168	-0.459	0.227	-4.191	0.610	3.529	0.339
[CNPrMIm]+	1	-0.735	0.087	0.110	0.105	1.015	0.191	-1.245	0.258	-4.184	0.694	3.353	0.386
[COC2mMOR]+	1	-0.216	0.077	0.054	0.093	1.059	0.168	-1.019	0.227	-4.564	0.610	3.082	0.339
[D2MIM]+	1	-0.093	0.077	-0.052	0.093	0.040	0.168	-1.620	0.227	-4.667	0.610	4.034	0.339
[DM3AM]+	1	-0.128	0.077	-0.131	0.093	0.329	0.168	-1.458	0.227	-4.550	0.610	3.816	0.339
[DMPyrr]+	1	-0.083	0.077	-0.142	0.093	0.419	0.168	-1.467	0.227	-4.859	0.610	3.824	0.339
[DoMIM]+	1	0.063	0.077	-0.055	0.093	0.275	0.168	-1.368	0.227	-4.897	0.610	3.824	0.339
[E3S]+	1	-0.062	0.077	-1.347	0.093	2.716	0.168	1.350	0.227	-5.274	0.610	3.242	0.339
[EMIM]+	8	-0.117	0.043	0.184	0.052	0.434	0.094	-1.433	0.127	-4.237	0.342	3.164	0.190
[EtOHM2iPAm]+	1	-0.669	0.077	0.236	0.093	0.617	0.168	-0.850	0.227	-3.356	0.610	3.270	0.339
[EtOHMIm]+	3	-0.374	0.051	0.077	0.062	0.717	0.112	-0.956	0.152	-3.341	0.408	3.003	0.227
[HexM3Am]+	1	-0.404	0.077	0.344	0.093	0.945	0.168	0.987	0.227	-4.526	0.610	2.957	0.339
[HM2iPam]+	1	-0.340	0.077	0.000	0.093	0.582	0.168	-1.194	0.227	-4.631	0.610	3.640	0.339
[HMIM]+	3	-0.051	0.051	0.072	0.062	0.330	0.112	-1.423	0.150	-4.552	0.405	3.555	0.225
[HMPyrr]+	1	-0.226	0.077	-0.083	0.093	0.560	0.168	-1.301	0.227	-4.501	0.610	3.673	0.339
[HxomMIm]+	1	-0.275	0.077	0.000	0.093	0.407	0.168	-1.478	0.227	4.320	0.610	3.510	0.339
[M2EIM]+	1	-0.095	0.077	0.299	0.093	0.360	0.168	-1.906	0.227	-3.805	0.610	3.177	0.339
[M3BAm]+	1	0.047	0.077	-0.051	0.093	0.356	0.168	-1.262	0.227	-4.400	0.610	3.209	0.339
[MDIm]+	1	0.131	0.094	-0.099	0.114	0.280	0.206	-1.702	0.278	-4.847	0.748	3.674	0.416
[MeOCH2CH2NEt3]+	1	-0.129	0.077	0.080	0.093	0.682	0.168	-1.084	0.227	-4.538	0.610	3.370	0.339
[MeOCH2CH2PBu3]+	1	-0.045	0.077	0.041	0.093	0.218	0.168	-1.396	0.227	-4.650	0.610	3.708	0.339
[MeOCH2CH2PEt3]+	1	-0.177	0.077	0.103	0.093	0.582	0.168	-1.022	0.227	-4.516	0.610	3.546	0.339
[MeoeM2EAm]+	1	-0.145	0.086	0.017	0.104	0.836	0.189	-1.164	0.254	-4.789	0.684	3.251	0.380
[MeoeMIm]+	1	-0.150	0.077	0.012	0.093	0.818	0.168	-1.289	0.227	-4.263	0.610	3.116	0.339
[MeoeMMorp]+	2	-0.183	0.058	-0.004	0.070	0.978	0.126	-1.149	0.170	-4.544	0.458	3.101	0.255
[MeoeMPip]+	2	-0.066	0.058	0.142	0.070	0.663	0.126	-1.163	0.170	-4.803	0.458	3.326	0.255
[MeoeMPyrr]+	1	-0.049	0.086	0.066	0.104	0.685	0.189	-1.239	0.254	-4.964	0.684	3.310	0.380

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[Mo1,3CN]+	1	-0.741	0.095	-0.429	0.114	1.147	0.207	-1.653	0.279	-8.945	0.752	3.536	0.418
[Mo1,3OH]+	1	-0.563	0.095	-0.215	0.114	0.689	0.207	-1.911	0.279	-8.449	0.752	3.467	0.418
[MOIm]+	2	-0.036	0.074	-0.093	0.089	0.088	0.162	-1.153	0.219	-3.595	0.588	3.962	0.327
[N112N113]+	1	-1.042	0.077	0.143	0.093	1.160	0.168	-0.335	0.227	-3.910	0.610	3.643	0.339
[N112N114]+	1	-0.397	0.077	0.000	0.093	0.779	0.168	0.712	0.227	-4.181	0.610	3.291	0.339
[N112O2N113]+	1	-0.339	0.077	-0.149	0.093	0.748	0.168	-0.945	0.227	-4.542	0.610	3.605	0.339
[N112O2N114]+	1	-0.205	0.077	-0.053	0.093	0.584	0.168	-1.037	0.227	-4.475	0.610	3.508	0.339
[N2,2,2,8]+	1	0.047	0.116	0.190	0.140	0.063	0.253	-1.554	0.341	-5.484	0.919	3.780	0.510
[N-C3CNMPyr]+	1	-0.522	0.087	0.065	0.105	1.323	0.191	-0.758	0.258	-4.719	0.694	3.172	0.386
[N-C3CNPy]+	1	-0.591	0.087	-0.011	0.105	1.340	0.191	-1.002	0.258	-4.713	0.694	3.091	0.386
[O4AM]+	1	0.226	0.077	0.000	0.093	-0.212	0.168	-1.756	0.227	-4.739	0.610	3.825	0.339
[OM3AM]+	1	-0.165	0.077	-0.181	0.093	0.569	0.168	-1.419	0.227	-4.677	0.610	3.711	0.339
[OMMIM]+	1	-0.354	0.077	0.200	0.093	0.130	0.168	-1.444	0.227	-4.224	0.610	3.826	0.339
[Ompyrr]+	1	-0.253	0.077	0.000	0.093	0.520	0.168	-1.460	0.227	-4.696	0.610	3.815	0.339
[P14,6,6,6]+	5	-0.246	0.053	-0.155	0.064	-0.227	0.116	-1.756	0.156	-4.677	0.421	4.081	0.234
[P8,8,8,8]+	1	0.153	0.077	-0.069	0.093	-0.011	0.168	-1.800	0.227	-5.186	0.610	3.888	0.339
[PDMIM]+	1	-0.643	0.098	0.462	0.118	1.119	0.215	0.394	0.289	-3.594	0.779	3.079	0.433
[PemPyrr]+	1	-0.303	0.077	0.000	0.093	0.727	0.168	-1.107	0.227	-4.622	0.610	3.630	0.339
[PM2iPAm]+	1	-0.378	0.077	0.115	0.093	0.723	0.168	-1.061	0.227	-4.594	0.610	3.388	0.339
[PMPip]+	1	-0.231	0.077	0.453	0.093	0.352	0.168	-1.263	0.227	-4.290	0.610	3.401	0.339
[PMPyrr]+	1	-0.236	0.077	0.000	0.093	0.908	0.168	-1.015	0.227	-4.691	0.610	3.446	0.339
[PrOHPy]+	2	-0.197	0.058	0.079	0.070	0.829	0.126	-0.925	0.170	-3.826	0.458	2.989	0.255
[QUIN6]+	1	-0.360	0.077	0.138	0.093	0.594	0.168	-0.936	0.227	-4.776	0.610	3.864	0.339
[QUIN8]+	1	-0.149	0.077	0.000	0.093	0.451	0.168	-1.080	0.227	-4.886	0.610	3.861	0.339
[sec-BMIm]+	1	-0.215	0.077	0.000	0.093	0.740	0.168	-1.119	0.227	-4.496	0.610	3.436	0.339
[TDC]+	2	-0.076	0.058	0.163	0.070	0.531	0.127	-0.944	0.172	-4.917	0.462	3.698	0.257
[tert-BMIm]+	1	-0.275	0.077	0.000	0.093	0.796	0.168	-0.926	0.227	-4.526	0.610	3.395	0.339
[[(CH3)2PO4]-	1	-0.149	0.086	0.226	0.104	-0.167	0.189	5.739	0.255	-0.695	0.685	-0.108	0.381
[BETI]-	1	0.129	0.086	-0.050	0.104	-0.345	0.189	-0.455	0.255	-0.110	0.685	-0.401	0.381
[Cl]-	1	-0.696	0.086	0.400	0.104	0.623	0.189	6.054	0.255	-0.949	0.685	-0.269	0.381
[TDI]-	2	-0.010	0.075	0.129	0.090	-0.189	0.163	0.816	0.220	0.014	0.592	0.076	0.329
[Trif]-	3	-0.205	0.061	0.068	0.073	0.135	0.132	1.627	0.178	0.117	0.480	-0.154	0.267

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[SCN]-	3	-0.537	0.064	0.213	0.077	0.763	0.140	2.629	0.188	-0.011	0.507	-0.224	0.282
[(MeO)(H)PO2]-	1	-0.413	0.088	0.136	0.106	0.616	0.193	5.523	0.260	-0.683	0.700	-0.284	0.389
[DEP]-	2	0.139	0.088	0.105	0.106	0.000	0.193	5.229	0.260	-0.804	0.700	0.182	0.389
[EtSO4]-	1	0.038	0.088	-0.205	0.106	0.120	0.193	2.924	0.260	-0.707	0.700	-0.269	0.389
[MeSO3]-	2	-0.535	0.064	0.259	0.077	0.291	0.139	4.247	0.188	-0.512	0.506	-0.215	0.281
[TCB]-	4	-0.023	0.055	-0.039	0.066	0.462	0.119	0.423	0.161	0.180	0.433	-0.148	0.241
[TCM]-	6	-0.442	0.055	0.537	0.067	0.814	0.121	2.602	0.163	3.982	0.439	-0.416	0.244
[FSI]-	2	-0.156	0.087	0.041	0.104	0.533	0.189	0.253	0.255	0.686	0.687	-0.176	0.382
[PF6]-	3	0.001	0.060	-0.064	0.072	0.118	0.131	0.051	0.177	-0.412	0.476	-0.355	0.265
[+CS]-	1	0.246	0.093	0.155	0.113	0.456	0.204	4.505	0.275	-0.666	0.741	0.474	0.412
[L-Lact]-	1	0.246	0.093	0.155	0.113	0.227	0.204	4.997	0.275	-0.652	0.741	0.077	0.412
[OS]-	2	0.220	0.066	0.071	0.079	-0.260	0.144	2.611	0.194	-0.689	0.522	0.261	0.290
[BF4]-	4	0.040	0.061	0.337	0.074	-0.295	0.134	0.489	0.180	-0.823	0.485	-0.443	0.269
[FAP]-	9	0.179	0.039	0.102	0.047	-0.208	0.085	-1.244	0.115	0.719	0.310	-0.095	0.172
[DCA]-	11	-0.193	0.042	0.263	0.050	0.209	0.091	2.287	0.123	-0.123	0.331	-0.307	0.184

Table D.12: Cation and anion ABSM parameters for log K values from method 3.

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[(C3COOMe)MIM]+	1	1.370	0.138	0.037	0.205	2.723	0.295	2.211	0.560	0.598	0.351	0.646	0.036
[(Hexom)2Im]+	1	-0.314	0.122	-0.479	0.181	2.076	0.260	2.376	0.494	0.287	0.309	0.835	0.032
[(Meo)2Im]+	1	-0.762	0.122	0.000	0.181	2.557	0.260	2.427	0.494	1.157	0.309	0.584	0.032
[1-PrOHPy]+	1	-0.897	0.138	0.619	0.205	1.592	0.295	2.414	0.560	2.441	0.351	0.673	0.036
[2,4,6-M3Py]+	1	0.000	0.122	0.280	0.181	1.610	0.260	1.400	0.494	0.590	0.309	0.420	0.032
[2,6-M2Py]+	1	0.000	0.122	0.180	0.181	1.700	0.260	1.350	0.494	0.300	0.309	0.370	0.032
[2-MPy]+	1	0.000	0.122	0.060	0.181	1.620	0.260	1.190	0.494	0.170	0.309	0.310	0.032
[3,5-M2Py]+	1	0.000	0.122	0.160	0.181	1.550	0.260	1.110	0.494	0.280	0.309	0.370	0.032
[3-MBPy]+	2	-0.407	0.124	-0.097	0.184	2.503	0.265	2.594	0.503	0.072	0.315	0.745	0.032
[4-CNBPy]+	1	-0.768	0.122	0.000	0.181	2.810	0.260	2.685	0.494	0.553	0.309	0.691	0.032
[AllMIm]+	2	-0.431	0.092	0.077	0.137	2.477	0.197	2.242	0.374	0.580	0.234	0.620	0.024
[B3EP]+	1	-0.543	0.184	-0.406	0.273	1.663	0.393	0.693	0.746	0.863	0.467	0.826	0.048
[B4MPy]+	1	-0.444	0.138	0.136	0.205	2.303	0.295	2.002	0.560	0.585	0.351	0.763	0.036

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[BM2Im]+	1	-0.641	0.122	0.000	0.181	2.429	0.260	2.663	0.494	0.521	0.309	0.721	0.032
[BMIM]+	15	-0.510	0.058	-0.045	0.087	2.385	0.125	2.651	0.237	0.383	0.148	0.735	0.015
[BMMOR]+	1	-0.578	0.149	0.144	0.221	2.626	0.319	2.961	0.604	0.295	0.378	0.690	0.039
[BMPIP]+	1	-0.347	0.122	0.000	0.181	2.241	0.260	2.472	0.494	0.294	0.309	0.687	0.032
[BMPy]+	3	-0.540	0.082	-0.016	0.121	2.513	0.174	2.231	0.330	0.514	0.207	0.734	0.021
[BMPyrr]+	8	-0.372	0.062	-0.043	0.093	2.381	0.133	2.590	0.253	0.169	0.158	0.711	0.016
[BzmIm]+	1	-0.535	0.122	0.000	0.181	2.523	0.260	2.333	0.494	0.575	0.309	0.668	0.032
[BzmPyrr]+	1	-0.652	0.122	0.154	0.181	2.371	0.260	2.285	0.494	0.531	0.309	0.691	0.032
[BzPy]+	1	-0.830	0.122	0.000	0.181	2.617	0.260	2.452	0.494	0.526	0.309	0.711	0.032
[C1,9(M2iPAm)2]2+	1	-0.894	0.122	0.175	0.181	2.533	0.260	2.544	0.494	0.492	0.309	0.690	0.032
[C3CNC1Pyr]+	1	-1.226	0.158	-0.029	0.234	3.404	0.337	3.139	0.639	0.075	0.400	0.662	0.041
[C3MPyrr]+	1	-0.466	0.122	2.562	0.181	0.000	0.260	2.505	0.494	0.271	0.309	0.682	0.032
[C5MPyrr]+	1	-0.549	0.122	0.000	0.181	2.317	0.260	2.425	0.494	0.385	0.309	0.747	0.032
[ChxmIm]+	1	-0.513	0.122	-0.203	0.181	2.418	0.260	2.688	0.494	0.334	0.309	0.745	0.032
[ChxmPyrr]+	1	0.545	0.122	-0.124	0.181	2.406	0.260	2.411	0.494	0.274	0.309	0.771	0.032
[ChxPy]+	1	-0.556	0.122	0.000	0.181	2.370	0.260	2.496	0.494	0.412	0.309	0.755	0.032
[CNMeM2iPam]+	1	-1.344	0.122	-0.140	0.181	3.283	0.260	3.118	0.494	0.819	0.309	0.735	0.032
[CnPrM2Im]+	1	0.000	0.122	0.250	0.181	1.810	0.260	1.250	0.494	0.300	0.309	0.350	0.032
[CNPrMIm]+	1	-1.116	0.138	-0.879	0.205	2.831	0.295	2.371	0.560	0.737	0.351	0.728	0.036
[COC2mMOR]+	1	-0.687	0.122	0.107	0.181	2.766	0.260	2.516	0.494	0.615	0.309	0.629	0.032
[COC2N112]+	1	-0.679	0.136	-0.002	0.202	2.856	0.291	2.717	0.553	0.150	0.346	0.702	0.035
[D2MIM]+	1	-0.252	0.122	-0.269	0.181	1.603	0.260	1.946	0.494	0.354	0.309	0.856	0.032
[DM3AM]+	1	-0.363	0.122	-0.339	0.181	1.986	0.260	2.144	0.494	0.422	0.309	0.809	0.032
[DMPyrr]+	1	-0.395	0.122	-0.241	0.181	1.991	0.260	2.112	0.494	0.268	0.309	0.822	0.032
[DoMIM]+	1	-0.290	0.122	-0.285	0.181	1.812	0.260	2.121	0.494	0.357	0.309	0.853	0.032
[E3S]+	1	-0.606	0.122	-0.196	0.181	2.992	0.260	2.444	0.494	0.355	0.309	0.690	0.032
[EMIM]+	10	-0.598	0.065	0.013	0.096	2.237	0.138	2.266	0.262	0.772	0.164	0.696	0.017
[EtOHM2iPAm]+	1	-0.934	0.122	0.200	0.181	2.361	0.260	2.695	0.494	1.532	0.309	0.641	0.032
[EtOHMIm]+	4	-0.950	0.072	-0.099	0.106	2.732	0.153	2.686	0.290	1.276	0.182	0.600	0.019
[HexM3Am]+	1	-0.469	0.122	0.000	0.181	2.085	0.260	2.185	0.494	0.617	0.309	0.617	0.032
[HM2iPam]+	1	-0.531	0.122	-0.124	0.181	2.232	0.260	2.297	0.494	0.344	0.309	0.736	0.032
[HMIM]+	3	-0.429	0.081	-0.112	0.120	2.164	0.172	2.279	0.327	0.475	0.205	0.753	0.021

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[HMPip]+	1	-0.404	0.122	-0.245	0.181	2.469	0.260	2.348	0.494	0.075	0.309	0.775	0.032
[HMPyrr]+	1	-0.533	0.122	-0.110	0.181	2.146	0.260	2.278	0.494	0.650	0.309	0.767	0.032
[HxomMIm]+	1	-0.462	0.122	0.000	0.181	2.073	0.260	2.022	0.494	0.637	0.309	0.684	0.032
[M2EIM]+	1	-0.565	0.122	0.214	0.181	2.347	0.260	2.075	0.494	0.896	0.309	0.655	0.032
[M2PIm]+	2	0.000	0.122	0.010	0.181	1.670	0.260	1.210	0.494	0.120	0.309	0.310	0.032
[M3BAm]+	1	-0.457	0.122	0.000	0.181	2.188	0.260	2.375	0.494	0.663	0.309	0.668	0.032
[MDIm]+	1	-0.412	0.149	-0.270	0.221	2.049	0.319	2.111	0.604	0.423	0.378	0.817	0.039
[MeOCH2CH2NEt3]+	1	-0.399	0.122	0.000	0.181	2.376	0.260	2.397	0.494	0.452	0.309	0.670	0.032
[MeOCH2CH2PBu3]+	1	-0.233	0.122	-0.176	0.181	1.902	0.260	2.121	0.494	0.239	0.309	0.769	0.032
[MeOCH2CH2PEt3]+	1	-0.437	0.122	0.000	0.181	2.291	0.260	2.503	0.494	0.431	0.309	0.725	0.032
[MeoeM2EAm]+	1	-0.620	0.136	-0.002	0.202	2.693	0.291	2.606	0.553	0.242	0.346	0.683	0.035
[MeoeMIm]+	1	-0.509	0.122	0.065	0.181	2.476	0.260	2.271	0.494	0.671	0.309	0.603	0.032
[MeoeMMorp]+	2	-0.655	0.091	0.070	0.136	2.764	0.195	2.536	0.371	0.500	0.232	0.630	0.024
[MeoeMPip]+	2	-0.464	0.091	-0.001	0.136	2.483	0.195	2.531	0.371	0.170	0.232	0.689	0.024
[MeoeMPyrr]+	1	-0.444	0.136	-0.002	0.202	2.496	0.291	2.525	0.553	0.043	0.346	0.681	0.035
[MMIm]+	2	-1.118	0.184	-0.327	0.273	2.537	0.393	4.056	0.746	0.772	0.467	0.806	0.048
[Mo1,3CN]+	1	-1.415	0.149	-0.072	0.221	3.504	0.319	3.757	0.604	-0.157	0.378	0.683	0.039
[Mo1,3OH]+	1	-1.268	0.149	0.183	0.221	3.014	0.319	3.462	0.604	0.530	0.378	0.668	0.039
[MOIm]+	3	-0.254	0.093	-0.299	0.138	1.515	0.199	1.773	0.377	0.732	0.236	0.862	0.024
[N112N113]+	1	-1.338	0.122	0.000	0.181	2.865	0.260	3.280	0.494	1.041	0.309	0.762	0.032
[N112N114]+	1	-0.725	0.122	0.000	0.181	2.522	0.260	2.863	0.494	0.751	0.309	0.656	0.032
[N112O2N113]+	1	-0.613	0.122	-0.225	0.181	2.440	0.260	2.608	0.494	0.420	0.309	0.748	0.032
[N112O2N114]+	1	-0.436	0.122	-0.108	0.181	2.279	0.260	2.505	0.494	0.435	0.309	0.707	0.032
[N2,2,2,8]+	1	-0.290	0.183	-0.200	0.272	2.101	0.392	2.435	0.743	-0.019	0.465	0.807	0.047
[N-C3CNMPyr]+	1	-0.799	0.138	0.017	0.205	2.989	0.295	2.564	0.560	0.427	0.351	0.637	0.036
[N-C3CNPy]+	1	-0.941	0.138	-0.062	0.205	3.051	0.295	2.374	0.560	0.433	0.351	0.630	0.036
[N-C3OHmMOR]+	1	-0.378	0.122	0.000	0.181	2.088	0.260	2.368	0.494	0.166	0.309	0.792	0.032
[O4AM]+	1	0.000	0.122	-0.287	0.181	1.478	0.260	1.845	0.494	0.189	0.309	0.816	0.032
[OM3AM]+	1	-0.426	0.122	-0.338	0.181	2.242	0.260	2.195	0.494	0.684	0.309	0.779	0.032
[OMMIM]+	1	-0.682	0.122	0.000	0.181	1.954	0.260	2.367	0.494	0.621	0.309	0.820	0.032
[Ompyrr]+	1	-0.587	0.122	0.000	0.181	2.080	0.260	2.176	0.494	0.486	0.309	0.822	0.032
[P14,6,6,6]+	8	-0.290	0.066	-0.751	0.098	1.409	0.141	0.789	0.267	0.372	0.167	0.966	0.017

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[P8,8,8,8]+	1	-0.212	0.122	-0.337	0.181	1.522	0.260	1.705	0.494	0.074	0.309	0.880	0.032
[PDMIM]+	2	-1.080	0.093	0.293	0.137	2.670	0.198	2.227	0.376	0.696	0.235	0.716	0.024
[PEMPip]+	1	-0.477	0.122	-0.186	0.181	2.639	0.260	2.450	0.494	0.103	0.309	0.761	0.032
[PemPyrr]+	1	-0.549	0.122	0.000	0.181	2.317	0.260	2.425	0.494	0.385	0.309	0.747	0.032
[PM2iPAm]+	1	-0.702	0.122	0.000	0.181	2.532	0.260	2.578	0.494	0.331	0.309	0.682	0.032
[PMPip]+	1	-0.432	0.122	0.145	0.181	2.287	0.260	2.489	0.494	0.402	0.309	0.674	0.032
[PMPyrr]+	1	-0.466	0.122	0.000	0.181	2.562	0.260	2.505	0.494	0.271	0.309	0.682	0.032
[PrOHM2Im]+	1	0.000	0.122	0.210	0.181	1.500	0.260	1.250	0.494	0.660	0.309	0.340	0.032
[PrOHPy]+	2	-0.688	0.091	0.157	0.136	2.595	0.195	2.799	0.371	1.221	0.232	0.599	0.024
[QUIN6]+	1	-0.562	0.122	0.000	0.181	2.201	0.260	2.569	0.494	0.238	0.309	0.815	0.032
[QUIN8]+	1	-0.363	0.122	-0.186	0.181	2.048	0.260	2.430	0.494	0.142	0.309	0.816	0.032
[sec-BMIm]+	1	-0.558	0.122	-0.097	0.181	2.519	0.260	2.497	0.494	0.456	0.309	0.705	0.032
[TDC]+	2	-0.187	0.092	-0.011	0.137	2.136	0.197	2.459	0.374	0.056	0.234	0.751	0.024
[tert-BMIm]+	1	-0.621	0.122	-0.118	0.181	2.603	0.260	2.689	0.494	0.410	0.309	0.693	0.032
[[(CH3)2PO4]-	1	-0.144	0.135	0.368	0.200	-0.256	0.289	5.321	0.548	-0.011	0.343	-0.035	0.035
[BETI]-	1	0.050	0.135	0.186	0.200	-0.179	0.289	-0.671	0.548	0.313	0.343	-0.122	0.035
[CH3SO4]-	1	0.004	0.135	0.307	0.200	-0.216	0.289	0.487	0.548	-0.383	0.343	-0.236	0.035
[Cl]-	3	-0.292	0.090	0.293	0.134	0.126	0.193	2.689	0.366	0.479	0.229	-0.056	0.023
[SbF6]-	1	-0.205	0.135	-0.218	0.200	0.479	0.289	-0.329	0.548	0.195	0.343	0.022	0.035
[TDI]-	2	0.033	0.117	0.123	0.173	-0.127	0.249	0.794	0.472	0.198	0.296	0.022	0.030
[Trif]-	3	-0.202	0.095	0.175	0.140	0.086	0.202	1.361	0.384	0.070	0.240	-0.040	0.024
[SCN]-	3	-0.521	0.100	0.746	0.148	0.143	0.214	2.464	0.406	0.212	0.254	-0.072	0.026
[(MeO)(H)PO2]-	2	-0.522	0.138	0.327	0.205	0.683	0.295	5.584	0.559	-0.772	0.350	-0.076	0.036
[DEP]-	2	0.186	0.138	0.182	0.205	0.000	0.295	5.166	0.559	-0.863	0.350	0.018	0.036
[EtSO4]-	1	-0.069	0.138	-0.013	0.205	0.320	0.295	3.061	0.559	-0.772	0.350	-0.108	0.036
[MeSO3]-	2	-0.586	0.100	0.452	0.148	0.316	0.214	4.047	0.405	-0.211	0.254	-0.075	0.026
[TFA]-	1	-0.212	0.138	-0.013	0.205	0.457	0.295	3.196	0.559	-0.038	0.350	-0.027	0.036
[Tf2C]-	1	0.000	0.172	0.070	0.256	-0.080	0.368	-0.060	0.699	0.030	0.437	0.050	0.045
[TCB]-	4	0.077	0.086	0.094	0.127	0.339	0.183	0.310	0.348	-0.051	0.218	-0.045	0.022
[M2PO4]-	1	0.508	0.221	1.187	0.327	0.053	0.472	3.214	0.895	-0.772	0.560	-0.456	0.057
[TCM]-	6	-0.196	0.086	0.227	0.127	0.136	0.183	0.746	0.348	0.157	0.218	-0.047	0.022
[FSI]-	2	-0.171	0.137	0.284	0.203	0.175	0.293	-0.040	0.555	0.187	0.347	-0.029	0.035

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[PF6]-	4	-0.001	0.080	0.340	0.118	-0.167	0.170	0.109	0.323	0.458	0.202	-0.100	0.021
[+CS]-	1	0.089	0.139	0.343	0.205	0.318	0.296	5.578	0.562	-0.613	0.352	0.069	0.036
[L-Lact]-	1	0.099	0.139	0.398	0.205	0.213	0.296	5.864	0.562	-0.704	0.352	-0.059	0.036
[OS]-	3	0.195	0.085	0.130	0.126	-0.567	0.181	2.722	0.344	-0.229	0.215	0.075	0.022
[BF4]-	6	-0.085	0.068	0.195	0.101	0.396	0.146	1.108	0.276	-0.465	0.173	-0.118	0.018
[FAP]-	10	0.299	0.061	0.002	0.091	-0.136	0.131	-1.277	0.248	0.480	0.155	-0.052	0.016
[DCA]-	12	-0.373	0.065	0.461	0.097	0.258	0.139	2.436	0.264	-0.111	0.165	-0.084	0.017

Table D.13: Cation and anion ABSM parameters for log P values from method 3.

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[(C3COOMe)MIM]+	1	-0.295	0.140	0.025	0.263	1.096	0.396	-1.307	0.578	-4.561	0.807	3.208	0.401
[(Hexom)2Im]+	1	0.107	0.123	-0.628	0.231	0.747	0.349	-1.441	0.510	-4.808	0.712	3.750	0.354
[(Meo)2Im]+	1	-0.412	0.123	0.000	0.231	0.761	0.349	-1.124	0.510	-3.776	0.712	3.055	0.354
[3-MBPy]+	2	0.030	0.126	0.173	0.236	0.822	0.356	-1.227	0.520	-4.993	0.726	3.523	0.361
[4-CNBPy]+	1	-0.316	0.123	0.132	0.231	1.015	0.349	-1.040	0.510	-4.399	0.712	3.272	0.354
[AllMIm]+	2	0.002	0.093	0.008	0.175	0.665	0.264	-1.468	0.385	-4.360	0.538	3.068	0.267
[B3EP]+	1	-0.144	0.186	-0.378	0.350	0.248	0.527	-3.418	0.770	-4.492	1.075	3.611	0.534
[B4MPy]+	1	-0.217	0.140	0.196	0.263	0.863	0.396	-1.527	0.578	-4.668	0.807	3.647	0.401
[BM2Im]+	1	-0.347	0.123	0.000	0.231	0.718	0.349	-1.195	0.510	-4.418	0.712	3.502	0.354
[BMIM]+	15	-0.188	0.059	0.242	0.111	0.632	0.168	-0.944	0.245	-4.217	0.343	3.481	0.170
[BMMOR]+	1	0.060	0.151	-0.068	0.283	0.039	0.427	-2.530	0.624	-8.495	0.871	3.573	0.433
[BMPIP]+	1	0.000	0.123	0.494	0.231	0.235	0.349	-1.165	0.510	-4.385	0.712	3.422	0.354
[BMPy]+	3	-0.294	0.083	0.260	0.156	0.892	0.236	-1.002	0.344	-3.359	0.481	3.480	0.239
[BMPyrr]+	8	-0.010	0.063	0.241	0.119	0.268	0.179	-1.364	0.261	-5.310	0.365	3.494	0.181
[BzmIm]+	1	-0.187	0.123	0.000	0.231	0.768	0.349	-1.284	0.510	-4.378	0.712	3.310	0.354
[BzmPyrr]+	1	-0.387	0.123	0.197	0.231	0.658	0.349	-1.275	0.510	-4.401	0.712	3.449	0.354
[BzPy]+	1	-0.516	0.123	0.000	0.231	0.865	0.349	-1.143	0.510	-4.432	0.712	3.485	0.354
[C1,9(M2iPAm)2]2+	1	-0.606	0.123	0.225	0.231	0.798	0.349	-1.034	0.510	-4.438	0.712	3.429	0.354
[C3CNC1Pyr]+	1	-0.904	0.160	0.466	0.300	1.155	0.451	-0.226	0.660	-4.931	0.921	3.303	0.458
[C3MPyrr]+	1	-0.236	0.123	0.000	0.231	0.908	0.349	-1.015	0.510	-4.691	0.712	3.446	0.354
[C5MPyrr]+	1	-0.303	0.123	0.000	0.231	0.727	0.349	-1.107	0.510	-4.622	0.712	3.630	0.354

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[ChxmIm]+	1	-0.299	0.123	0.000	0.231	0.754	0.349	-0.851	0.510	-4.618	0.712	3.653	0.354
[ChxmPyrr]+	1	-0.297	0.123	0.000	0.231	0.697	0.349	-1.157	0.510	-4.687	0.712	3.709	0.354
[ChxPy]+	1	-0.344	0.123	0.146	0.231	0.703	0.349	-1.047	0.510	-4.535	0.712	3.681	0.354
[CNMeM2iPam]+	1	-1.001	0.123	0.000	0.231	1.512	0.349	-0.459	0.510	-4.191	0.712	3.529	0.354
[CNPrMIm]+	1	-0.723	0.140	0.030	0.263	1.071	0.396	-1.383	0.578	-4.210	0.807	3.402	0.401
[COC2mMOR]+	1	-0.216	0.123	0.000	0.231	1.059	0.349	-1.019	0.510	-4.564	0.712	3.082	0.354
[D2MIM]+	1	0.000	0.123	0.000	0.231	0.000	0.349	-1.620	0.510	-4.667	0.712	4.034	0.354
[DM3AM]+	1	0.000	0.123	0.000	0.231	0.329	0.349	-1.458	0.510	-4.550	0.712	3.816	0.354
[DMPyrr]+	1	0.000	0.123	-0.142	0.231	0.419	0.349	-1.467	0.510	-4.859	0.712	3.824	0.354
[DoMIM]+	1	0.000	0.123	0.000	0.231	0.275	0.349	-1.368	0.510	-4.897	0.712	3.824	0.354
[E3S]+	1	0.000	0.123	-1.347	0.231	2.716	0.349	1.350	0.510	-5.274	0.712	3.242	0.354
[EMIM]+	10	-0.144	0.065	0.153	0.123	0.373	0.185	-1.521	0.270	-4.188	0.377	3.234	0.187
[EtOHM2iPAm]+	1	-0.669	0.123	0.236	0.231	0.617	0.349	-0.850	0.510	-3.356	0.712	3.270	0.354
[EtOHMIm]+	3	-0.362	0.080	-0.004	0.151	0.879	0.227	-1.047	0.332	-3.583	0.463	3.007	0.230
[HexM3Am]+	1	-0.322	0.123	0.242	0.231	0.287	0.349	-1.383	0.510	-4.265	0.712	3.513	0.354
[HM2iPam]+	1	-0.340	0.123	0.000	0.231	0.582	0.349	-1.194	0.510	-4.631	0.712	3.640	0.354
[HMIM]+	3	-0.049	0.082	0.001	0.153	0.328	0.231	-1.440	0.338	-4.567	0.472	3.576	0.234
[HMPyrr]+	1	-0.226	0.123	0.000	0.231	0.560	0.349	-1.301	0.510	-4.501	0.712	3.673	0.354
[HxomMIm]+	1	-0.275	0.123	0.000	0.231	0.407	0.349	-1.478	0.510	4.320	0.712	3.510	0.354
[M2EIM]+	1	0.000	0.123	0.299	0.231	0.360	0.349	-1.906	0.510	-3.805	0.712	3.177	0.354
[M3BAm]+	1	0.000	0.123	0.000	0.231	0.356	0.349	-1.262	0.510	-4.400	0.712	3.209	0.354
[MDIm]+	1	-0.017	0.151	-0.164	0.283	0.254	0.427	-1.725	0.623	-4.846	0.871	3.715	0.433
[MeOCH2CH2NEt3]+	1	0.000	0.123	0.000	0.231	0.682	0.349	-1.084	0.510	-4.538	0.712	3.370	0.354
[MeOCH2CH2PBu3]+	1	0.000	0.123	0.000	0.231	0.218	0.349	-1.396	0.510	-4.650	0.712	3.708	0.354
[MeOCH2CH2PEt3]+	1	-0.177	0.123	0.000	0.231	0.582	0.349	-1.022	0.510	-4.516	0.712	3.546	0.354
[MeoeM2EAm]+	1	-0.130	0.138	-0.091	0.259	0.856	0.391	-1.193	0.571	-4.833	0.798	3.274	0.396
[MeoeMIm]+	1	-0.150	0.123	0.000	0.231	0.818	0.349	-1.289	0.510	-4.263	0.712	3.116	0.354
[MeoeMMorp]+	2	-0.159	0.093	-0.045	0.174	0.988	0.262	-1.163	0.383	-4.565	0.534	3.112	0.266
[MeoeMPip]+	2	-0.065	0.093	0.148	0.174	0.673	0.262	-1.177	0.383	-4.825	0.534	3.337	0.266
[MeoeMPyrr]+	1	-0.130	0.138	0.077	0.259	0.705	0.391	-1.268	0.571	-5.008	0.798	3.333	0.396
[MMIm]+	1	0.386	0.186	0.183	0.350	-0.677	0.527	-1.461	0.770	-3.148	1.075	2.994	0.534
[Mo1,3CN]+	1	-0.805	0.151	-0.442	0.283	1.049	0.427	-1.581	0.624	-8.974	0.871	3.571	0.433

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[Mo1,3OH]+	1	-0.627	0.151	-0.120	0.283	0.591	0.427	-1.839	0.624	-8.478	0.871	3.502	0.433
[MOIm]+	3	-0.166	0.095	-0.326	0.178	0.603	0.268	-1.845	0.392	-4.772	0.548	4.043	0.272
[N112N113]+	1	-1.042	0.123	0.143	0.231	1.160	0.349	-0.335	0.510	-3.910	0.712	3.643	0.354
[N112N114]+	1	-0.397	0.123	0.000	0.231	0.779	0.349	0.712	0.510	-4.181	0.712	3.291	0.354
[N112O2N113]+	1	-0.339	0.123	-0.149	0.231	0.748	0.349	-0.945	0.510	-4.542	0.712	3.605	0.354
[N112O2N114]+	1	-0.205	0.123	0.000	0.231	0.584	0.349	-1.037	0.510	-4.475	0.712	3.508	0.354
[N2,2,2,8]+	1	0.132	0.186	0.207	0.348	0.047	0.525	-1.516	0.766	-5.516	1.071	3.811	0.532
[N-C3CNMPyr]+	1	-0.510	0.140	-0.015	0.263	1.379	0.396	-0.896	0.578	-4.745	0.807	3.221	0.401
[N-C3CNPy]+	1	-0.579	0.140	-0.091	0.263	1.396	0.396	-1.140	0.578	-4.739	0.807	3.140	0.401
[O4AM]+	1	0.226	0.123	0.000	0.231	-0.212	0.349	-1.756	0.510	-4.739	0.712	3.825	0.354
[OM3AM]+	1	-0.165	0.123	-0.181	0.231	0.569	0.349	-1.419	0.510	-4.677	0.712	3.711	0.354
[OMMIM]+	1	-0.354	0.123	0.200	0.231	0.130	0.349	-1.444	0.510	-4.224	0.712	3.826	0.354
[Ompyrr]+	1	-0.253	0.123	0.000	0.231	0.520	0.349	-1.460	0.510	-4.696	0.712	3.815	0.354
[P14,6,6,6]+	8	-0.031	0.067	-0.621	0.126	0.176	0.190	-2.699	0.277	-4.729	0.387	4.189	0.192
[P8,8,8,8]+	1	0.153	0.123	0.000	0.231	0.000	0.349	-1.800	0.510	-5.186	0.712	3.888	0.354
[PDMIM]+	2	-0.873	0.095	0.480	0.178	0.783	0.268	-1.150	0.392	-3.897	0.548	3.538	0.272
[PemPyrr]+	1	-0.303	0.123	0.000	0.231	0.727	0.349	-1.107	0.510	-4.622	0.712	3.630	0.354
[PM2iPAm]+	1	-0.378	0.123	0.115	0.231	0.723	0.349	-1.061	0.510	-4.594	0.712	3.388	0.354
[PMPip]+	1	-0.231	0.123	0.453	0.231	0.352	0.349	-1.263	0.510	-4.290	0.712	3.401	0.354
[PMPyrr]+	1	-0.236	0.123	0.000	0.231	0.908	0.349	-1.015	0.510	-4.691	0.712	3.446	0.354
[PrOHPy]+	2	-0.124	0.093	0.102	0.174	0.839	0.262	-0.939	0.383	-3.847	0.534	3.000	0.266
[QUIN6]+	1	-0.360	0.123	0.138	0.231	0.594	0.349	-0.936	0.510	-4.776	0.712	3.864	0.354
[QUIN8]+	1	-0.149	0.123	0.000	0.231	0.451	0.349	-1.080	0.510	-4.886	0.712	3.861	0.354
[sec-BMIm]+	1	-0.215	0.123	0.000	0.231	0.740	0.349	-1.119	0.510	-4.496	0.712	3.436	0.354
[TDC]+	2	-0.070	0.093	0.122	0.175	0.559	0.264	-1.013	0.385	-4.929	0.538	3.723	0.267
[tert-BMIm]+	1	-0.275	0.123	0.000	0.231	0.796	0.349	-0.926	0.510	-4.526	0.712	3.395	0.354
[[(CH3)2PO4]-	1	-0.067	0.137	0.117	0.257	-0.120	0.387	5.437	0.566	-0.604	0.790	-0.147	0.392
[BETI]-	1	0.188	0.137	-0.242	0.257	-0.298	0.387	-0.757	0.566	-0.019	0.790	-0.440	0.392
[CH3SO4]-	1	0.188	0.137	-0.242	0.257	-0.632	0.387	0.149	0.566	-0.613	0.790	-0.790	0.392
[Cl]-	3	-0.009	0.092	-0.585	0.172	1.109	0.259	2.542	0.379	-1.014	0.529	-0.404	0.263
[SbF6]-	1	-0.050	0.137	-1.068	0.257	1.364	0.387	0.294	0.566	-1.340	0.790	0.015	0.392
[TDI]-	2	0.079	0.118	-0.069	0.221	-0.147	0.334	0.542	0.488	0.097	0.681	0.039	0.338

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[Trif]-	3	-0.139	0.096	0.000	0.180	0.169	0.271	1.409	0.396	0.183	0.553	-0.189	0.275
[SCN]-	3	-0.484	0.101	0.122	0.190	0.794	0.287	2.458	0.419	0.051	0.585	-0.259	0.291
[(MeO)(H)PO2]-	2	-0.386	0.140	0.167	0.262	0.677	0.395	5.611	0.577	-0.732	0.806	-0.354	0.400
[DEP]-	2	0.144	0.140	0.136	0.262	0.061	0.395	5.317	0.577	-0.853	0.806	0.112	0.400
[EtSO4]-	1	0.144	0.140	-0.153	0.262	0.181	0.395	3.012	0.577	-0.756	0.806	-0.339	0.400
[MeSO3]-	2	-0.481	0.101	0.221	0.190	0.344	0.286	4.140	0.418	-0.491	0.585	-0.269	0.290
[TFA]-	1	0.015	0.140	-1.404	0.262	1.983	0.395	2.410	0.577	-0.285	0.806	-0.190	0.400
[TCB]-	4	0.017	0.087	0.026	0.163	0.488	0.246	0.446	0.359	0.179	0.501	-0.189	0.249
[TCM]-	6	-0.378	0.087	0.442	0.163	0.912	0.246	2.530	0.360	4.011	0.503	-0.451	0.250
[FSI]-	2	-0.132	0.139	0.024	0.260	0.549	0.392	0.215	0.572	0.718	0.800	-0.207	0.397
[PF6]-	4	0.012	0.081	0.226	0.152	-0.346	0.228	0.294	0.334	0.268	0.466	-0.346	0.232
[+CS]-	1	0.031	0.141	0.621	0.263	0.053	0.397	5.448	0.580	-0.614	0.810	0.366	0.403
[L-Lact]-	1	0.031	0.141	0.621	0.263	-0.176	0.397	5.940	0.580	-0.600	0.810	-0.031	0.403
[OS]-	3	0.121	0.086	0.201	0.161	-0.576	0.243	2.751	0.356	-0.452	0.497	0.279	0.247
[BF4]-	5	0.268	0.075	-0.042	0.141	0.305	0.212	0.932	0.310	-0.958	0.433	-0.511	0.215
[FAP]-	9	0.130	0.062	0.091	0.117	-0.228	0.176	-1.215	0.257	0.763	0.360	-0.118	0.179
[DCA]-	11	-0.205	0.066	0.343	0.124	0.153	0.187	2.425	0.273	-0.097	0.381	-0.356	0.189

Table D.14: Cation and anion ABSM parameters for log K values from method 4.

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[(C3COOMe)MIM]+	1	1.354	0.081	0.103	0.082	2.690	0.092	2.390	0.132	0.620	0.134	0.628	0.019
[(Hexom)2Im]+	1	-0.314	0.071	-0.479	0.072	2.076	0.081	2.376	0.116	0.287	0.118	0.835	0.017
[(Meo)2Im]+	1	-0.762	0.071	0.000	0.072	2.557	0.081	2.427	0.116	1.157	0.118	0.584	0.017
[1-PrOHPy]+	1	-0.913	0.081	0.685	0.082	1.559	0.092	2.593	0.132	2.463	0.134	0.655	0.019
[3-MBPy]+	2	-0.329	0.073	-0.063	0.074	2.346	0.083	2.325	0.119	0.260	0.121	0.741	0.017
[4-CNBPy]+	1	-0.768	0.071	0.000	0.072	2.810	0.081	2.685	0.116	0.553	0.118	0.691	0.017
[AllMIm]+	2	-0.439	0.054	0.110	0.055	2.460	0.061	2.331	0.088	0.591	0.089	0.612	0.013
[B3EP]+	1	-0.524	0.108	-0.393	0.110	1.778	0.123	0.875	0.176	0.672	0.179	0.801	0.026
[B4MPy]+	1	-0.460	0.081	0.202	0.082	2.270	0.092	2.181	0.132	0.607	0.134	0.745	0.019
[BM2Im]+	1	-0.641	0.071	0.000	0.072	2.429	0.081	2.663	0.116	0.521	0.118	0.721	0.017
[BMIM]+	13	-0.415	0.036	-0.008	0.037	2.186	0.041	2.290	0.059	0.621	0.060	0.733	0.009

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[BMMOR]+	1	-0.502	0.087	0.160	0.089	2.546	0.099	2.828	0.143	0.391	0.145	0.684	0.021
[BMPIP]+	1	-0.347	0.071	0.000	0.072	2.241	0.081	2.472	0.116	0.294	0.118	0.687	0.017
[BMPy]+	3	-0.441	0.049	-0.031	0.050	2.524	0.056	2.235	0.080	0.500	0.081	0.727	0.012
[BMPyrr]+	8	-0.336	0.037	-0.016	0.037	2.328	0.042	2.550	0.060	0.231	0.061	0.703	0.009
[BzmIm]+	1	-0.535	0.071	0.000	0.072	2.523	0.081	2.333	0.116	0.575	0.118	0.668	0.017
[BzmPyrr]+	1	-0.652	0.071	0.154	0.072	2.371	0.081	2.285	0.116	0.531	0.118	0.691	0.017
[BzPy]+	1	-0.830	0.071	0.000	0.072	2.617	0.081	2.452	0.116	0.526	0.118	0.711	0.017
[C1,9(M2iPAm)2]2+	1	-0.894	0.071	0.175	0.072	2.533	0.081	2.544	0.116	0.492	0.118	0.690	0.017
[C3CNC1Pyr]+	1	-1.161	0.092	0.003	0.094	3.277	0.105	2.938	0.151	0.225	0.153	0.656	0.022
[C3MPyrr]+	1	-0.466	0.071	2.562	0.072	0.000	0.081	2.505	0.116	0.271	0.118	0.682	0.017
[C5MPyrr]+	1	-0.549	0.071	0.000	0.072	2.317	0.081	2.425	0.116	0.385	0.118	0.747	0.017
[ChxmIm]+	1	-0.513	0.071	-0.203	0.072	2.418	0.081	2.688	0.116	0.334	0.118	0.745	0.017
[ChxmPyrr]+	1	0.545	0.071	-0.124	0.072	2.406	0.081	2.411	0.116	0.274	0.118	0.771	0.017
[ChxPy]+	1	-0.556	0.071	0.000	0.072	2.370	0.081	2.496	0.116	0.412	0.118	0.755	0.017
[CNMeM2iPam]+	1	-1.344	0.071	-0.140	0.072	3.283	0.081	3.118	0.116	0.819	0.118	0.735	0.017
[CNPrMIm]+	1	-1.132	0.081	-0.813	0.082	2.798	0.092	2.550	0.132	0.759	0.134	0.710	0.019
[COC2mMOR]+	1	-0.687	0.071	0.107	0.072	2.766	0.081	2.516	0.116	0.615	0.118	0.629	0.017
[COC2N112]+	1	-0.652	0.080	0.022	0.081	2.843	0.090	2.754	0.130	0.169	0.132	0.693	0.019
[D2MIM]+	1	-0.252	0.071	-0.269	0.072	1.603	0.081	1.946	0.116	0.354	0.118	0.856	0.017
[DM3AM]+	1	-0.363	0.071	-0.339	0.072	1.986	0.081	2.144	0.116	0.422	0.118	0.809	0.017
[DMPyrr]+	1	-0.395	0.071	-0.241	0.072	1.991	0.081	2.112	0.116	0.268	0.118	0.822	0.017
[DoMIM]+	1	-0.290	0.071	-0.285	0.072	1.812	0.081	2.121	0.116	0.357	0.118	0.853	0.017
[E3S]+	1	-0.606	0.071	-0.196	0.072	2.992	0.081	2.444	0.116	0.355	0.118	0.690	0.017
[EMIM]+	8	-0.579	0.040	0.026	0.041	2.352	0.045	2.448	0.065	0.672	0.066	0.671	0.010
[EtOHM2iPAm]+	1	-0.934	0.071	0.200	0.072	2.361	0.081	2.695	0.116	1.532	0.118	0.641	0.017
[EtOHMIm]+	4	-0.872	0.044	-0.020	0.045	2.596	0.050	2.715	0.072	1.415	0.073	0.593	0.010
[HexM3Am]+	1	-0.469	0.071	0.000	0.072	2.085	0.081	2.185	0.116	0.617	0.118	0.617	0.017
[HM2iPam]+	1	-0.531	0.071	-0.124	0.072	2.232	0.081	2.297	0.116	0.344	0.118	0.736	0.017
[HMIM]+	3	-0.412	0.047	-0.098	0.048	2.167	0.054	2.310	0.077	0.478	0.078	0.745	0.011
[HMPip]+	1	-0.404	0.071	-0.245	0.072	2.469	0.081	2.348	0.116	0.075	0.118	0.775	0.017
[HMPyrr]+	1	-0.533	0.071	-0.110	0.072	2.146	0.081	2.278	0.116	0.650	0.118	0.767	0.017
[HxomMIm]+	1	-0.462	0.071	0.000	0.072	2.073	0.081	2.022	0.116	0.637	0.118	0.684	0.017

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[M2EIM]+	1	-0.565	0.071	0.214	0.072	2.347	0.081	2.075	0.116	0.896	0.118	0.655	0.017
[M3BAm]+	1	-0.457	0.071	0.000	0.072	2.188	0.081	2.375	0.116	0.663	0.118	0.668	0.017
[MDIm]+	1	-0.388	0.087	-0.252	0.089	2.071	0.099	2.169	0.142	0.412	0.145	0.804	0.021
[MeOCH2CH2NEt3]+	1	-0.399	0.071	0.000	0.072	2.376	0.081	2.397	0.116	0.452	0.118	0.670	0.017
[MeOCH2CH2PBu3]+	1	-0.233	0.071	-0.176	0.072	1.902	0.081	2.121	0.116	0.239	0.118	0.769	0.017
[MeOCH2CH2PEt3]+	1	-0.437	0.071	0.000	0.072	2.291	0.081	2.503	0.116	0.431	0.118	0.725	0.017
[MeoeM2EAm]+	1	-0.593	0.080	0.022	0.081	2.680	0.090	2.643	0.130	0.261	0.132	0.674	0.019
[MeoeMIm]+	1	-0.509	0.071	0.065	0.072	2.476	0.081	2.271	0.116	0.671	0.118	0.603	0.017
[MeoeMMorp]+	2	-0.642	0.053	0.082	0.054	2.758	0.061	2.554	0.087	0.510	0.089	0.626	0.013
[MeoeMPip]+	2	-0.451	0.053	0.011	0.054	2.477	0.061	2.549	0.087	0.180	0.089	0.685	0.013
[MeoeMPyrr]+	1	-0.417	0.080	0.022	0.081	2.483	0.090	2.562	0.130	0.062	0.132	0.672	0.019
[Mo1,3CN]+	1	-1.339	0.087	-0.056	0.089	3.424	0.099	3.624	0.143	-0.061	0.145	0.677	0.021
[Mo1,3OH]+	1	-1.192	0.087	0.199	0.089	2.934	0.099	3.329	0.143	0.626	0.145	0.662	0.021
[MOIm]+	2	-0.018	0.067	-0.121	0.068	1.170	0.076	1.959	0.109	1.185	0.111	0.840	0.016
[N112N113]+	1	-1.338	0.071	0.000	0.072	2.865	0.081	3.280	0.116	1.041	0.118	0.762	0.017
[N112N114]+	1	-0.725	0.071	0.000	0.072	2.522	0.081	2.863	0.116	0.751	0.118	0.656	0.017
[N112O2N113]+	1	-0.613	0.071	-0.225	0.072	2.440	0.081	2.608	0.116	0.420	0.118	0.748	0.017
[N112O2N114]+	1	-0.436	0.071	-0.108	0.072	2.279	0.081	2.505	0.116	0.435	0.118	0.707	0.017
[N2,2,2,8]+	1	-0.254	0.107	-0.173	0.109	2.048	0.121	2.395	0.175	0.043	0.177	0.799	0.026
[N-C3CNMPyr]+	1	-0.815	0.081	0.083	0.082	2.956	0.092	2.743	0.132	0.449	0.134	0.619	0.019
[N-C3CNPy]+	1	-0.957	0.081	0.004	0.082	3.018	0.092	2.553	0.132	0.455	0.134	0.612	0.019
[N-C3OHmMOR]+	1	-0.378	0.071	0.000	0.072	2.088	0.081	2.368	0.116	0.166	0.118	0.792	0.017
[O4AM]+	1	0.000	0.071	-0.287	0.072	1.478	0.081	1.845	0.116	0.189	0.118	0.816	0.017
[OM3AM]+	1	-0.426	0.071	-0.338	0.072	2.242	0.081	2.195	0.116	0.684	0.118	0.779	0.017
[OMMIM]+	1	-0.682	0.071	0.000	0.072	1.954	0.081	2.367	0.116	0.621	0.118	0.820	0.017
[Ompyrr]+	1	-0.587	0.071	0.000	0.072	2.080	0.081	2.176	0.116	0.486	0.118	0.822	0.017
[P14,6,6,6]+	5	-0.519	0.049	-0.498	0.050	1.382	0.056	1.899	0.080	0.280	0.081	0.914	0.012
[P8,8,8,8]+	1	-0.212	0.071	-0.337	0.072	1.522	0.081	1.705	0.116	0.000	0.118	0.880	0.017
[PDMIM]+	1	-0.719	0.087	0.741	0.088	2.444	0.098	3.562	0.141	0.846	0.143	0.559	0.021
[PEMPip]+	1	-0.477	0.071	-0.186	0.072	2.639	0.081	2.450	0.116	0.103	0.118	0.761	0.017
[PemPyrr]+	1	-0.549	0.071	0.000	0.072	2.317	0.081	2.425	0.116	0.385	0.118	0.747	0.017
[PM2iPAm]+	1	-0.702	0.071	0.000	0.072	2.532	0.081	2.578	0.116	0.331	0.118	0.682	0.017

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*l*	*l* error
[PMPip]+	1	-0.432	0.071	0.145	0.072	2.287	0.081	2.489	0.116	0.402	0.118	0.674	0.017
[PMPyrr]+	1	-0.466	0.071	0.000	0.072	2.562	0.081	2.505	0.116	0.271	0.118	0.682	0.017
[PrOHPy]+	2	-0.675	0.053	0.169	0.054	2.589	0.061	2.818	0.087	1.231	0.089	0.594	0.013
[QUIN6]+	1	-0.562	0.071	0.000	0.072	2.201	0.081	2.569	0.116	0.238	0.118	0.815	0.017
[QUIN8]+	1	-0.363	0.071	-0.186	0.072	2.048	0.081	2.430	0.116	0.142	0.118	0.816	0.017
[sec-BMIm]+	1	-0.558	0.071	-0.097	0.072	2.519	0.081	2.497	0.116	0.456	0.118	0.705	0.017
[TDC]+	2	-0.195	0.054	0.022	0.055	2.119	0.061	2.548	0.088	0.066	0.089	0.742	0.013
[tert-BMIm]+	1	-0.621	0.071	-0.118	0.072	2.603	0.081	2.689	0.116	0.410	0.118	0.693	0.017
[[(CH3)2PO4]-	1	-0.239	0.080	0.331	0.081	-0.057	0.090	5.682	0.130	-0.249	0.132	-0.033	0.019
[BETI]-	1	-0.045	0.080	0.149	0.081	0.020	0.090	-0.310	0.130	0.075	0.132	-0.120	0.019
[Cl]-	1	-0.784	0.080	0.568	0.081	0.764	0.090	5.961	0.130	-0.520	0.132	-0.089	0.019
[TDI]-	2	-0.053	0.069	0.087	0.070	0.052	0.078	1.109	0.112	-0.015	0.114	0.025	0.016
[Trif]-	3	-0.271	0.056	0.142	0.057	0.223	0.063	1.585	0.091	-0.092	0.092	-0.035	0.013
[SCN]-	3	-0.586	0.059	0.714	0.060	0.270	0.067	2.665	0.096	0.062	0.098	-0.066	0.014
[(MeO)(H)PO2]-	1	-0.541	0.082	0.314	0.083	0.568	0.092	5.402	0.133	-0.672	0.135	-0.051	0.019
[DEP]-	2	0.167	0.082	0.169	0.083	-0.115	0.092	4.984	0.133	-0.672	0.135	0.043	0.019
[EtSO4]-	1	-0.088	0.082	-0.026	0.083	0.205	0.092	2.879	0.133	-0.672	0.135	-0.083	0.019
[MeSO3]-	2	-0.643	0.059	0.428	0.060	0.359	0.067	4.136	0.096	-0.280	0.098	-0.061	0.014
[TCB]-	4	0.053	0.050	0.076	0.051	0.317	0.057	0.252	0.082	-0.040	0.084	-0.032	0.012
[M2PO4]-	1	-0.610	0.071	0.860	0.072	2.590	0.081	7.270	0.116	0.000	0.118	0.350	0.017
[TCM]-	6	-0.272	0.051	0.211	0.052	0.216	0.058	0.879	0.083	0.061	0.084	-0.041	0.012
[FSI]-	2	-0.207	0.080	0.257	0.082	0.228	0.091	0.000	0.130	0.125	0.133	-0.021	0.019
[PF6]-	3	-0.066	0.055	-0.014	0.057	0.474	0.063	0.175	0.090	-0.215	0.092	-0.097	0.013
[+CS]-	1	0.318	0.086	0.090	0.088	0.345	0.098	4.468	0.141	-0.521	0.143	0.121	0.021
[L-Lact]-	1	0.328	0.086	0.145	0.088	0.240	0.098	4.754	0.141	-0.612	0.143	-0.007	0.021
[OS]-	2	0.262	0.061	-0.051	0.062	-0.133	0.069	2.711	0.099	-0.601	0.101	0.068	0.014
[BF4]-	5	-0.306	0.049	0.256	0.050	0.284	0.056	0.963	0.080	-0.328	0.082	-0.101	0.012
[FAP]-	10	0.272	0.036	-0.022	0.037	-0.123	0.041	-1.314	0.059	0.461	0.060	-0.043	0.009
[DCA]-	12	-0.357	0.038	0.395	0.039	0.291	0.044	2.257	0.063	-0.133	0.064	-0.066	0.009

Table D.15: Cation and anion ABSM parameters for log P values from method 4.

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[(C3COOMe)MIM]+	1	-0.314	0.085	0.096	0.105	1.046	0.195	-1.169	0.260	-4.535	0.697	3.159	0.387
[(Hexom)2Im]+	1	0.107	0.075	-0.628	0.092	0.747	0.172	-1.441	0.228	-4.808	0.613	3.750	0.340
[(Meo)2Im]+	1	-0.412	0.075	0.000	0.092	0.761	0.172	-1.124	0.228	-3.776	0.613	3.055	0.340
[3-MBPy]+	2	0.118	0.077	0.067	0.095	0.850	0.177	-1.456	0.235	-4.918	0.631	3.487	0.350
[4-CNBPy]+	1	-0.316	0.075	0.132	0.092	1.015	0.172	-1.040	0.228	-4.399	0.613	3.272	0.340
[AllMIm]+	2	-0.008	0.057	0.044	0.070	0.640	0.130	-1.399	0.173	-4.348	0.464	3.043	0.258
[B3EP]+	1	-0.134	0.114	-0.333	0.140	0.303	0.261	-3.330	0.347	-4.541	0.932	3.541	0.518
[B4MPy]+	1	-0.236	0.085	0.267	0.105	0.813	0.195	-1.389	0.260	-4.642	0.697	3.598	0.387
[BM2Im]+	1	-0.347	0.075	0.000	0.092	0.718	0.172	-1.195	0.228	-4.418	0.613	3.502	0.340
[BMIM]+	13	-0.079	0.038	0.105	0.047	0.666	0.088	-1.251	0.117	-4.126	0.313	3.442	0.174
[BMMOR]+	1	0.133	0.093	-0.179	0.113	0.131	0.211	-2.603	0.281	-8.466	0.755	3.538	0.419
[BMPIP]+	1	0.000	0.075	0.494	0.092	0.235	0.172	-1.165	0.228	-4.385	0.613	3.422	0.340
[BMPy]+	3	-0.219	0.053	0.093	0.065	1.119	0.122	-0.879	0.162	-3.394	0.434	3.446	0.241
[BMPyrr]+	8	0.023	0.039	0.214	0.047	0.281	0.089	-1.398	0.118	-5.278	0.316	3.463	0.176
[BzmIm]+	1	-0.187	0.075	0.000	0.092	0.768	0.172	-1.284	0.228	-4.378	0.613	3.310	0.340
[BzmPyrr]+	1	-0.387	0.075	0.197	0.092	0.658	0.172	-1.275	0.228	-4.401	0.613	3.449	0.340
[BzPy]+	1	-0.516	0.075	0.000	0.092	0.865	0.172	-1.143	0.228	-4.432	0.613	3.485	0.340
[C1,9(M2iPAm)2]2+	1	-0.606	0.075	0.225	0.092	0.798	0.172	-1.034	0.228	-4.438	0.613	3.429	0.340
[C3CNC1Pyr]+	1	-0.833	0.098	0.384	0.120	1.178	0.223	-0.397	0.297	-4.869	0.796	3.268	0.443
[C3MPyrr]+	1	-0.236	0.075	0.000	0.092	0.908	0.172	-1.015	0.228	-4.691	0.613	3.446	0.340
[C5MPyrr]+	1	-0.303	0.075	0.000	0.092	0.727	0.172	-1.107	0.228	-4.622	0.613	3.630	0.340
[ChxmIm]+	1	-0.299	0.075	0.000	0.092	0.754	0.172	-0.851	0.228	-4.618	0.613	3.653	0.340
[ChxmPyrr]+	1	-0.297	0.075	0.000	0.092	0.697	0.172	-1.157	0.228	-4.687	0.613	3.709	0.340
[ChxPy]+	1	-0.344	0.075	0.146	0.092	0.703	0.172	-1.047	0.228	-4.535	0.613	3.681	0.340
[CNMeM2iPam]+	1	-1.001	0.075	0.000	0.092	1.512	0.172	-0.459	0.228	-4.191	0.613	3.529	0.340
[CNPrMIm]+	1	-0.742	0.085	0.101	0.105	1.021	0.195	-1.245	0.260	-4.184	0.697	3.353	0.387
[COC2mMOR]+	1	-0.216	0.075	0.000	0.092	1.059	0.172	-1.019	0.228	-4.564	0.613	3.082	0.340
[D2MIM]+	1	0.000	0.075	0.000	0.092	0.000	0.172	-1.620	0.228	-4.667	0.613	4.034	0.340
[DM3AM]+	1	0.000	0.075	0.000	0.092	0.329	0.172	-1.458	0.228	-4.550	0.613	3.816	0.340
[DMPyrr]+	1	0.000	0.075	-0.142	0.092	0.419	0.172	-1.467	0.228	-4.859	0.613	3.824	0.340
[DoMIM]+	1	0.000	0.075	0.000	0.092	0.275	0.172	-1.368	0.228	-4.897	0.613	3.824	0.340

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[E3S]+	1	0.000	0.075	-1.347	0.092	2.716	0.172	1.350	0.228	-5.274	0.613	3.242	0.340
[EMIM]+	8	-0.134	0.042	0.198	0.052	0.428	0.096	-1.433	0.128	-4.237	0.344	3.164	0.191
[EtOHM2iPAm]+	1	-0.669	0.075	0.236	0.092	0.617	0.172	-0.850	0.228	-3.356	0.613	3.270	0.340
[EtOHMIm]+	3	-0.346	0.050	0.065	0.062	0.716	0.115	-0.957	0.153	-3.341	0.410	3.003	0.228
[HexM3Am]+	1	-0.404	0.075	0.344	0.092	0.945	0.172	0.987	0.228	-4.526	0.613	2.957	0.340
[HM2iPam]+	1	-0.340	0.075	0.000	0.092	0.582	0.172	-1.194	0.228	-4.631	0.613	3.640	0.340
[HMIM]+	3	-0.039	0.050	0.010	0.061	0.330	0.114	-1.422	0.152	-4.552	0.407	3.555	0.226
[HMPyrr]+	1	-0.226	0.075	0.000	0.092	0.560	0.172	-1.301	0.228	-4.501	0.613	3.673	0.340
[HxomMIm]+	1	-0.275	0.075	0.000	0.092	0.407	0.172	-1.478	0.228	4.320	0.613	3.510	0.340
[M2EIM]+	1	0.000	0.075	0.299	0.092	0.360	0.172	-1.906	0.228	-3.805	0.613	3.177	0.340
[M3BAm]+	1	0.000	0.075	0.000	0.092	0.356	0.172	-1.262	0.228	-4.400	0.613	3.209	0.340
[MDIm]+	1	0.000	0.092	-0.155	0.113	0.278	0.210	-1.701	0.280	-4.847	0.751	3.674	0.417
[MeOCH2CH2NEt3]+	1	0.000	0.075	0.000	0.092	0.682	0.172	-1.084	0.228	-4.538	0.613	3.370	0.340
[MeOCH2CH2PBu3]+	1	0.000	0.075	0.000	0.092	0.218	0.172	-1.396	0.228	-4.650	0.613	3.708	0.340
[MeOCH2CH2PEt3]+	1	-0.177	0.075	0.000	0.092	0.582	0.172	-1.022	0.228	-4.516	0.613	3.546	0.340
[MeoeM2EAm]+	1	-0.118	0.084	-0.073	0.103	0.839	0.193	-1.164	0.256	-4.789	0.687	3.251	0.382
[MeoeMIm]+	1	-0.150	0.075	0.000	0.092	0.818	0.172	-1.289	0.228	-4.263	0.613	3.116	0.340
[MeoeMMorp]+	2	-0.153	0.056	-0.037	0.069	0.980	0.129	-1.149	0.172	-4.544	0.460	3.101	0.256
[MeoeMPip]+	2	-0.059	0.056	0.156	0.069	0.664	0.129	-1.163	0.172	-4.803	0.460	3.326	0.256
[MeoeMPyrr]+	1	-0.118	0.084	0.095	0.103	0.688	0.193	-1.239	0.256	-4.964	0.687	3.310	0.382
[Mo1,3CN]+	1	-0.732	0.093	-0.553	0.113	1.141	0.211	-1.654	0.281	-8.945	0.755	3.536	0.419
[Mo1,3OH]+	1	-0.554	0.093	-0.231	0.113	0.683	0.211	-1.912	0.281	-8.449	0.755	3.467	0.419
[MOIm]+	2	-0.045	0.072	-0.087	0.089	0.080	0.166	-1.156	0.220	-3.595	0.591	3.962	0.328
[N112N113]+	1	-1.042	0.075	0.143	0.092	1.160	0.172	-0.335	0.228	-3.910	0.613	3.643	0.340
[N112N114]+	1	-0.397	0.075	0.000	0.092	0.779	0.172	0.712	0.228	-4.181	0.613	3.291	0.340
[N112O2N113]+	1	-0.339	0.075	-0.149	0.092	0.748	0.172	-0.945	0.228	-4.542	0.613	3.605	0.340
[N112O2N114]+	1	-0.205	0.075	0.000	0.092	0.584	0.172	-1.037	0.228	-4.475	0.613	3.508	0.340
[N2,2,2,8]+	1	0.165	0.113	0.180	0.138	0.060	0.258	-1.550	0.344	-5.484	0.922	3.780	0.513
[N-C3CNMPyr]+	1	-0.529	0.085	0.056	0.105	1.329	0.195	-0.758	0.260	-4.719	0.697	3.172	0.387
[N-C3CNPy]+	1	-0.598	0.085	-0.020	0.105	1.346	0.195	-1.002	0.260	-4.713	0.697	3.091	0.387
[O4AM]+	1	0.226	0.075	0.000	0.092	-0.212	0.172	-1.756	0.228	-4.739	0.613	3.825	0.340
[OM3AM]+	1	-0.165	0.075	-0.181	0.092	0.569	0.172	-1.419	0.228	-4.677	0.613	3.711	0.340

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[OMMIM]+	1	-0.354	0.075	0.200	0.092	0.130	0.172	-1.444	0.228	-4.224	0.613	3.826	0.340
[Ompyrr]+	1	-0.253	0.075	0.000	0.092	0.520	0.172	-1.460	0.228	-4.696	0.613	3.815	0.340
[P14,6,6,6]+	5	-0.281	0.052	-0.149	0.063	-0.180	0.118	-1.757	0.157	-4.677	0.422	4.081	0.235
[P8,8,8,8]+	1	0.153	0.075	0.000	0.092	0.000	0.172	-1.800	0.228	-5.186	0.613	3.888	0.340
[PDMIM]+	1	-0.717	0.096	0.452	0.117	1.110	0.219	0.392	0.292	-3.594	0.782	3.079	0.435
[PemPyrr]+	1	-0.303	0.075	0.000	0.092	0.727	0.172	-1.107	0.228	-4.622	0.613	3.630	0.340
[PM2iPAm]+	1	-0.378	0.075	0.115	0.092	0.723	0.172	-1.061	0.228	-4.594	0.613	3.388	0.340
[PMPip]+	1	-0.231	0.075	0.453	0.092	0.352	0.172	-1.263	0.228	-4.290	0.613	3.401	0.340
[PMPyrr]+	1	-0.236	0.075	0.000	0.092	0.908	0.172	-1.015	0.228	-4.691	0.613	3.446	0.340
[PrOHPy]+	2	-0.117	0.056	0.110	0.069	0.830	0.129	-0.925	0.172	-3.826	0.460	2.989	0.256
[QUIN6]+	1	-0.360	0.075	0.138	0.092	0.594	0.172	-0.936	0.228	-4.776	0.613	3.864	0.340
[QUIN8]+	1	-0.149	0.075	0.000	0.092	0.451	0.172	-1.080	0.228	-4.886	0.613	3.861	0.340
[sec-BMIm]+	1	-0.215	0.075	0.000	0.092	0.740	0.172	-1.119	0.228	-4.496	0.613	3.436	0.340
[TDC]+	2	-0.080	0.057	0.158	0.070	0.533	0.130	-0.944	0.173	-4.917	0.464	3.698	0.258
[tert-BMIm]+	1	-0.275	0.075	0.000	0.092	0.796	0.172	-0.926	0.228	-4.526	0.613	3.395	0.340
[[(CH3)2PO4]-	1	-0.176	0.084	0.254	0.103	-0.154	0.193	5.744	0.256	-0.695	0.688	-0.108	0.382
[BETI]-	1	0.079	0.084	-0.105	0.103	-0.332	0.193	-0.450	0.256	-0.110	0.688	-0.401	0.382
[Cl]-	1	-0.723	0.084	0.428	0.103	0.636	0.193	6.059	0.256	-0.949	0.688	-0.269	0.382
[TDI]-	2	-0.019	0.073	0.053	0.089	-0.178	0.166	0.810	0.221	0.014	0.594	0.076	0.330
[Trif]-	3	-0.216	0.059	0.090	0.072	0.144	0.135	1.599	0.180	0.117	0.482	-0.154	0.268
[SCN]-	3	-0.555	0.062	0.204	0.076	0.771	0.143	2.629	0.190	-0.011	0.509	-0.224	0.283
[(MeO)(H)PO2]-	1	-0.396	0.086	0.122	0.105	0.622	0.197	5.523	0.262	-0.683	0.702	-0.284	0.390
[DEP]-	2	0.134	0.086	0.091	0.105	0.006	0.197	5.229	0.262	-0.804	0.702	0.182	0.390
[EtSO4]-	1	0.134	0.086	-0.198	0.105	0.126	0.197	2.924	0.262	-0.707	0.702	-0.269	0.390
[MeSO3]-	2	-0.540	0.062	0.267	0.076	0.300	0.142	4.249	0.189	-0.512	0.508	-0.215	0.282
[TCB]-	4	0.000	0.053	0.017	0.065	0.464	0.122	0.422	0.162	0.180	0.435	-0.148	0.242
[TCM]-	6	-0.451	0.054	0.553	0.066	0.820	0.124	2.603	0.164	3.982	0.441	-0.416	0.245
[FSI]-	2	-0.165	0.085	0.051	0.103	0.536	0.193	0.249	0.257	0.686	0.690	-0.176	0.383
[PF6]-	3	-0.024	0.059	0.037	0.072	0.126	0.134	0.054	0.178	-0.412	0.478	-0.355	0.266
[+CS]-	1	0.281	0.091	0.149	0.112	0.409	0.208	4.506	0.277	-0.666	0.744	0.474	0.414
[L-Lact]-	1	0.281	0.091	0.149	0.112	0.180	0.208	4.998	0.277	-0.652	0.744	0.077	0.414
[OS]-	2	0.180	0.064	0.121	0.079	-0.367	0.147	2.613	0.195	-0.689	0.524	0.261	0.291

Ion	# of Inst	*c*	*c* errors	*e*	*e* error	*s*	*s* error	*a*	*a* error	*b*	*b* error	*v*	*v* error
[BF4]-	4	0.114	0.060	0.347	0.073	-0.286	0.136	0.491	0.181	-0.823	0.487	-0.443	0.270
[FAP]-	9	0.118	0.038	0.073	0.047	-0.211	0.087	-1.244	0.116	0.719	0.312	-0.095	0.173
[DCA]-	11	-0.186	0.041	0.272	0.050	0.203	0.093	2.287	0.124	-0.123	0.332	-0.307	0.185

Table D.16: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter c for log K.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[(Hexom)2Im]+	1	-0.314	-0.118	-0.314	0.121	-0.314	0.070	-0.314	0.122	-0.314	0.071
[(Meo)2Im]+	1	-0.762	-0.090	-0.762	0.121	-0.762	0.070	-0.762	0.122	-0.762	0.071
[1-PrOHPy]+	1	-0.713	-0.055	-0.897	0.137	-0.913	0.080	-0.897	0.138	-0.913	0.081
[3-MBPy]+	2	-0.338	-0.098	-0.408	0.123	-0.328	0.072	-0.407	0.124	-0.329	0.073
[AllMIm]+	2	-0.432	0.058	-0.431	0.092	-0.439	0.053	-0.431	0.092	-0.439	0.054
[B3EP]+	1	-0.450	0.000	-0.543	0.183	-0.524	0.107	-0.543	0.184	-0.524	0.108
[BMIm]+	13	-0.421	-0.022	-0.512	0.058	-0.414	0.035	-0.510	0.058	-0.415	0.036
[BMMOR]+	1	-0.676	0.000	-0.580	0.148	-0.503	0.086	-0.578	0.149	-0.502	0.087
[BMPip]+	1	-0.364	-0.054	-0.347	0.121	-0.347	0.070	-0.347	0.122	-0.347	0.071
[BMPy]+	3	-0.449	-0.054	-0.543	0.081	-0.446	0.048	-0.540	0.082	-0.441	0.049
[BMPyrr]+	8	-0.363	-0.033	-0.372	0.062	-0.336	0.036	-0.372	0.062	-0.336	0.037
[BzmIm]+	1	-0.535	0.055	-0.535	0.121	-0.535	0.070	-0.535	0.122	-0.535	0.071
[BzmPyrr]+	1	-0.652	0.064	-0.652	0.121	-0.652	0.070	-0.652	0.122	-0.652	0.071
[BzPy]+	1	-0.830	0.074	-0.830	0.121	-0.830	0.070	-0.830	0.122	-0.830	0.071
[C1,9(M2iPAm)2]2+	1	-0.894	0.064	-0.894	0.121	-0.894	0.070	-0.894	0.122	-0.894	0.071
[C3MPyrr]+	1	-0.466	0.115	-0.466	0.121	-0.466	0.070	-0.466	0.122	-0.466	0.071
[C5MPyrr]+	1	-0.549	0.087	-0.549	0.121	-0.549	0.070	-0.549	0.122	-0.549	0.071
[ChxmIm]+	1	-0.513	0.075	-0.513	0.121	-0.513	0.070	-0.513	0.122	-0.513	0.071
[ChxmPyrr]+	1	0.545	0.077	0.545	0.121	0.545	0.070	0.545	0.122	0.545	0.071
[ChxPy]+	1	-0.556	0.065	-0.556	0.121	-0.556	0.070	-0.556	0.122	-0.556	0.071
[CNMeM2iPam]+	1	-1.344	0.114	-1.344	0.121	-1.344	0.070	-1.344	0.122	-1.344	0.071
[CNPrMIm]+	1	-1.119	-0.110	-1.116	0.137	-1.132	0.080	-1.116	0.138	-1.132	0.081
[D2MIM]+	1	-0.252	-0.089	-0.252	0.121	-0.252	0.070	-0.252	0.122	-0.252	0.071
[DM3AM]+	1	-0.363	-0.089	-0.363	0.121	-0.363	0.070	-0.363	0.122	-0.363	0.071

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[DMPyrr]+	1	-0.395	-0.062	-0.395	0.121	-0.395	0.070	-0.395	0.122	-0.395	0.071
[E3S]+	1	-0.606	-0.121	-0.606	0.121	-0.606	0.070	-0.606	0.122	-0.606	0.071
[EMIM]+	10	-0.505	-0.024	-0.598	0.064	-0.579	0.039	-0.598	0.065	-0.579	0.040
[EtOHM2iPAm]+	1	-0.934	0.075	-0.934	0.121	-0.934	0.070	-0.934	0.122	-0.934	0.071
[EtOHMIm]+	4	-0.843	-0.042	-0.946	0.071	-0.870	0.043	-0.950	0.072	-0.872	0.044
[HexM3Am]+	2	-0.469	-0.056	-0.469	0.121	-0.469	0.070	-0.469	0.122	-0.469	0.071
[HM2iPam]+	1	-0.531	0.077	-0.531	0.121	-0.531	0.070	-0.531	0.122	-0.531	0.071
[HMIM]+	3	-0.379	-0.025	-0.428	0.080	-0.412	0.047	-0.429	0.081	-0.412	0.047
[HMPip]+	1	-0.404	-0.057	-0.404	0.121	-0.404	0.070	-0.404	0.122	-0.404	0.071
[HMPyrr]+	1	-0.533	-0.093	-0.533	0.121	-0.533	0.070	-0.533	0.122	-0.533	0.071
[HxomMIm]+	1	-0.463	-0.118	-0.462	0.121	-0.462	0.070	-0.462	0.122	-0.462	0.071
[M2EIm]+	1	-0.611	-0.078	-0.565	0.121	-0.565	0.070	-0.565	0.122	-0.565	0.071
[M3BAm]+	1	-0.457	0.049	-0.457	0.121	-0.457	0.070	-0.457	0.122	-0.457	0.071
[MDIm]+	1	-0.391	-0.091	-0.412	0.148	-0.388	0.086	-0.412	0.149	-0.388	0.087
[MeoeMim]+	1	-0.507	-0.089	-0.509	0.121	-0.509	0.070	-0.509	0.122	-0.509	0.071
[MeoeMMorp]+	2	-0.675	-0.051	-0.655	0.091	-0.642	0.053	-0.655	0.091	-0.642	0.053
[MeoeMPip]+	2	-0.440	-0.051	-0.464	0.091	-0.451	0.053	-0.464	0.091	-0.451	0.053
[MeoeMPyrr]+	1	-0.380	-0.064	-0.443	0.136	-0.416	0.079	-0.444	0.136	-0.417	0.080
[MOIm]+	3	-0.197	-0.033	-0.297	0.092	-0.073	0.066	-0.254	0.093	-0.018	0.067
[N112N113]+	1	-1.338	0.079	-1.338	0.121	-1.338	0.070	-1.338	0.122	-1.338	0.071
[N112N114]+	1	-0.725	0.089	-0.725	0.121	-0.725	0.070	-0.725	0.122	-0.725	0.071
[N112O2N113]+	1	-0.613	0.073	-0.613	0.121	-0.613	0.070	-0.613	0.122	-0.613	0.071
[N112O2N114]+	1	-0.436	0.087	-0.436	0.121	-0.436	0.070	-0.436	0.122	-0.436	0.071
[N2,2,2,8]+	1	-0.347	0.047	-0.290	0.182	-0.254	0.106	-0.290	0.183	-0.254	0.107
[O4AM]+	1	0.000	0.000	0.000	0.121	0.000	0.070	0.000	0.122	0.000	0.071
[OM3AM]+	1	-0.426	-0.082	-0.426	0.121	-0.426	0.070	-0.426	0.122	-0.426	0.071
[Ompyrr]+	1	-0.587	-0.082	-0.587	0.121	-0.587	0.070	-0.587	0.122	-0.587	0.071
[PDMIM]+	2	-0.822	-0.129	-1.083	0.092	-0.733	0.085	-1.080	0.093	-0.719	0.087
[PEMPip]+	1	-0.477	-0.065	-0.477	0.121	-0.477	0.070	-0.477	0.122	-0.477	0.071
[PeMPyrr]+	1	-0.549	-0.087	-0.549	0.121	-0.549	0.070	-0.549	0.122	-0.549	0.071
[PM2iPAm]+	1	-0.702	0.071	-0.702	0.121	-0.702	0.070	-0.702	0.122	-0.702	0.071

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[PMPip]+	1	-0.435	-0.068	-0.432	0.121	-0.432	0.070	-0.432	0.122	-0.432	0.071
[PMPyrr]+	1	-0.466	-0.115	-0.466	0.121	-0.466	0.070	-0.466	0.122	-0.466	0.071
[sec-BMIm]+	1	-0.558	0.064	-0.558	0.121	-0.558	0.070	-0.558	0.122	-0.558	0.071
[tert-BMIm]+	1	-0.621	0.068	-0.621	0.121	-0.621	0.070	-0.621	0.122	-0.621	0.071

Table D.17: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter e for log K.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[(Hexom)2Im]+	1	-0.479	-0.230	-0.479	0.180	-0.479	0.067	-0.479	0.181	-0.479	0.072
[(Meo)2Im]+	1	-0.013	-0.112	-0.013	0.180	-0.013	0.067	0.000	0.181	0.000	0.072
[1-PrOHPy]+	1	0.151	-0.088	0.639	0.204	0.705	0.076	0.619	0.205	0.685	0.082
[3-MBPy]+	2	0.035	-0.203	-0.033	0.183	0.004	0.069	-0.097	0.184	-0.063	0.074
[AllMIm]+	2	0.135	0.071	0.087	0.136	0.120	0.051	0.077	0.137	0.110	0.055
[B3EP]+	1	-0.331	0.000	-0.372	0.272	-0.357	0.102	-0.406	0.273	-0.393	0.110
[BMIm]+	13	0.033	-0.051	-0.017	0.086	0.024	0.034	-0.045	0.087	-0.008	0.037
[BMMOR]+	1	0.277	0.000	0.141	0.220	0.160	0.082	0.144	0.221	0.160	0.089
[BMPip]+	1	0.134	-0.081	0.111	0.180	0.111	0.067	0.000	0.181	0.000	0.072
[BMPy]+	3	0.157	-0.106	0.018	0.120	0.004	0.046	-0.016	0.121	-0.031	0.050
[BMPyrr]+	8	0.119	-0.058	-0.025	0.092	0.004	0.035	-0.043	0.093	-0.016	0.037
[BzmIm]+	1	0.000	0.000	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[BzmPyrr]+	1	0.154	0.087	0.154	0.180	0.154	0.067	0.154	0.181	0.154	0.072
[BzPy]+	1	0.000	0.000	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[C1,9(M2iPAm)2]2+	1	0.175	0.082	0.175	0.180	0.175	0.067	0.175	0.181	0.175	0.072
[C3MPyrr]+	1	2.562	0.000	2.562	0.180	2.562	0.067	2.562	0.181	2.562	0.072
[C5MPyrr]+	1	0.000	0.000	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[ChxmIm]+	1	-0.203	0.100	-0.203	0.180	-0.203	0.067	-0.203	0.181	-0.203	0.072
[ChxmPyrr]+	1	-0.124	0.102	-0.124	0.180	-0.124	0.067	-0.124	0.181	-0.124	0.072
[ChxPy]+	1	0.000	0.000	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[CNMeM2iPam]+	1	-0.140	0.122	-0.140	0.180	-0.140	0.067	-0.140	0.181	-0.140	0.072

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[CNPrMIm]+	1	0.073	-0.150	-0.859	0.204	-0.793	0.076	-0.879	0.205	-0.813	0.082
[D2MIM]+	1	-0.269	-0.088	-0.269	0.180	-0.269	0.067	-0.269	0.181	-0.269	0.072
[DM3AM]+	1	-0.339	-0.098	-0.339	0.180	-0.339	0.067	-0.339	0.181	-0.339	0.072
[DMPyrr]+	1	-0.241	-0.070	-0.241	0.180	-0.241	0.067	-0.241	0.181	-0.241	0.072
[E3S]+	1	-0.196	-0.302	-0.196	0.180	-0.196	0.067	-0.196	0.181	-0.196	0.072
[EMIM]+	10	0.088	-0.058	0.047	0.095	0.062	0.038	0.013	0.096	0.026	0.041
[EtOHM2iPAm]+	1	0.200	0.088	0.200	0.180	0.200	0.067	0.200	0.181	0.200	0.072
[EtOHMIm]+	4	0.095	-0.064	-0.091	0.106	-0.011	0.041	-0.099	0.106	-0.020	0.045
[HexM3Am]+	2	-0.056	-0.071	-0.058	0.180	-0.058	0.067	0.000	0.181	0.000	0.072
[HM2iPam]+	1	-0.124	0.092	-0.124	0.180	-0.124	0.067	-0.124	0.181	-0.124	0.072
[HMIM]+	3	-0.103	-0.058	-0.147	0.119	-0.133	0.045	-0.112	0.120	-0.098	0.048
[HMPip]+	1	-0.245	-0.088	-0.245	0.180	-0.245	0.067	-0.245	0.181	-0.245	0.072
[HMPyrr]+	1	-0.110	-0.099	-0.110	0.180	-0.110	0.067	-0.110	0.181	-0.110	0.072
[HxomMIm]+	1	-0.394	-0.230	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[M2EIm]+	1	0.188	-0.146	0.214	0.180	0.214	0.067	0.214	0.181	0.214	0.072
[M3BAm]+	1	-0.005	0.133	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[MDIm]+	1	-0.162	-0.178	-0.277	0.220	-0.257	0.082	-0.270	0.221	-0.252	0.089
[MeoeMim]+	1	-0.015	-0.111	0.065	0.180	0.065	0.067	0.065	0.181	0.065	0.072
[MeoeMMorp]+	2	0.021	-0.021	0.074	0.135	0.087	0.050	0.070	0.136	0.082	0.054
[MeoeMPip]+	2	0.065	-0.073	0.041	0.135	0.053	0.050	-0.001	0.136	0.011	0.054
[MeoeMPyrr]+	1	0.018	-0.092	0.006	0.201	0.032	0.075	-0.002	0.202	0.022	0.081
[MOIm]+	3	-0.216	-0.082	-0.335	0.137	-0.175	0.063	-0.299	0.138	-0.121	0.068
[N112N113]+	1	0.044	0.096	0.044	0.180	0.044	0.067	0.000	0.181	0.000	0.072
[N112N114]+	1	0.053	0.105	0.053	0.180	0.053	0.067	0.000	0.181	0.000	0.072
[N112O2N113]+	1	-0.225	0.101	-0.225	0.180	-0.225	0.067	-0.225	0.181	-0.225	0.072
[N112O2N114]+	1	-0.108	0.110	-0.108	0.180	-0.108	0.067	-0.108	0.181	-0.108	0.072
[N2,2,2,8]+	1	-0.063	0.068	-0.182	0.271	-0.153	0.101	-0.200	0.272	-0.173	0.109
[O4AM]+	1	-0.287	-0.134	-0.287	0.180	-0.287	0.067	-0.287	0.181	-0.287	0.072
[OM3AM]+	1	-0.338	-0.089	-0.338	0.180	-0.338	0.067	-0.338	0.181	-0.338	0.072
[Ompyrr]+	1	-0.064	-0.090	-0.064	0.180	-0.064	0.067	0.000	0.181	0.000	0.072

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[PDMIM]+	2	0.780	-0.181	0.302	0.137	0.759	0.082	0.293	0.137	0.741	0.088
[PEMPip]+	1	-0.186	-0.099	-0.186	0.180	-0.186	0.067	-0.186	0.181	-0.186	0.072
[PeMPyrr]+	1	0.000	0.000	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[PM2iPAm]+	1	0.000	0.000	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[PMPip]+	1	0.149	-0.086	0.145	0.180	0.145	0.067	0.145	0.181	0.145	0.072
[PMPyrr]+	1	0.000	0.000	0.000	0.180	0.000	0.067	0.000	0.181	0.000	0.072
[sec-BMIm]+	1	-0.097	0.082	-0.097	0.180	-0.097	0.067	-0.097	0.181	-0.097	0.072
[tert-BMIm]+	1	-0.118	0.087	-0.118	0.180	-0.118	0.067	-0.118	0.181	-0.118	0.072

Table D.18: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter s for log K.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[(Hexom)2Im]+	1	2.076	-0.295	2.076	0.258	2.076	0.081	2.076	0.260	2.076	0.081
[(Meo)2Im]+	1	2.557	-0.104	2.557	0.258	2.557	0.081	2.557	0.260	2.557	0.081
[1-PrOHPy]+	1	2.663	-0.098	1.593	0.293	1.559	0.092	1.592	0.295	1.559	0.092
[3-MBPy]+	2	2.325	-0.249	2.502	0.263	2.346	0.083	2.503	0.265	2.346	0.083
[AllMIm]+	2	2.368	0.072	2.477	0.195	2.460	0.061	2.477	0.197	2.460	0.061
[B3EP]+	1	1.731	0.000	1.664	0.390	1.778	0.123	1.663	0.393	1.778	0.123
[BMIm]+	15	2.134	-0.057	2.384	0.124	2.186	0.041	2.385	0.125	2.186	0.041
[BMMOR]+	1	2.472	0.000	2.625	0.316	2.546	0.099	2.626	0.319	2.546	0.099
[BMPip]+	1	2.271	-0.092	2.241	0.258	2.241	0.081	2.241	0.260	2.241	0.081
[BMPy]+	3	2.270	-0.124	2.512	0.173	2.524	0.056	2.513	0.174	2.524	0.056
[BMPyrr]+	8	2.207	-0.061	2.381	0.132	2.328	0.042	2.381	0.133	2.328	0.042
[BzmIm]+	1	2.523	0.051	2.523	0.258	2.523	0.081	2.523	0.260	2.523	0.081
[BzmPyrr]+	1	2.371	0.089	2.371	0.258	2.371	0.081	2.371	0.260	2.371	0.081
[BzPy]+	1	2.617	0.069	2.617	0.258	2.617	0.081	2.617	0.260	2.617	0.081
[C1,9(M2iPAm)2]2+	1	2.533	0.086	2.533	0.258	2.533	0.081	2.533	0.260	2.533	0.081
[C3MPyrr]+	1	0.000	0.087	0.000	0.258	0.000	0.081	0.000	0.260	0.000	0.081
[C5MPyrr]+	1	2.317	0.092	2.317	0.258	2.317	0.081	2.317	0.260	2.317	0.081

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[ChxmIm]+	1	2.418	0.094	2.418	0.258	2.418	0.081	2.418	0.260	2.418	0.081
[ChxmPyrr]+	1	2.406	0.097	2.406	0.258	2.406	0.081	2.406	0.260	2.406	0.081
[ChxPy]+	1	2.370	0.062	2.370	0.258	2.370	0.081	2.370	0.260	2.370	0.081
[CNMeM2iPam]+	1	3.283	0.116	3.283	0.258	3.283	0.081	3.283	0.260	3.283	0.081
[CNPrMIm]+	1	2.617	-0.147	2.832	0.293	2.798	0.092	2.831	0.295	2.798	0.092
[D2MIM]+	1	1.603	-0.082	1.603	0.258	1.603	0.081	1.603	0.260	1.603	0.081
[DM3AM]+	1	1.986	-0.090	1.986	0.258	1.986	0.081	1.986	0.260	1.986	0.081
[DMPyrr]+	1	1.991	-0.069	1.991	0.258	1.991	0.081	1.991	0.260	1.991	0.081
[E3S]+	1	2.992	-0.399	2.992	0.258	2.992	0.081	2.992	0.260	2.992	0.081
[EMIM]+	10	2.305	-0.065	2.238	0.137	2.352	0.045	2.237	0.138	2.352	0.045
[EtOHM2iPAm]+	1	2.361	0.086	2.361	0.258	2.361	0.081	2.361	0.260	2.361	0.081
[EtOHMIm]+	4	2.462	-0.066	2.728	0.152	2.596	0.050	2.732	0.153	2.596	0.050
[HexM3Am]+	1	2.083	-0.075	2.085	0.258	2.085	0.081	2.085	0.260	2.085	0.081
[HM2iPam]+	1	2.232	0.091	2.232	0.258	2.232	0.081	2.232	0.260	2.232	0.081
[HMIM]+	3	2.081	-0.063	2.164	0.171	2.167	0.054	2.164	0.172	2.167	0.054
[HMPip]+	1	2.469	-0.109	2.469	0.258	2.469	0.081	2.469	0.260	2.469	0.081
[HMPyrr]+	1	2.146	-0.095	2.146	0.258	2.146	0.081	2.146	0.260	2.146	0.081
[HxomMIm]+	1	2.478	-0.295	2.073	0.258	2.073	0.081	2.073	0.260	2.073	0.081
[M2EIm]+	1	2.380	-0.154	2.347	0.258	2.347	0.081	2.347	0.260	2.347	0.081
[M3BAm]+	1	2.188	0.153	2.188	0.258	2.188	0.081	2.188	0.260	2.188	0.081
[MDIm]+	1	2.036	-0.211	2.049	0.316	2.071	0.099	2.049	0.319	2.071	0.099
[MeoeMim]+	1	2.644	-0.112	2.476	0.258	2.476	0.081	2.476	0.260	2.476	0.081
[MeoeMMorp]+	2	2.823	-0.073	2.764	0.194	2.758	0.061	2.764	0.195	2.758	0.061
[MeoeMPip]+	2	2.484	-0.074	2.483	0.194	2.477	0.061	2.483	0.195	2.477	0.061
[MeoeMPyrr]+	1	2.497	-0.095	2.495	0.289	2.483	0.090	2.496	0.291	2.483	0.090
[MOIm]+	3	1.301	-0.095	1.511	0.197	1.170	0.076	1.515	0.199	1.170	0.076
[N112N113]+	1	2.865	0.101	2.865	0.258	2.865	0.081	2.865	0.260	2.865	0.081
[N112N114]+	1	2.522	0.100	2.522	0.258	2.522	0.081	2.522	0.260	2.522	0.081
[N112O2N113]+	1	2.440	0.111	2.440	0.258	2.440	0.081	2.440	0.260	2.440	0.081
[N112O2N114]+	1	2.279	0.112	2.279	0.258	2.279	0.081	2.279	0.260	2.279	0.081

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[N2,2,2,8]+	1	2.034	0.058	2.101	0.389	2.048	0.121	2.101	0.392	2.048	0.121
[O4AM]+	1	1.478	-0.110	1.478	0.258	1.478	0.081	1.478	0.260	1.478	0.081
[OM3AM]+	1	2.242	-0.082	2.242	0.258	2.242	0.081	2.242	0.260	2.242	0.081
[Ompyrr]+	1	2.080	-0.086	2.080	0.258	2.080	0.081	2.080	0.260	2.080	0.081
[PDMIM]+	2	2.357	-0.210	2.670	0.196	2.444	0.098	2.670	0.198	2.444	0.098
[PEMPip]+	1	2.639	-0.123	2.639	0.258	2.639	0.081	2.639	0.260	2.639	0.081
[PeMPyrr]+	1	2.317	-0.092	2.317	0.258	2.317	0.081	2.317	0.260	2.317	0.081
[PM2iPAm]+	1	2.532	0.064	2.532	0.258	2.532	0.081	2.532	0.260	2.532	0.081
[PMPip]+	1	2.281	-0.098	2.287	0.258	2.287	0.081	2.287	0.260	2.287	0.081
[PMPyrr]+	1	2.562	-0.087	2.562	0.258	2.562	0.081	2.562	0.260	2.562	0.081
[sec-BMIm]+	1	2.519	0.078	2.519	0.258	2.519	0.081	2.519	0.260	2.519	0.081
[tert-BMIm]+	1	2.603	0.083	2.603	0.258	2.603	0.081	2.603	0.260	2.603	0.081

Table D.19: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter a for log K.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[(Hexom)2Im]+	1	2.376	-0.222	2.376	0.494	2.376	0.116	2.376	0.494	2.376	0.116
[(Meo)2Im]+	1	2.427	-0.152	2.427	0.494	2.427	0.116	2.427	0.494	2.427	0.116
[1-PrOHPy]+	1	2.874	-0.095	2.414	0.560	2.593	0.132	2.414	0.560	2.593	0.132
[3-MBPy]+	2	2.289	-0.246	2.594	0.503	2.325	0.119	2.594	0.503	2.325	0.119
[AllMIm]+	2	2.324	0.094	2.242	0.374	2.331	0.088	2.242	0.374	2.331	0.088
[B3EP]+	1	0.788	0.000	0.693	0.746	0.875	0.176	0.693	0.746	0.875	0.176
[BMIm]+	15	2.281	-0.071	2.651	0.237	2.290	0.059	2.651	0.237	2.290	0.059
[BMMOR]+	1	2.369	0.000	2.961	0.604	2.828	0.143	2.961	0.604	2.828	0.143
[BMPip]+	1	2.467	-0.095	2.472	0.494	2.472	0.116	2.472	0.494	2.472	0.116
[BMPy]+	3	2.416	-0.131	2.231	0.330	2.235	0.080	2.231	0.330	2.235	0.080
[BMPyrr]+	8	2.363	-0.076	2.590	0.253	2.550	0.060	2.590	0.253	2.550	0.060
[BzmIm]+	1	2.333	0.097	2.333	0.494	2.333	0.116	2.333	0.494	2.333	0.116
[BzmPyrr]+	1	2.285	0.121	2.285	0.494	2.285	0.116	2.285	0.494	2.285	0.116

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[BzPy]+	1	2.452	0.130	2.452	0.494	2.452	0.116	2.452	0.494	2.452	0.116
[C1,9(M2iPAm)2]2+	1	2.544	0.116	2.544	0.494	2.544	0.116	2.544	0.494	2.544	0.116
[C3MPyrr]+	1	2.505	0.184	2.505	0.494	2.505	0.116	2.505	0.494	2.505	0.116
[C5MPyrr]+	1	2.425	0.155	2.425	0.494	2.425	0.116	2.425	0.494	2.425	0.116
[ChxmIm]+	1	2.688	0.136	2.688	0.494	2.688	0.116	2.688	0.494	2.688	0.116
[ChxmPyrr]+	1	2.411	0.138	2.411	0.494	2.411	0.116	2.411	0.494	2.411	0.116
[ChxPy]+	1	2.496	0.117	2.496	0.494	2.496	0.116	2.496	0.494	2.496	0.116
[CNMeM2iPam]+	1	3.118	0.174	3.118	0.494	3.118	0.116	3.118	0.494	3.118	0.116
[CNPrMIm]+	1	2.543	-0.204	2.371	0.560	2.550	0.132	2.371	0.560	2.550	0.132
[D2MIM]+	1	1.946	-0.125	1.946	0.494	1.946	0.116	1.946	0.494	1.946	0.116
[DM3AM]+	1	2.144	-0.135	2.144	0.494	2.144	0.116	2.144	0.494	2.144	0.116
[DMPyrr]+	1	2.112	-0.110	2.112	0.494	2.112	0.116	2.112	0.494	2.112	0.116
[E3S]+	1	2.444	-0.261	2.444	0.494	2.444	0.116	2.444	0.494	2.444	0.116
[EMIM]+	10	2.381	-0.079	2.266	0.262	2.448	0.065	2.266	0.262	2.448	0.065
[EtOHM2iPAm]+	1	2.695	0.115	2.695	0.494	2.695	0.116	2.695	0.494	2.695	0.116
[EtOHMIm]+	4	2.694	-0.079	2.686	0.290	2.715	0.072	2.686	0.290	2.715	0.072
[HexM3Am]+	1	2.176	-0.085	2.185	0.494	2.185	0.116	2.185	0.494	2.185	0.116
[HM2iPam]+	1	2.297	0.137	2.297	0.494	2.297	0.116	2.297	0.494	2.297	0.116
[HMIM]+	3	2.298	-0.071	2.279	0.327	2.310	0.077	2.279	0.327	2.310	0.077
[HMPip]+	1	2.348	-0.105	2.348	0.494	2.348	0.116	2.348	0.494	2.348	0.116
[HMPyrr]+	1	2.278	-0.196	2.278	0.494	2.278	0.116	2.278	0.494	2.278	0.116
[HxomMIm]+	1	2.428	-0.222	2.022	0.494	2.022	0.116	2.022	0.494	2.022	0.116
[M2EIm]+	1	2.101	-0.190	2.075	0.494	2.075	0.116	2.075	0.494	2.075	0.116
[M3BAm]+	1	2.375	0.202	2.375	0.494	2.375	0.116	2.375	0.494	2.375	0.116
[MDIm]+	1	2.054	-0.173	2.111	0.604	2.169	0.142	2.111	0.604	2.169	0.142
[MeoeMim]+	1	2.378	-0.153	2.271	0.494	2.271	0.116	2.271	0.494	2.271	0.116
[MeoeMMorp]+	2	2.588	-0.080	2.536	0.371	2.554	0.087	2.536	0.371	2.554	0.087
[MeoeMPip]+	2	2.537	-0.091	2.531	0.371	2.549	0.087	2.531	0.371	2.549	0.087
[MeoeMPyrr]+	1	2.534	-0.107	2.525	0.553	2.562	0.130	2.525	0.553	2.562	0.130
[MOIm]+	3	2.021	-0.102	1.773	0.377	1.959	0.109	1.773	0.377	1.959	0.109

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[N112N113]+	1	3.280	0.128	3.280	0.494	3.280	0.116	3.280	0.494	3.280	0.116
[N112N114]+	1	2.863	0.138	2.863	0.494	2.863	0.116	2.863	0.494	2.863	0.116
[N112O2N113]+	1	2.608	0.125	2.608	0.494	2.608	0.116	2.608	0.494	2.608	0.116
[N112O2N114]+	1	2.505	0.153	2.505	0.494	2.505	0.116	2.505	0.494	2.505	0.116
[N2,2,2,8]+	1	2.317	0.076	2.435	0.743	2.395	0.175	2.435	0.743	2.395	0.175
[O4AM]+	1	1.845	-0.158	1.845	0.494	1.845	0.116	1.845	0.494	1.845	0.116
[OM3AM]+	1	2.195	-0.123	2.195	0.494	2.195	0.116	2.195	0.494	2.195	0.116
[Ompyrr]+	1	2.176	-0.160	2.176	0.494	2.176	0.116	2.176	0.494	2.176	0.116
[PDMIM]+	2	3.432	-0.243	2.227	0.376	3.562	0.141	2.227	0.376	3.562	0.141
[PEMPip]+	1	2.450	-0.119	2.450	0.494	2.450	0.116	2.450	0.494	2.450	0.116
[PeMPyrr]+	1	2.425	-0.155	2.425	0.494	2.425	0.116	2.425	0.494	2.425	0.116
[PM2iPAm]+	1	2.578	0.139	2.578	0.494	2.578	0.116	2.578	0.494	2.578	0.116
[PMPip]+	1	2.476	-0.097	2.489	0.494	2.489	0.116	2.489	0.494	2.489	0.116
[PMPyrr]+	1	2.505	-0.184	2.505	0.494	2.505	0.116	2.505	0.494	2.505	0.116
[sec-BMIm]+	1	2.497	0.111	2.497	0.494	2.497	0.116	2.497	0.494	2.497	0.116
[tert-BMIm]+	1	2.689	0.119	2.689	0.494	2.689	0.116	2.689	0.494	2.689	0.116

Table D.20: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter b for log K.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[(Hexom)2Im]+	1	0.287	-0.235	0.287	0.310	0.287	0.118	0.287	0.309	0.287	0.118
[(Meo)2Im]+	1	1.154	-0.110	1.157	0.310	1.157	0.118	1.157	0.309	1.157	0.118
[1-PrOHPy]+	1	1.311	-0.106	2.447	0.351	2.468	0.135	2.441	0.351	2.463	0.134
[3-MBPy]+	2	0.189	-0.232	0.045	0.315	0.233	0.122	0.072	0.315	0.260	0.121
[AllMIm]+	2	0.624	0.074	0.583	0.234	0.594	0.090	0.580	0.234	0.591	0.089
[B3EP]+	1	0.774	0.000	0.865	0.468	0.765	0.180	0.863	0.467	0.672	0.179
[BMIm]+	15	0.603	-0.071	0.383	0.148	0.621	0.060	0.383	0.148	0.621	0.060
[BMMOR]+	1	0.597	0.000	0.296	0.379	0.392	0.146	0.295	0.378	0.391	0.145
[BMPip]+	1	0.327	-0.111	0.294	0.310	0.294	0.118	0.294	0.309	0.294	0.118

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[BMPy]+	3	0.566	-0.114	0.514	0.207	0.501	0.082	0.514	0.207	0.500	0.081
[BMPyrr]+	8	0.388	-0.067	0.172	0.158	0.234	0.061	0.169	0.158	0.231	0.061
[BzmIm]+	1	0.575	0.068	0.575	0.310	0.575	0.118	0.575	0.309	0.575	0.118
[BzmPyrr]+	1	0.531	0.104	0.531	0.310	0.531	0.118	0.531	0.309	0.531	0.118
[BzPy]+	1	0.526	0.088	0.526	0.310	0.526	0.118	0.526	0.309	0.526	0.118
[C1,9(M2iPAm)2]2+	1	0.492	0.103	0.492	0.310	0.492	0.118	0.492	0.309	0.492	0.118
[C3MPyrr]+	1	0.271	0.107	0.271	0.310	0.271	0.118	0.271	0.309	0.271	0.118
[C5MPyrr]+	1	0.385	0.096	0.385	0.310	0.385	0.118	0.385	0.309	0.385	0.118
[ChxmIm]+	1	0.334	0.099	0.334	0.310	0.334	0.118	0.334	0.309	0.334	0.118
[ChxmPyrr]+	1	0.274	0.101	0.274	0.310	0.274	0.118	0.274	0.309	0.274	0.118
[ChxPy]+	1	0.412	0.079	0.412	0.310	0.412	0.118	0.412	0.309	0.412	0.118
[CNMeM2iPam]+	1	0.819	0.129	0.819	0.310	0.819	0.118	0.819	0.309	0.819	0.118
[CNPrMIm]+	1	0.816	-0.166	0.743	0.351	0.764	0.135	0.737	0.351	0.759	0.134
[D2MIM]+	1	0.354	-0.093	0.354	0.310	0.354	0.118	0.354	0.309	0.354	0.118
[DM3AM]+	1	0.422	-0.094	0.422	0.310	0.422	0.118	0.422	0.309	0.422	0.118
[DMPyrr]+	1	0.268	-0.076	0.268	0.310	0.268	0.118	0.268	0.309	0.268	0.118
[E3S]+	1	0.355	-0.276	0.355	0.310	0.355	0.118	0.355	0.309	0.355	0.118
[EMIM]+	10	0.683	-0.074	0.774	0.164	0.674	0.066	0.772	0.164	0.672	0.066
[EtOHM2iPAm]+	1	1.532	0.086	1.532	0.310	1.532	0.118	1.532	0.309	1.532	0.118
[EtOHMIm]+	4	1.331	-0.078	1.276	0.182	1.415	0.073	1.276	0.182	1.415	0.073
[HexM3Am]+	1	0.620	-0.090	0.617	0.310	0.617	0.118	0.617	0.309	0.617	0.118
[HM2iPam]+	1	0.344	0.100	0.344	0.310	0.344	0.118	0.344	0.309	0.344	0.118
[HMIM]+	3	0.533	-0.069	0.476	0.205	0.479	0.079	0.475	0.205	0.478	0.078
[HMPip]+	1	0.075	-0.099	0.075	0.310	0.075	0.118	0.075	0.309	0.075	0.118
[HMPyrr]+	1	0.650	-0.114	0.650	0.310	0.650	0.118	0.650	0.309	0.650	0.118
[HxomMIm]+	1	0.337	-0.235	0.637	0.310	0.637	0.118	0.637	0.309	0.637	0.118
[M2EIm]+	1	0.899	-0.149	0.896	0.310	0.896	0.118	0.896	0.309	0.896	0.118
[M3BAm]+	1	0.663	0.201	0.663	0.310	0.663	0.118	0.663	0.309	0.663	0.118
[MDIm]+	1	0.524	-0.191	0.425	0.379	0.414	0.145	0.423	0.378	0.412	0.145
[MeoeMim]+	1	0.413	-0.130	0.671	0.310	0.671	0.118	0.671	0.309	0.671	0.118

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[MeoeMMorp]+	2	0.542	-0.081	0.501	0.232	0.511	0.089	0.500	0.232	0.510	0.089
[MeoeMPip]+	2	0.241	-0.085	0.171	0.232	0.181	0.089	0.170	0.232	0.180	0.089
[MeoeMPyrr]+	1	0.162	-0.113	0.044	0.346	0.063	0.133	0.043	0.346	0.062	0.132
[MOIm]+	3	0.994	-0.108	0.732	0.236	1.186	0.112	0.732	0.236	1.185	0.111
[N112N113]+	1	1.041	0.107	1.041	0.310	1.041	0.118	1.041	0.309	1.041	0.118
[N112N114]+	1	0.751	0.097	0.751	0.310	0.751	0.118	0.751	0.309	0.751	0.118
[N112O2N113]+	1	0.420	0.115	0.420	0.310	0.420	0.118	0.420	0.309	0.420	0.118
[N112O2N114]+	1	0.435	0.131	0.435	0.310	0.435	0.118	0.435	0.309	0.435	0.118
[N2,2,2,8]+	1	0.179	0.060	-0.016	0.466	0.046	0.178	-0.019	0.465	0.043	0.177
[O4AM]+	1	0.189	-0.121	0.189	0.310	0.189	0.118	0.189	0.309	0.189	0.118
[OM3AM]+	1	0.684	-0.021	0.684	0.310	0.684	0.118	0.684	0.309	0.684	0.118
[Ompyrr]+	1	0.486	-0.103	0.486	0.310	0.486	0.118	0.486	0.309	0.486	0.118
[PDMIM]+	2	0.926	-0.220	0.697	0.235	0.847	0.144	0.696	0.235	0.846	0.143
[PEMPip]+	1	0.103	-0.112	0.103	0.310	0.103	0.118	0.103	0.309	0.103	0.118
[PeMPyrr]+	1	0.385	-0.096	0.385	0.310	0.385	0.118	0.385	0.309	0.385	0.118
[PM2iPAm]+	1	0.331	0.083	0.331	0.310	0.331	0.118	0.331	0.309	0.331	0.118
[PMPip]+	1	0.410	-0.124	0.402	0.310	0.402	0.118	0.402	0.309	0.402	0.118
[PMPyrr]+	1	0.271	-0.107	0.271	0.310	0.271	0.118	0.271	0.309	0.271	0.118
[sec-BMIm]+	1	0.456	0.081	0.456	0.310	0.456	0.118	0.456	0.309	0.456	0.118
[tert-BMIm]+	1	0.410	0.087	0.410	0.310	0.410	0.118	0.410	0.309	0.410	0.118

Table D.21: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter l for log K.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		l (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)
[(Hexom)2Im]+	1	0.835	-0.035	0.835	0.032	0.835	0.017	0.835	0.032	0.835	0.017
[(Meo)2Im]+	1	0.584	-0.021	0.584	0.032	0.584	0.017	0.584	0.032	0.584	0.017
[1-PrOHPy]+	1	0.611	-0.016	0.673	0.036	0.655	0.019	0.673	0.036	0.655	0.019
[3-MBPy]+	2	0.714	-0.030	0.745	0.032	0.741	0.017	0.745	0.032	0.741	0.017
[AllMIm]+	2	0.606	0.017	0.620	0.024	0.612	0.013	0.620	0.024	0.612	0.013

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		l (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)
[B3EP]+	1	0.783	-	0.826	0.048	0.801	0.026	0.826	0.048	0.801	0.026
[BMIm]+	15	0.712	-0.007	0.735	0.015	0.733	0.009	0.735	0.015	0.733	0.009
[BMMOR]+	1	0.638	-	0.690	0.039	0.684	0.021	0.690	0.039	0.684	0.021
[BMPip]+	1	0.679	-0.016	0.687	0.032	0.687	0.017	0.687	0.032	0.687	0.017
[BMPy]+	3	0.714	-0.016	0.734	0.021	0.727	0.012	0.734	0.021	0.727	0.012
[BMPyrr]+	8	0.679	-0.010	0.711	0.016	0.703	0.009	0.711	0.016	0.703	0.009
[BzmIm]+	1	0.668	0.014	0.668	0.032	0.668	0.017	0.668	0.032	0.668	0.017
[BzmPyrr]+	1	0.691	0.015	0.691	0.032	0.691	0.017	0.691	0.032	0.691	0.017
[BzPy]+	1	0.711	0.017	0.711	0.032	0.711	0.017	0.711	0.032	0.711	0.017
[C1,9(M2iPAm)2]2+	1	0.690	0.015	0.690	0.032	0.690	0.017	0.690	0.032	0.690	0.017
[C3MPyrr]+	1	0.682	0.032	0.682	0.032	0.682	0.017	0.682	0.032	0.682	0.017
[C5MPyrr]+	1	0.747	0.023	0.747	0.032	0.747	0.017	0.747	0.032	0.747	0.017
[ChxmIm]+	1	0.745	0.018	0.745	0.032	0.745	0.017	0.745	0.032	0.745	0.017
[ChxmPyrr]+	1	0.771	0.018	0.771	0.032	0.771	0.017	0.771	0.032	0.771	0.017
[ChxPy]+	1	0.755	0.015	0.755	0.032	0.755	0.017	0.755	0.032	0.755	0.017
[CNMeM2iPam]+	1	0.735	0.025	0.735	0.032	0.735	0.017	0.735	0.032	0.735	0.017
[CNPrMIm]+	1	0.699	-0.029	0.728	0.036	0.710	0.019	0.728	0.036	0.710	0.019
[D2MIM]+	1	0.856	-0.027	0.856	0.032	0.856	0.017	0.856	0.032	0.856	0.017
[DM3AM]+	1	0.809	-0.024	0.809	0.032	0.809	0.017	0.809	0.032	0.809	0.017
[DMPyrr]+	1	0.822	-0.018	0.822	0.032	0.822	0.017	0.822	0.032	0.822	0.017
[E3S]+	1	0.690	-0.036	0.690	0.032	0.690	0.017	0.690	0.032	0.690	0.017
[EMIM]+	10	0.654	-0.008	0.696	0.017	0.671	0.010	0.696	0.017	0.671	0.010
[EtOHM2iPAm]+	1	0.641	0.017	0.641	0.032	0.641	0.017	0.641	0.032	0.641	0.017
[EtOHMIm]+	4	0.580	-0.011	0.600	0.019	0.593	0.010	0.600	0.019	0.593	0.010
[HexM3Am]+	1	0.689	-0.014	0.617	0.032	0.617	0.017	0.617	0.032	0.617	0.017
[HM2iPam]+	1	0.736	0.018	0.736	0.032	0.736	0.017	0.736	0.032	0.736	0.017
[HMIM]+	3	0.751	-0.008	0.753	0.021	0.745	0.011	0.753	0.021	0.745	0.011
[HMPip]+	1	0.775	-0.016	0.775	0.032	0.775	0.017	0.775	0.032	0.775	0.017
[HMPyrr]+	1	0.767	-0.026	0.767	0.032	0.767	0.017	0.767	0.032	0.767	0.017
[HxomMIm]+	1	0.786	-0.035	0.684	0.032	0.684	0.017	0.684	0.032	0.684	0.017

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		l (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)
[M2EIm]+	1	0.667	-0.023	0.655	0.032	0.655	0.017	0.655	0.032	0.655	0.017
[M3BAm]+	1	0.668	0.013	0.668	0.032	0.668	0.017	0.668	0.032	0.668	0.017
[MDIm]+	1	0.786	-0.028	0.817	0.039	0.804	0.021	0.817	0.039	0.804	0.021
[MeoeMim]+	1	0.602	-0.021	0.603	0.032	0.603	0.017	0.603	0.032	0.603	0.017
[MeoeMMorp]+	2	0.644	-0.015	0.630	0.024	0.626	0.013	0.630	0.024	0.626	0.013
[MeoeMPip]+	2	0.688	-0.015	0.689	0.024	0.685	0.013	0.689	0.024	0.685	0.013
[MeoeMPyrr]+	1	0.671	-0.019	0.681	0.035	0.672	0.019	0.681	0.035	0.672	0.019
[MOIm]+	3	0.837	-0.010	0.862	0.024	0.840	0.016	0.862	0.024	0.840	0.016
[N112N113]+	1	0.762	0.021	0.762	0.032	0.762	0.017	0.762	0.032	0.762	0.017
[N112N114]+	1	0.656	0.024	0.656	0.032	0.656	0.017	0.656	0.032	0.656	0.017
[N112O2N113]+	1	0.748	0.019	0.748	0.032	0.748	0.017	0.748	0.032	0.748	0.017
[N112O2N114]+	1	0.707	0.020	0.707	0.032	0.707	0.017	0.707	0.032	0.707	0.017
[N2,2,2,8]+	1	0.787	0.014	0.807	0.047	0.799	0.026	0.807	0.047	0.799	0.026
[O4AM]+	1	0.816	-0.013	0.816	0.032	0.816	0.017	0.816	0.032	0.816	0.017
[OM3AM]+	1	0.779	-0.022	0.779	0.032	0.779	0.017	0.779	0.032	0.779	0.017
[Ompyrr]+	1	0.822	-0.023	0.822	0.032	0.822	0.017	0.822	0.032	0.822	0.017
[PDMIM]+	2	0.526	-0.038	0.716	0.024	0.559	0.021	0.716	0.024	0.559	0.021
[PEMPip]+	1	0.761	-0.018	0.761	0.032	0.761	0.017	0.761	0.032	0.761	0.017
[PeMPyrr]+	1	0.747	-0.023	0.747	0.032	0.747	0.017	0.747	0.032	0.747	0.017
[PM2iPAm]+	1	0.682	0.017	0.682	0.032	0.682	0.017	0.682	0.032	0.682	0.017
[PMPip]+	1	0.675	-0.018	0.674	0.032	0.674	0.017	0.674	0.032	0.674	0.017
[PMPyrr]+	1	0.682	-0.032	0.682	0.032	0.682	0.017	0.682	0.032	0.682	0.017
[sec-BMIm]+	1	0.705	0.015	0.705	0.032	0.705	0.017	0.705	0.032	0.705	0.017
[tert-BMIm]+	1	0.693	0.015	0.693	0.032	0.693	0.017	0.693	0.032	0.693	0.017

Table D.22: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter c for log P.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[(Hexom)2Im]+	1	0.074	0.172	0.107	0.122	0.107	0.077	0.107	0.123	0.107	0.075
[(Meo)2Im]+	1	-0.414	0.150	-0.412	0.122	-0.412	0.077	-0.412	0.123	-0.412	0.075
[3-MBPy]+	2	0.040	0.146	-0.073	0.125	0.033	0.079	0.030	0.126	0.118	0.077
[AllMIm]+	2	0.028	0.090	-0.002	0.093	-0.004	0.058	0.002	0.093	-0.008	0.057
[B3EP]+	1	0.049	0.000	-0.032	0.185	-0.019	0.117	-0.144	0.186	-0.134	0.114
[BMIm]+	15	-0.048	0.035	-0.235	0.061	-0.106	0.039	-0.188	0.059	-0.079	0.038
[BMMOR]+	1	-0.239	0.000	0.008	0.154	0.124	0.095	0.060	0.151	0.133	0.093
[BMPip]+	1	-0.115	0.081	-0.129	0.122	-0.129	0.077	0.000	0.123	0.000	0.075
[BMPy]+	2	-0.090	0.082	-0.378	0.112	-0.207	0.055	-0.294	0.083	-0.219	0.053
[BMPyrr]+	8	-0.340	0.053	-0.034	0.064	0.014	0.040	-0.010	0.063	0.023	0.039
[BzmIm]+	1	-0.187	0.083	-0.187	0.122	-0.187	0.077	-0.187	0.123	-0.187	0.075
[BzmPyrr]+	1	-0.387	0.120	-0.387	0.122	-0.387	0.077	-0.387	0.123	-0.387	0.075
[BzPy]+	1	-0.516	0.118	-0.516	0.122	-0.516	0.077	-0.516	0.123	-0.516	0.075
[C1,9(M2iPAm)2]2+	1	-0.606	0.137	-0.606	0.122	-0.606	0.077	-0.606	0.123	-0.606	0.075
[C3MPyrr]+	1	-0.236	0.170	-0.236	0.122	-0.236	0.077	-0.236	0.123	-0.236	0.075
[C5MPyrr]+	1	-0.303	0.134	-0.303	0.122	-0.303	0.077	-0.303	0.123	-0.303	0.075
[ChxmIm]+	1	-0.299	0.128	-0.299	0.122	-0.299	0.077	-0.299	0.123	-0.299	0.075
[ChxmPyrr]+	1	-0.297	0.116	-0.297	0.122	-0.297	0.077	-0.297	0.123	-0.297	0.075
[ChxPy]+	1	-0.344	0.118	-0.344	0.122	-0.344	0.077	-0.344	0.123	-0.344	0.075
[CNMeM2iPam]+	1	-1.001	0.151	-1.001	0.122	-1.001	0.077	-1.001	0.123	-1.001	0.075
[CNPrMIm]+	1	-0.680	0.175	-0.729	0.139	-0.735	0.087	-0.723	0.140	-0.742	0.085
[D2MIM]+	1	-0.093	0.147	-0.093	0.122	-0.093	0.077	0.000	0.123	0.000	0.075
[DM3AM]+	1	-0.128	0.135	-0.128	0.122	-0.128	0.077	0.000	0.123	0.000	0.075
[DMPyrr]+	1	-0.083	0.128	-0.083	0.122	-0.083	0.077	0.000	0.123	0.000	0.075
[E3S]+	1	-0.062	0.179	-0.062	0.122	-0.062	0.077	0.000	0.123	0.000	0.075
[EMIM]+	10	-0.049	0.039	-0.130	0.065	-0.117	0.043	-0.144	0.065	-0.134	0.042
[EtOHM2iPAm]+	1	-0.669	0.143	-0.669	0.122	-0.669	0.077	-0.669	0.123	-0.669	0.075
[EtOHMIm]+	3	-0.404	0.065	-0.394	0.080	-0.374	0.051	-0.362	0.080	-0.346	0.050
[HexM3Am]+	1	-0.404	0.085	-0.322	0.122	-0.404	0.077	-0.322	0.123	-0.404	0.075

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[HM2iPam]+	1	-0.340	0.129	-0.340	0.122	-0.340	0.077	-0.340	0.123	-0.340	0.075
[HMIM]+	3	-0.083	0.036	-0.065	0.081	-0.051	0.051	-0.049	0.082	-0.039	0.050
[HMPyrr]+	1	-0.226	0.152	-0.226	0.122	-0.226	0.077	-0.226	0.123	-0.226	0.075
[HxomMIm]+	1	-0.071	0.172	-0.275	0.122	-0.275	0.077	-0.275	0.123	-0.275	0.075
[M2EIm]+	1	-0.095	0.122	-0.095	0.122	-0.095	0.077	0.000	0.123	0.000	0.075
[M3BAm]+	1	0.047	0.074	0.047	0.122	0.047	0.077	0.000	0.123	0.000	0.075
[MDIm]+	1	0.036	0.171	0.106	0.150	0.131	0.094	-0.017	0.151	0.000	0.092
[MeoeMIm]+	1	-0.150	0.131	-0.150	0.122	-0.150	0.077	-0.150	0.123	-0.150	0.075
[MeoeMMorp]+	2	-0.264	0.077	-0.192	0.092	-0.183	0.058	-0.159	0.093	-0.153	0.056
[MeoeMPip]+	2	-0.102	0.077	-0.075	0.092	-0.066	0.058	-0.065	0.093	-0.059	0.056
[MeoeMPyrr]+	1	-0.068	0.098	-0.066	0.137	-0.049	0.086	-0.130	0.138	-0.118	0.084
[MOIm]+	3	-0.011	0.054	-0.188	0.096	-0.036	0.074	-0.166	0.095	-0.045	0.072
[N112N113]+	1	-1.042	0.133	-1.042	0.122	-1.042	0.077	-1.042	0.123	-1.042	0.075
[N112N114]+	1	-0.397	0.136	-0.397	0.122	-0.397	0.077	-0.397	0.123	-0.397	0.075
[N112O2N113]+	1	-0.339	0.132	-0.339	0.122	-0.339	0.077	-0.339	0.123	-0.339	0.075
[N112O2N114]+	1	-0.205	0.143	-0.205	0.122	-0.205	0.077	-0.205	0.123	-0.205	0.075
[N2,2,2,8]+	1	-0.003	0.086	-0.001	0.184	0.047	0.116	0.132	0.186	0.165	0.113
[O4AM]+	1	0.226	0.198	0.226	0.122	0.226	0.077	0.226	0.123	0.226	0.075
[OM3AM]+	1	-0.165	0.129	-0.165	0.122	-0.165	0.077	-0.165	0.123	-0.165	0.075
[Ompyrr]+	1	-0.253	0.121	-0.253	0.122	-0.253	0.077	-0.253	0.123	-0.253	0.075
[PDMIM]+	2	-0.499	0.182	-0.864	0.095	-0.643	0.098	-0.873	0.095	-0.717	0.096
[PeMPyrr]+	1	-0.303	0.134	-0.303	0.122	-0.303	0.077	-0.303	0.123	-0.303	0.075
[PM2iPAm]+	1	-0.378	0.118	-0.378	0.122	-0.378	0.077	-0.378	0.123	-0.378	0.075
[PMPip]+	1	-0.230	0.100	-0.231	0.122	-0.231	0.077	-0.231	0.123	-0.231	0.075
[PMPyrr]+	1	-0.236	0.170	-0.236	0.122	-0.236	0.077	-0.236	0.123	-0.236	0.075
[sec-BMIm]+	1	-0.215	0.105	-0.215	0.122	-0.215	0.077	-0.215	0.123	-0.215	0.075
[tert-BMIm]+	1	-0.275	0.110	-0.275	0.122	-0.275	0.077	-0.275	0.123	-0.275	0.075

Table D.23: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter e for log P.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[(Hexom)2Im]+	1	-0.541	-0.269	-0.628	0.224	-0.628	0.093	-0.628	0.231	-0.628	0.092
[(Meo)2Im]+	1	-0.103	-0.138	-0.104	0.224	-0.104	0.093	0.000	0.231	0.000	0.092
[3-MBPy]+	2	0.087	-0.226	0.158	0.230	-0.015	0.095	0.173	0.236	0.067	0.095
[AllMIm]+	2	0.127	0.000	0.070	0.170	0.078	0.070	0.008	0.175	0.044	0.070
[B3EP]+	1	-0.315	0.000	-0.341	0.339	-0.347	0.141	-0.378	0.350	-0.333	0.140
[BMIm]+	15	0.328	-0.059	0.340	0.111	0.133	0.047	0.242	0.111	0.105	0.047
[BMMOR]+	1	0.318	0.000	0.125	0.281	-0.163	0.114	-0.068	0.283	-0.179	0.113
[BMPip]+	1	0.448	-0.096	0.494	0.224	0.494	0.093	0.494	0.231	0.494	0.092
[BMPy]+	2	0.238	-0.119	0.671	0.205	0.102	0.066	0.260	0.156	0.093	0.065
[BMPyrr]+	8	0.380	-0.068	0.313	0.117	0.224	0.048	0.241	0.119	0.214	0.047
[BzmIm]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[BzmPyrr]+	1	0.197	0.120	0.197	0.224	0.197	0.093	0.197	0.231	0.197	0.092
[BzPy]+	1	0.092	0.112	0.092	0.224	0.092	0.093	0.000	0.231	0.000	0.092
[C1,9(M2iPAm)2]2+	1	0.225	0.127	0.225	0.224	0.225	0.093	0.225	0.231	0.225	0.092
[C3MPyrr]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[C5MPyrr]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[ChxmIm]+	1	-0.094	0.125	-0.094	0.224	-0.094	0.093	0.000	0.231	0.000	0.092
[ChxmPyrr]+	1	0.073	0.113	0.073	0.224	0.073	0.093	0.000	0.231	0.000	0.092
[ChxPy]+	1	0.146	0.116	0.146	0.224	0.146	0.093	0.146	0.231	0.146	0.092
[CNMeM2iPam]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[CNPrMIm]+	1	0.206	-0.180	0.095	0.255	0.110	0.105	0.030	0.263	0.101	0.105
[D2MIM]+	1	-0.052	-0.118	-0.052	0.224	-0.052	0.093	0.000	0.231	0.000	0.092
[DM3AM]+	1	-0.131	-0.125	-0.131	0.224	-0.131	0.093	0.000	0.231	0.000	0.092
[DMPyrr]+	1	-0.142	-0.114	-0.142	0.224	-0.142	0.093	-0.142	0.231	-0.142	0.092
[E3S]+	1	-1.347	-0.367	-1.347	0.224	-1.347	0.093	-1.347	0.231	-1.347	0.092
[EMIM]+	10	0.215	-0.067	0.190	0.120	0.184	0.052	0.153	0.123	0.198	0.052
[EtOHM2iPAm]+	1	0.236	0.129	0.236	0.224	0.236	0.093	0.236	0.231	0.236	0.092
[EtOHMIm]+	3	0.229	-0.074	0.023	0.146	0.077	0.062	-0.004	0.151	0.065	0.062
[HexM3Am]+	1	0.344	-0.082	0.242	0.224	0.344	0.093	0.242	0.231	0.344	0.092

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[HM2iPam]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[HMIM]+	3	0.098	-0.068	0.088	0.149	0.072	0.062	0.001	0.153	0.010	0.061
[HMPyrr]+	1	-0.083	-0.132	-0.083	0.224	-0.083	0.093	0.000	0.231	0.000	0.092
[HxomMIm]+	1	-0.558	-0.269	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[M2EIm]+	1	0.292	-0.165	0.299	0.224	0.299	0.093	0.299	0.231	0.299	0.092
[M3BAm]+	1	-0.021	-0.163	-0.051	0.224	-0.051	0.093	0.000	0.231	0.000	0.092
[MDIm]+	1	-0.064	-0.227	-0.062	0.274	-0.099	0.114	-0.164	0.283	-0.155	0.113
[MeoeMIm]+	1	0.012	0.026	0.012	0.224	0.012	0.093	0.000	0.231	0.000	0.092
[MeoeMMorp]+	2	0.067	-0.081	0.001	0.168	-0.004	0.070	-0.045	0.174	-0.037	0.069
[MeoeMPip]+	2	0.191	-0.082	0.147	0.168	0.142	0.070	0.148	0.174	0.156	0.069
[MeoeMPyrr]+	1	0.119	-0.105	0.076	0.251	0.066	0.104	0.077	0.259	0.095	0.103
[MOIm]+	3	0.009	0.097	-0.249	0.176	-0.093	0.089	-0.326	0.178	-0.087	0.089
[N112N113]+	1	0.143	0.129	0.143	0.224	0.143	0.093	0.143	0.231	0.143	0.092
[N112N114]+	1	0.000	0.131	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[N112O2N113]+	1	-0.149	0.000	-0.149	0.224	-0.149	0.093	-0.149	0.231	-0.149	0.092
[N112O2N114]+	1	-0.053	0.135	-0.053	0.224	-0.053	0.093	0.000	0.231	0.000	0.092
[N2,2,2,8]+	1	0.192	0.080	0.279	0.338	0.190	0.140	0.207	0.348	0.180	0.138
[O4AM]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[OM3AM]+	1	-0.181	-0.118	-0.181	0.224	-0.181	0.093	-0.181	0.231	-0.181	0.092
[Ompyrr]+	1	0.000		0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[PDMIM]+	2	0.685	-0.200	0.555	0.174	0.462	0.118	0.480	0.178	0.452	0.117
[PeMPyrr]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[PM2iPAm]+	1	0.115	0.114	0.115	0.224	0.115	0.093	0.115	0.231	0.115	0.092
[PMPip]+	1	0.458	-0.101	0.453	0.224	0.453	0.093	0.453	0.231	0.453	0.092
[PMPyrr]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[sec-BMIm]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092
[tert-BMIm]+	1	0.000	0.000	0.000	0.224	0.000	0.093	0.000	0.231	0.000	0.092

Table D.24: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter s for log P.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[(Hexom)2Im]+	1	0.642	-0.353	0.747	0.343	0.747	0.168	0.747	0.349	0.747	0.172
[(Meo)2Im]+	1	0.764	-0.139	0.761	0.343	0.761	0.168	0.761	0.349	0.761	0.172
[3-MBPy]+	2	0.657	-0.300	0.751	0.352	0.859	0.173	0.822	0.356	0.850	0.177
[AllMIm]+	2	0.519	0.096	0.641	0.260	0.637	0.127	0.665	0.264	0.640	0.130
[B3EP]+	1	0.303	0.000	0.213	0.518	0.309	0.256	0.248	0.527	0.303	0.261
[BMIm]+	15	0.296	-0.071	0.558	0.170	0.679	0.086	0.632	0.168	0.666	0.088
[BMMOR]+	1	0.675	0.000	-0.129	0.431	0.137	0.207	0.039	0.427	0.131	0.211
[BMPip]+	1	0.322	-0.115	0.235	0.343	0.235	0.168	0.235	0.349	0.235	0.172
[BMPy]+	2	0.549	-0.153	0.523	0.315	1.124	0.119	0.892	0.236	1.119	0.122
[BMPyrr]+	8	0.308	-0.077	0.207	0.179	0.284	0.087	0.268	0.179	0.281	0.089
[BzmIm]+	1	0.768	0.071	0.768	0.343	0.768	0.168	0.768	0.349	0.768	0.172
[BzmPyrr]+	1	0.658	0.133	0.658	0.343	0.658	0.168	0.658	0.349	0.658	0.172
[BzPy]+	1	0.865	0.120	0.865	0.343	0.865	0.168	0.865	0.349	0.865	0.172
[C1,9(M2iPAm)2]2+	1	0.798	0.142	0.798	0.343	0.798	0.168	0.798	0.349	0.798	0.172
[C3MPyrr]+	1	0.908	0.172	0.908	0.343	0.908	0.168	0.908	0.349	0.908	0.172
[C5MPyrr]+	1	0.727	0.113	0.727	0.343	0.727	0.168	0.727	0.349	0.727	0.172
[ChxmIm]+	1	0.754	0.131	0.754	0.343	0.754	0.168	0.754	0.349	0.754	0.172
[ChxmPyrr]+	1	0.697	0.120	0.697	0.343	0.697	0.168	0.697	0.349	0.697	0.172
[ChxPy]+	1	0.703	0.121	0.703	0.343	0.703	0.168	0.703	0.349	0.703	0.172
[CNMeM2iPam]+	1	1.512	0.126	1.512	0.343	1.512	0.168	1.512	0.349	1.512	0.172
[CNPrMIm]+	1	0.782	-0.191	1.023	0.390	1.015	0.191	1.071	0.396	1.021	0.195
[D2MIM]+	1	0.040	-0.128	0.040	0.343	0.040	0.168	0.000	0.349	0.000	0.172
[DM3AM]+	1	0.329	-0.126	0.329	0.343	0.329	0.168	0.329	0.349	0.329	0.172
[DMPyrr]+	1	0.419	-0.124	0.419	0.343	0.419	0.168	0.419	0.349	0.419	0.172
[E3S]+	1	2.716	-0.482	2.716	0.343	2.716	0.168	2.716	0.349	2.716	0.172
[EMIM]+	10	0.428	-0.081	0.338	0.183	0.434	0.094	0.373	0.185	0.428	0.096
[EtOHM2iPAm]+	1	0.617	0.138	0.617	0.343	0.617	0.168	0.617	0.349	0.617	0.172
[EtOHMIm]+	3	0.517	-0.084	0.845	0.224	0.717	0.112	0.879	0.227	0.716	0.115
[HexM3Am]+	1	0.945	-0.095	0.287	0.343	0.945	0.168	0.287	0.349	0.945	0.172

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[HM2iPam]+	1	0.582	0.115	0.582	0.343	0.582	0.168	0.582	0.349	0.582	0.172
[HMIM]+	3	0.348	-0.077	0.304	0.228	0.330	0.112	0.328	0.231	0.330	0.114
[HMPyrr]+	1	0.560	-0.144	0.560	0.343	0.560	0.168	0.560	0.349	0.560	0.172
[HxomMIm]+	1	1.080	-0.353	0.407	0.343	0.407	0.168	0.407	0.349	0.407	0.172
[M2EIm]+	1	0.443	-0.198	0.360	0.343	0.360	0.168	0.360	0.349	0.360	0.172
[M3BAm]+	1	0.356	-0.189	0.356	0.343	0.356	0.168	0.356	0.349	0.356	0.172
[MDIm]+	1	0.395	-0.269	0.214	0.420	0.280	0.206	0.254	0.427	0.278	0.210
[MeoeMIm]+	1	0.653	0.127	0.818	0.343	0.818	0.168	0.818	0.349	0.818	0.172
[MeoeMMorp]+	2	0.995	-0.092	0.972	0.258	0.978	0.126	0.988	0.262	0.980	0.129
[MeoeMPip]+	2	0.660	-0.093	0.656	0.258	0.663	0.126	0.673	0.262	0.664	0.129
[MeoeMPyrr]+	1	0.691	-0.122	0.672	0.385	0.685	0.189	0.705	0.391	0.688	0.193
[MOIm]+	3	-0.150	0.117	0.508	0.269	0.088	0.162	0.603	0.268	0.080	0.166
[N112N113]+	1	1.160	0.151	1.160	0.343	1.160	0.168	1.160	0.349	1.160	0.172
[N112N114]+	1	0.779	0.139	0.779	0.343	0.779	0.168	0.779	0.349	0.779	0.172
[N112O2N113]+	1	0.748	0.113	0.748	0.343	0.748	0.168	0.748	0.349	0.748	0.172
[N112O2N114]+	1	0.584	0.149	0.584	0.343	0.584	0.168	0.584	0.349	0.584	0.172
[N2,2,2,8]+	1	0.294	0.095	-0.014	0.517	0.063	0.253	0.047	0.525	0.060	0.258
[O4AM]+	1	-0.212	-0.144	-0.212	0.343	-0.212	0.168	-0.212	0.349	-0.212	0.172
[OM3AM]+	1	0.569	-0.118	0.569	0.343	0.569	0.168	0.569	0.349	0.569	0.172
[Ompyrr]+	1	0.520	-0.096	0.520	0.343	0.520	0.168	0.520	0.349	0.520	0.172
[PDMIM]+	2	0.568	-0.267	0.715	0.267	1.119	0.215	0.783	0.268	1.110	0.219
[PeMPyrr]+	1	0.727	-0.113	0.727	0.343	0.727	0.168	0.727	0.349	0.727	0.172
[PM2iPAm]+	1	0.723	0.117	0.723	0.343	0.723	0.168	0.723	0.349	0.723	0.172
[PMPip]+	1	0.342	-0.120	0.352	0.343	0.352	0.168	0.352	0.349	0.352	0.172
[PMPyrr]+	1	0.908	-0.172	0.908	0.343	0.908	0.168	0.908	0.349	0.908	0.172
[sec-BMIm]+	1	0.740	0.093	0.740	0.343	0.740	0.168	0.740	0.349	0.740	0.172
[tert-BMIm]+	1	0.796	0.097	0.796	0.343	0.796	0.168	0.796	0.349	0.796	0.172

Table D.25: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter a for log P.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[(Hexom)2Im]+	1	-1.419	-0.269	-1.441	0.507	-1.441	0.227	-1.441	0.510	-1.441	0.228
[(Meo)2Im]+	1	-1.120	-0.192	-1.124	0.507	-1.124	0.227	-1.124	0.510	-1.124	0.228
[3-MBPy]+	2	-1.197	-0.300	-1.241	0.520	-1.473	0.233	-1.227	0.520	-1.456	0.235
[AllMIm]+	2	-1.365	0.115	-1.467	0.384	-1.399	0.172	-1.468	0.385	-1.399	0.173
[B3EP]+	1	-3.190	0.000	-3.416	0.766	-3.330	0.345	-3.418	0.770	-3.330	0.347
[BMIm]+	15	-1.382	-0.089	-0.937	0.252	-1.246	0.116	-0.944	0.245	-1.251	0.117
[BMMOR]+	1	-1.223	0.000	-2.523	0.637	-2.602	0.279	-2.530	0.624	-2.603	0.281
[BMPip]+	1	-1.108	-0.117	-1.165	0.507	-1.165	0.227	-1.165	0.510	-1.165	0.228
[BMPy]+	2	-1.246	-0.161	-0.985	0.465	-0.878	0.161	-1.002	0.344	-0.879	0.162
[BMPyrr]+	8	-1.276	-0.094	-1.365	0.264	-1.402	0.117	-1.364	0.261	-1.398	0.118
[BzmIm]+	1	-1.284	0.119	-1.284	0.507	-1.284	0.227	-1.284	0.510	-1.284	0.228
[BzmPyrr]+	1	-1.275	0.174	-1.275	0.507	-1.275	0.227	-1.275	0.510	-1.275	0.228
[BzPy]+	1	-1.143	0.181	-1.143	0.507	-1.143	0.227	-1.143	0.510	-1.143	0.228
[C1,9(M2iPAm)2]2+	1	-1.034	0.190	-1.034	0.507	-1.034	0.227	-1.034	0.510	-1.034	0.228
[C3MPyrr]+	1	-1.015	0.239	-1.015	0.507	-1.015	0.227	-1.015	0.510	-1.015	0.228
[C5MPyrr]+	1	-1.107	0.212	-1.107	0.507	-1.107	0.227	-1.107	0.510	-1.107	0.228
[ChxmIm]+	1	-0.851	0.180	-0.851	0.507	-0.851	0.227	-0.851	0.510	-0.851	0.228
[ChxmPyrr]+	1	-1.157	0.162	-1.157	0.507	-1.157	0.227	-1.157	0.510	-1.157	0.228
[ChxPy]+	1	-1.047	0.166	-1.047	0.507	-1.047	0.227	-1.047	0.510	-1.047	0.228
[CNMeM2iPam]+	1	-0.459	0.198	-0.459	0.507	-0.459	0.227	-0.459	0.510	-0.459	0.228
[CNPrMIm]+	1	-1.167	-0.255	-1.381	0.576	-1.245	0.258	-1.383	0.578	-1.245	0.260
[D2MIM]+	1	-1.620	-0.176	-1.620	0.507	-1.620	0.227	-1.620	0.510	-1.620	0.228
[DM3AM]+	1	-1.458	-0.175	-1.458	0.507	-1.458	0.227	-1.458	0.510	-1.458	0.228
[DMPyrr]+	1	-1.467	-0.197	-1.467	0.507	-1.467	0.227	-1.467	0.510	-1.467	0.228
[E3S]+	1	-1.550	-0.318	1.350	0.507	1.350	0.227	1.350	0.510	1.350	0.228
[EMIM]+	10	-1.294	-0.098	-1.519	0.271	-1.433	0.127	-1.521	0.270	-1.433	0.128
[EtOHM2iPAm]+	1	-0.850	0.178	-0.850	0.507	-0.850	0.227	-0.850	0.510	-0.850	0.228
[EtOHMIm]+	3	-1.026	-0.097	-1.045	0.331	-0.956	0.152	-1.047	0.332	-0.957	0.153
[HexM3Am]+	1	0.987	-0.107	-1.383	0.507	0.987	0.227	-1.383	0.510	0.987	0.228

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[HM2iPam]+	1	-1.194	0.183	-1.194	0.507	-1.194	0.227	-1.194	0.510	-1.194	0.228
[HMIM]+	3	-1.275	-0.087	-1.440	0.336	-1.423	0.150	-1.440	0.338	-1.422	0.152
[HMPyrr]+	1	-1.301	-0.275	-1.301	0.507	-1.301	0.227	-1.301	0.510	-1.301	0.228
[HxomMIm]+	1	-1.351	-0.269	-1.478	0.507	-1.478	0.227	-1.478	0.510	-1.478	0.228
[M2EIm]+	1	-1.681	-0.237	-1.906	0.507	-1.906	0.227	-1.906	0.510	-1.906	0.228
[M3BAm]+	1	-1.262	-0.249	-1.262	0.507	-1.262	0.227	-1.262	0.510	-1.262	0.228
[MDIm]+	1	-1.611	-0.219	-1.724	0.621	-1.702	0.278	-1.725	0.623	-1.701	0.280
[MeoeMIm]+	1	-1.289	0.173	-1.289	0.507	-1.289	0.227	-1.289	0.510	-1.289	0.228
[MeoeMMorp]+	2	-1.058	-0.099	-1.163	0.381	-1.149	0.170	-1.163	0.383	-1.149	0.172
[MeoeMPip]+	2	-1.094	-0.112	-1.177	0.381	-1.163	0.170	-1.177	0.383	-1.163	0.172
[MeoeMPyrr]+	1	-1.140	-0.132	-1.268	0.568	-1.239	0.254	-1.268	0.571	-1.239	0.256
[MOIm]+	3	-1.641	0.126	-1.842	0.398	-1.153	0.219	-1.845	0.392	-1.156	0.220
[N112N113]+	1	-0.335	0.182	-0.335	0.507	-0.335	0.227	-0.335	0.510	-0.335	0.228
[N112N114]+	1	0.712	0.182	0.712	0.507	0.712	0.227	0.712	0.510	0.712	0.228
[N112O2N113]+	1	-0.945	0.184	-0.945	0.507	-0.945	0.227	-0.945	0.510	-0.945	0.228
[N112O2N114]+	1	-1.037	0.200	-1.037	0.507	-1.037	0.227	-1.037	0.510	-1.037	0.228
[N2,2,2,8]+	1	-1.339	0.119	-1.517	0.764	-1.554	0.341	-1.516	0.766	-1.550	0.344
[O4AM]+	1	-1.756	-0.240	-1.756	0.507	-1.756	0.227	-1.756	0.510	-1.756	0.228
[OM3AM]+	1	-1.419	-0.164	-1.419	0.507	-1.419	0.227	-1.419	0.510	-1.419	0.228
[Ompyrr]+	1	-1.460	-0.203	-1.460	0.507	-1.460	0.227	-1.460	0.510	-1.460	0.228
[PDMIM]+	2	-0.238	-0.294	-1.147	0.394	0.394	0.289	-1.150	0.392	0.392	0.292
[PeMPyrr]+	1	-1.107	-0.212	-1.107	0.507	-1.107	0.227	-1.107	0.510	-1.107	0.228
[PM2iPAm]+	1	-1.061	0.178	-1.061	0.507	-1.061	0.227	-1.061	0.510	-1.061	0.228
[PMPip]+	1	-1.259	-0.122	-1.263	0.507	-1.263	0.227	-1.263	0.510	-1.263	0.228
[PMPyrr]+	1	-1.015	-0.239	-1.015	0.507	-1.015	0.227	-1.015	0.510	-1.015	0.228
[sec-BMIm]+	1	-1.119	0.145	-1.119	0.507	-1.119	0.227	-1.119	0.510	-1.119	0.228
[tert-BMIm]+	1	-0.926	0.151	-0.926	0.507	-0.926	0.227	-0.926	0.510	-0.926	0.228

Table D.26: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter b for log P.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[(Hexom)2Im]+	1	-4.748	-0.290	-4.808	0.696	-4.808	0.610	-4.808	0.712	-4.808	0.613
[(Meo)2Im]+	1	-3.781	-0.132	-3.776	0.696	-3.776	0.610	-3.776	0.712	-3.776	0.613
[3-MBPy]+	2	-4.970	-0.279	-4.824	0.714	-4.918	0.628	-4.993	0.726	-4.918	0.631
[AllMIm]+	2	-4.282	0.103	-4.304	0.527	-4.348	0.462	-4.360	0.538	-4.348	0.464
[B3EP]+	1	-4.153	0.000	-4.400	1.052	-4.541	0.928	-4.492	1.075	-4.541	0.932
[BMIm]+	15	-4.337	-0.087	-4.040	0.346	-4.126	0.312	-4.217	0.343	-4.126	0.313
[BMMOR]+	1	-4.414	0.000	-8.088	0.874	-8.466	0.752	-8.495	0.871	-8.466	0.755
[BMPip]+	1	-4.452	-0.138	-4.385	0.696	-4.385	0.610	-4.385	0.712	-4.385	0.613
[BMPy]+	2	-4.417	-0.138	-2.460	0.638	-3.394	0.432	-3.359	0.481	-3.394	0.434
[BMPyrr]+	8	-4.474	-0.081	-5.166	0.363	-5.278	0.315	-5.310	0.365	-5.278	0.316
[BzmIm]+	1	-4.378	0.077	-4.378	0.696	-4.378	0.610	-4.378	0.712	-4.378	0.613
[BzmPyrr]+	1	-4.401	0.142	-4.401	0.696	-4.401	0.610	-4.401	0.712	-4.401	0.613
[BzPy]+	1	-4.432	0.110	-4.432	0.696	-4.432	0.610	-4.432	0.712	-4.432	0.613
[C1,9(M2iPAm)2]2+	1	-4.438	0.156	-4.438	0.696	-4.438	0.610	-4.438	0.712	-4.438	0.613
[C3MPyrr]+	1	-4.691	0.149	-4.691	0.696	-4.691	0.610	-4.691	0.712	-4.691	0.613
[C5MPyrr]+	1	-4.622	0.116	-4.622	0.696	-4.622	0.610	-4.622	0.712	-4.622	0.613
[ChxmIm]+	1	-4.618	0.124	-4.618	0.696	-4.618	0.610	-4.618	0.712	-4.618	0.613
[ChxmPyrr]+	1	-4.687	0.111	-4.687	0.696	-4.687	0.610	-4.687	0.712	-4.687	0.613
[ChxPy]+	1	-4.535	0.114	-4.535	0.696	-4.535	0.610	-4.535	0.712	-4.535	0.613
[CNMeM2iPam]+	1	-4.191	0.120	-4.191	0.696	-4.191	0.610	-4.191	0.712	-4.191	0.613
[CNPrMIm]+	1	-4.055	-0.201	-4.096	0.791	-4.184	0.694	-4.210	0.807	-4.184	0.697
[D2MIM]+	1	-4.667	-0.132	-4.667	0.696	-4.667	0.610	-4.667	0.712	-4.667	0.613
[DM3AM]+	1	-4.550	-0.120	-4.550	0.696	-4.550	0.610	-4.550	0.712	-4.550	0.613
[DMPyrr]+	1	-4.859	-0.129	-4.859	0.696	-4.859	0.610	-4.859	0.712	-4.859	0.613
[E3S]+	1	-5.274	-0.343	-5.274	0.696	-5.274	0.610	-5.274	0.712	-5.274	0.613
[EMIM]+	10	-4.209	-0.091	-4.096	0.372	-4.237	0.342	-4.188	0.377	-4.237	0.344
[EtOHM2iPAm]+	1	-3.356	0.123	-3.356	0.696	-3.356	0.610	-3.356	0.712	-3.356	0.613
[EtOHMIm]+	3	-3.493	-0.095	-3.508	0.455	-3.341	0.408	-3.583	0.463	-3.341	0.410
[HexM3Am]+	1	-4.526	-0.109	-4.265	0.696	-4.526	0.610	-4.265	0.712	-4.526	0.613

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[HM2iPam]+	1	-4.631	0.118	-4.631	0.696	-4.631	0.610	-4.631	0.712	-4.631	0.613
[HMIM]+	3	-4.426	-0.084	-4.512	0.462	-4.552	0.405	-4.567	0.472	-4.552	0.407
[HMPyrr]+	1	-4.501	-0.159	-4.501	0.696	-4.501	0.610	-4.501	0.712	-4.501	0.613
[HxomMIm]+	1	-4.718	-0.290	4.320	0.696	4.320	0.610	4.320	0.712	4.320	0.613
[M2EIm]+	1	-4.024	-0.182	-3.805	0.696	-3.805	0.610	-3.805	0.712	-3.805	0.613
[M3BAm]+	1	-4.400	-0.244	-4.400	0.696	-4.400	0.610	-4.400	0.712	-4.400	0.613
[MDIm]+	1	-4.546	-0.253	-4.749	0.853	-4.847	0.748	-4.846	0.871	-4.847	0.751
[MeoeMIm]+	1	-4.263	0.124	-4.263	0.696	-4.263	0.610	-4.263	0.712	-4.263	0.613
[MeoeMMorp]+	2	-4.381	-0.097	-4.532	0.523	-4.544	0.458	-4.565	0.534	-4.544	0.460
[MeoeMPip]+	2	-4.665	-0.103	-4.792	0.523	-4.803	0.458	-4.825	0.534	-4.803	0.460
[MeoeMPyrr]+	1	-4.694	-0.138	-4.941	0.781	-4.964	0.684	-5.008	0.798	-4.964	0.687
[MOIm]+	3	-3.980	0.132	-4.551	0.546	-3.595	0.588	-4.772	0.548	-3.595	0.591
[N112N113]+	1	-3.910	0.151	-3.910	0.696	-3.910	0.610	-3.910	0.712	-3.910	0.613
[N112N114]+	1	-4.181	0.124	-4.181	0.696	-4.181	0.610	-4.181	0.712	-4.181	0.613
[N112O2N113]+	1	-4.542	0.135	-4.542	0.696	-4.542	0.610	-4.542	0.712	-4.542	0.613
[N112O2N114]+	1	-4.475	0.131	-4.475	0.696	-4.475	0.610	-4.475	0.712	-4.475	0.613
[N2,2,2,8]+	1	-4.769	0.093	-5.372	1.049	-5.484	0.919	-5.516	1.071	-5.484	0.922
[O4AM]+	1	-4.739	-0.139	-4.739	0.696	-4.739	0.610	-4.739	0.712	-4.739	0.613
[OM3AM]+	1	-4.677	-0.115	-4.677	0.696	-4.677	0.610	-4.677	0.712	-4.677	0.613
[Ompyrr]+	1	-4.696	-0.116	-4.696	0.696	-4.696	0.610	-4.696	0.712	-4.696	0.613
[PDMIM]+	2	-4.006	-0.266	-3.735	0.541	-3.594	0.779	-3.897	0.548	-3.594	0.782
[PeMPyrr]+	1	-4.622	-0.116	-4.622	0.696	-4.622	0.610	-4.622	0.712	-4.622	0.613
[PM2iPAm]+	1	-4.594	0.109	-4.594	0.696	-4.594	0.610	-4.594	0.712	-4.594	0.613
[PMPip]+	1	-4.296	-0.152	-4.290	0.696	-4.290	0.610	-4.290	0.712	-4.290	0.613
[PMPyrr]+	1	-4.691	-0.149	-4.691	0.696	-4.691	0.610	-4.691	0.712	-4.691	0.613
[sec-BMIm]+	1	-4.496	0.091	-4.496	0.696	-4.496	0.610	-4.496	0.712	-4.496	0.613
[tert-BMIm]+	1	-4.526	0.095	-4.526	0.696	-4.526	0.610	-4.526	0.712	-4.526	0.613

Table D.27: Comparison of cation literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter v for log P.

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		v (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)
[(Hexom)2Im]+	1	3.787	-0.150	3.750	0.352	3.750	0.339	3.750	0.354	3.750	0.340
[(Meo)2Im]+	1	3.056	-0.119	3.055	0.352	3.055	0.339	3.055	0.354	3.055	0.340
[3-MBPy]+	2	3.435	-0.132	3.512	0.361	3.487	0.349	3.523	0.361	3.487	0.350
[AllMIm]+	2	3.102	0.025	3.065	0.267	3.043	0.257	3.068	0.267	3.043	0.258
[B3EP]+	1	3.539	0.000	3.605	0.532	3.541	0.516	3.611	0.534	3.541	0.518
[BMIm]+	15	3.390	-0.033	3.470	0.175	3.442	0.173	3.481	0.170	3.442	0.174
[BMMOR]+	1	3.130	0.000	3.548	0.442	3.538	0.418	3.573	0.433	3.538	0.419
[BMPip]+	1	3.390	-0.070	3.422	0.352	3.422	0.339	3.422	0.354	3.422	0.340
[BMPy]+	2	3.433	-0.073	3.426	0.323	3.446	0.240	3.480	0.239	3.446	0.241
[BMPyrr]+	8	3.330	-0.046	3.485	0.184	3.463	0.175	3.494	0.181	3.463	0.176
[BzmIm]+	1	3.310	0.070	3.310	0.352	3.310	0.339	3.310	0.354	3.310	0.340
[BzmPyrr]+	1	3.449	0.096	3.449	0.352	3.449	0.339	3.449	0.354	3.449	0.340
[BzPy]+	1	3.485	0.083	3.485	0.352	3.485	0.339	3.485	0.354	3.485	0.340
[C1,9(M2iPAm)2]2+	1	3.429	0.110	3.429	0.352	3.429	0.339	3.429	0.354	3.429	0.340
[C3MPyrr]+	1	3.446	0.143	3.446	0.352	3.446	0.339	3.446	0.354	3.446	0.340
[C5MPyrr]+	1	3.630	0.109	3.630	0.352	3.630	0.339	3.630	0.354	3.630	0.340
[ChxmIm]+	1	3.653	0.102	3.653	0.352	3.653	0.339	3.653	0.354	3.653	0.340
[ChxmPyrr]+	1	3.709	0.092	3.709	0.352	3.709	0.339	3.709	0.354	3.709	0.340
[ChxPy]+	1	3.681	0.095	3.681	0.352	3.681	0.339	3.681	0.354	3.681	0.340
[CNMeM2iPam]+	1	3.529	0.117	3.529	0.352	3.529	0.339	3.529	0.354	3.529	0.340
[CNPrMIm]+	1	3.301	-0.145	3.395	0.400	3.353	0.386	3.402	0.401	3.353	0.387
[D2MIM]+	1	4.034	-0.132	4.034	0.352	4.034	0.339	4.034	0.354	4.034	0.340
[DM3AM]+	1	3.816	-0.108	3.816	0.352	3.816	0.339	3.816	0.354	3.816	0.340
[DMPyrr]+	1	3.824	-0.108	3.824	0.352	3.824	0.339	3.824	0.354	3.824	0.340
[E3S]+	1	3.242	-0.156	3.242	0.352	3.242	0.339	3.242	0.354	3.242	0.340
[EMIM]+	10	3.163	-0.039	3.228	0.188	3.164	0.190	3.234	0.187	3.164	0.191
[EtOHM2iPAm]+	1	3.270	0.109	3.270	0.352	3.270	0.339	3.270	0.354	3.270	0.340
[EtOHMIm]+	3	2.931	-0.055	3.003	0.230	3.003	0.227	3.007	0.230	3.003	0.228
[HexM3Am]+	1	2.957	-0.070	3.513	0.352	2.957	0.339	3.513	0.354	2.957	0.340

Cation	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		v (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)
[HM2iPam]+	1	3.640	0.104	3.640	0.352	3.640	0.339	3.640	0.354	3.640	0.340
[HMIM]+	3	3.585	-0.033	3.573	0.234	3.555	0.225	3.576	0.234	3.555	0.226
[HMPyrr]+	1	3.673	-0.128	3.673	0.352	3.673	0.339	3.673	0.354	3.673	0.340
[HxomMIm]+	1	3.646	-0.150	3.510	0.352	3.510	0.339	3.510	0.354	3.510	0.340
[M2EIm]+	1	3.174	-0.109	3.177	0.352	3.177	0.339	3.177	0.354	3.177	0.340
[M3BAm]+	1	3.209	-0.061	3.209	0.352	3.209	0.339	3.209	0.354	3.209	0.340
[MDIm]+	1	3.587	-0.146	3.709	0.431	3.674	0.416	3.715	0.433	3.674	0.417
[MeoeMIm]+	1	3.116	0.104	3.116	0.352	3.116	0.339	3.116	0.354	3.116	0.340
[MeoeMMorp]+	2	3.168	-0.067	3.110	0.264	3.101	0.255	3.112	0.266	3.101	0.256
[MeoeMPip]+	2	3.360	-0.068	3.335	0.264	3.326	0.255	3.337	0.266	3.326	0.256
[MeoeMPyrr]+	1	3.324	-0.086	3.329	0.395	3.310	0.380	3.333	0.396	3.310	0.382
[MOIm]+	3	3.872	0.051	4.030	0.276	3.962	0.327	4.043	0.272	3.962	0.328
[N112N113]+	1	3.643	0.106	3.643	0.352	3.643	0.339	3.643	0.354	3.643	0.340
[N112N114]+	1	3.291	0.108	3.291	0.352	3.291	0.339	3.291	0.354	3.291	0.340
[N112O2N113]+	1	3.605	0.107	3.605	0.352	3.605	0.339	3.605	0.354	3.605	0.340
[N112O2N114]+	1	3.508	0.114	3.508	0.352	3.508	0.339	3.508	0.354	3.508	0.340
[N2,2,2,8]+	1	3.663	0.075	3.802	0.531	3.780	0.510	3.811	0.532	3.780	0.513
[O4AM]+	1	3.825	-0.174	3.825	0.352	3.825	0.339	3.825	0.354	3.825	0.340
[OM3AM]+	1	3.711	-0.103	3.711	0.352	3.711	0.339	3.711	0.354	3.711	0.340
[Ompyrr]+	1	3.815	-0.103	3.815	0.352	3.815	0.339	3.815	0.354	3.815	0.340
[PDMIM]+	2	2.907	-0.159	3.528	0.274	3.079	0.433	3.538	0.272	3.079	0.435
[PeMPyrr]+	1	3.630	-0.109	3.630	0.352	3.630	0.339	3.630	0.354	3.630	0.340
[PM2iPAm]+	1	3.388	0.094	3.388	0.352	3.388	0.339	3.388	0.354	3.388	0.340
[PMPip]+	1	3.409	-0.082	3.401	0.352	3.401	0.339	3.401	0.354	3.401	0.340
[PMPyrr]+	1	3.446	-0.143	3.446	0.352	3.446	0.339	3.446	0.354	3.446	0.340
[sec-BMIm]+	1	3.436	0.084	3.436	0.352	3.436	0.339	3.436	0.354	3.436	0.340
[tert-BMIm]+	1	3.395	0.087	3.395	0.352	3.395	0.339	3.395	0.354	3.395	0.340

Table D.28: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter c for log K.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[+CS]-	1	0.157	0.000	0.086	0.138	0.317	0.085	0.089	0.139	0.318	0.086
[BETI]-	1	0.068	0.064	0.052	0.134	-0.046	0.079	0.050	0.135	-0.045	0.080
[BF4]-	6	-0.192	0.028	-0.078	0.068	-0.292	0.049	-0.085	0.068	-0.306	0.049
[DCA]-	12	-0.372	0.051	-0.373	0.065	-0.357	0.038	-0.373	0.065	-0.357	0.038
[DEP]-	2	0.093	0.113	0.186	0.137	0.167	0.080	0.186	0.138	0.167	0.082
[EtSO4]-	1	-0.173	0.066	-0.069	0.137	-0.088	0.080	-0.069	0.138	-0.088	0.082
[FAP]-	10	0.229	0.030	0.298	0.061	0.271	0.036	0.299	0.061	0.272	0.036
[FSI]-	2	-0.147	0.047	-0.171	0.136	-0.207	0.079	-0.171	0.137	-0.207	0.080
[L-Lact]-	1	0.197	0.000	0.096	0.138	0.327	0.085	0.099	0.139	0.328	0.086
[MeSO3]-	2	-0.827	0.094	-0.585	0.099	-0.644	0.058	-0.586	0.100	-0.643	0.059
[OS]-	3	0.057	0.063	0.195	0.084	0.262	0.060	0.195	0.085	0.262	0.061
[PF6]-	4	-0.016	0.029	-0.021	0.079	-0.088	0.055	-0.001	0.080	-0.066	0.055
[SCN]-	3	-0.566	0.044	-0.520	0.099	-0.587	0.058	-0.521	0.100	-0.586	0.059
[TCB]-	4	0.048	0.044	0.077	0.085	0.053	0.050	0.077	0.086	0.053	0.050
[TCM]-	6	-0.098	0.072	-0.194	0.085	-0.271	0.050	-0.196	0.086	-0.272	0.051
[TDI]-	2	-0.046	0.000	0.035	0.116	-0.054	0.068	0.033	0.117	-0.053	0.069
[TFA]-	1	-0.295	0.059	-0.212	0.137	#N/A	#N/A	-0.212	0.138	#N/A	#N/A
[Trif]-	3	-0.275	0.039	-0.201	0.094	-0.272	0.055	-0.202	0.095	-0.271	0.056

Table D.29: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter e for log K.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[+CS]-	1	0.058	0.000	0.324	0.204	0.075	0.081	0.343	0.205	0.090	0.088
[BETI]-	1	-0.334	0.121	0.158	0.199	0.117	0.075	0.186	0.200	0.149	0.081
[BF4]-	6	0.227	0.067	0.176	0.101	0.238	0.046	0.195	0.101	0.256	0.050
[DCA]-	12	0.345	0.095	0.441	0.096	0.375	0.036	0.461	0.097	0.395	0.039
[DEP]-	2	0.107	0.181	0.148	0.204	0.133	0.077	0.182	0.205	0.169	0.083
[EtSO4]-	1	-0.072	0.145	-0.047	0.204	-0.062	0.077	-0.013	0.205	-0.026	0.083

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[FAP]-	10	-0.049	0.053	-0.006	0.090	-0.032	0.034	0.002	0.091	-0.022	0.037
[FSI]-	2	0.134	0.058	0.266	0.202	0.237	0.075	0.284	0.203	0.257	0.082
[L-Lact]-	1	0.113	0.000	0.379	0.204	0.130	0.081	0.398	0.205	0.145	0.088
[MeSO3]-	2	0.463	0.135	0.422	0.148	0.394	0.056	0.452	0.148	0.428	0.060
[OS]-	3	-0.126	0.091	0.103	0.125	-0.074	0.057	0.130	0.126	-0.051	0.062
[PF6]-	4	-0.158	0.066	0.292	0.118	-0.067	0.052	0.340	0.118	-0.014	0.057
[SCN]-	3	0.431	0.077	0.723	0.148	0.688	0.056	0.746	0.148	0.714	0.060
[TCB]-	4	-0.009	0.079	0.101	0.127	0.081	0.048	0.094	0.127	0.076	0.051
[TCM]-	6	0.094	0.101	0.230	0.127	0.211	0.048	0.227	0.127	0.211	0.052
[TDI]-	2	0.013	0.000	0.055	0.172	0.016	0.065	0.123	0.173	0.087	0.070
[TFA]-	1	-0.186	0.249	-0.047	0.204	#N/A	#N/A	-0.013	0.205	#N/A	#N/A
[Trif]-	3	0.035	0.083	0.150	0.140	0.115	0.053	0.175	0.140	0.142	0.057

Table D.30: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter s for log K.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[+CS]-	1	0.229	0.000	0.312	0.294	0.345	0.098	0.318	0.296	0.345	0.098
[BETI]-	1	0.217	0.115	-0.178	0.286	0.020	0.090	-0.179	0.289	0.020	0.090
[BF4]-	6	0.343	0.072	0.397	0.144	0.284	0.056	0.396	0.146	0.284	0.056
[DCA]-	12	0.476	0.092	0.257	0.138	0.291	0.044	0.258	0.139	0.291	0.044
[DEP]-	2	-0.068	0.184	-0.001	0.292	-0.115	0.092	0.000	0.295	-0.115	0.092
[EtSO4]-	1	0.239	0.161	0.319	0.292	0.205	0.092	0.320	0.295	0.205	0.092
[FAP]-	10	-0.114	0.057	-0.135	0.130	-0.123	0.041	-0.136	0.131	-0.123	0.041
[FSI]-	2	0.295	0.058	0.175	0.290	0.228	0.091	0.175	0.293	0.228	0.091
[L-Lact]-	1	0.124	0.000	0.207	0.294	0.240	0.098	0.213	0.296	0.240	0.098
[MeSO3]-	2	0.417	0.133	0.317	0.212	0.359	0.067	0.316	0.214	0.359	0.067
[OS]-	3	-0.077	0.099	-0.568	0.180	-0.133	0.069	-0.567	0.181	-0.133	0.069
[PF6]-	4	0.529	0.071	-0.155	0.169	0.474	0.063	-0.167	0.170	0.474	0.063
[SCN]-	3	0.534	0.089	0.144	0.212	0.270	0.067	0.143	0.214	0.270	0.067

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[TCB]-	4	0.345	0.088	0.339	0.182	0.317	0.057	0.339	0.183	0.317	0.057
[TCM]-	6	0.290	0.101	0.137	0.182	0.216	0.058	0.136	0.183	0.216	0.058
[TDI]-	2	0.088	0.000	-0.126	0.247	0.052	0.078	-0.127	0.249	0.052	0.078
[TFA]-	1	0.545	0.368	0.456	0.292	#N/A	#N/A	0.457	0.295	#N/A	#N/A
[Trif]-	3	0.323	0.093	0.087	0.201	0.223	0.063	0.086	0.202	0.223	0.063

Table D.31: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter a for log K.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[+CS]-	1	4.084	0.000	5.578	0.562	4.468	0.141	5.578	0.562	4.468	0.141
[BETI]-	1	-0.196	0.158	-0.671	0.548	-0.310	0.130	-0.671	0.548	-0.310	0.130
[BF4]-	6	0.978	0.090	1.108	0.276	0.963	0.080	1.108	0.276	0.963	0.080
[DCA]-	12	2.270	0.124	2.436	0.264	2.257	0.063	2.436	0.264	2.257	0.063
[DEP]-	2	5.071	0.240	5.166	0.559	4.984	0.133	5.166	0.559	4.984	0.133
[EtSO4]-	1	2.931	0.202	3.061	0.559	2.879	0.133	3.061	0.559	2.879	0.133
[FAP]-	10	-1.277	0.064	-1.277	0.248	-1.314	0.059	-1.277	0.248	-1.314	0.059
[FSI]-	2	0.133	0.076	-0.040	0.555	0.000	0.130	-0.040	0.555	0.000	0.130
[L-Lact]-	1	4.370	0.000	5.864	0.562	4.754	0.141	5.864	0.562	4.754	0.141
[MeSO3]-	2	4.083	0.216	4.047	0.405	4.136	0.096	4.047	0.405	4.136	0.096
[OS]-	3	2.575	0.152	2.722	0.344	2.711	0.099	2.722	0.344	2.711	0.099
[PF6]-	4	0.035	0.083	0.109	0.323	0.175	0.090	0.109	0.323	0.175	0.090
[SCN]-	3	2.806	0.104	2.464	0.406	2.665	0.096	2.464	0.406	2.665	0.096
[TCB]-	4	0.371	0.099	0.310	0.348	0.252	0.082	0.310	0.348	0.252	0.082
[TCM]-	6	1.338	0.129	0.746	0.348	0.879	0.083	0.746	0.348	0.879	0.083
[TDI]-	2	1.132	0.000	0.794	0.472	1.109	0.112	0.794	0.472	1.109	0.112
[TFA]-	1	3.113	0.735	3.196	0.559	#N/A	#N/A	3.196	0.559	#N/A	#N/A
[Trif]-	3	1.709	0.109	1.361	0.384	1.585	0.091	1.361	0.384	1.585	0.091

Table D.32: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter b for log K.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[+CS]-	1	-0.522	0.000	-0.612	0.352	-0.519	0.144	-0.613	0.352	-0.521	0.143
[BETI]-	1	-0.238	0.129	0.313	0.343	0.075	0.133	0.313	0.343	0.075	0.132
[BF4]-	6	-0.287	0.083	-0.465	0.173	-0.329	0.082	-0.465	0.173	-0.328	0.082
[DCA]-	12	-0.198	0.097	-0.117	0.166	-0.138	0.064	-0.111	0.165	-0.133	0.064
[DEP]-	2	-0.774	0.184	-0.865	0.350	-0.765	0.136	-0.863	0.350	-0.672	0.135
[EtSO4]-	1	-0.668	0.189	-0.774	0.350	-0.674	0.136	-0.772	0.350	-0.672	0.135
[FAP]-	10	0.341	0.063	0.479	0.156	0.460	0.060	0.480	0.155	0.461	0.060
[FSI]-	2	-0.021	0.060	0.184	0.348	0.122	0.133	0.187	0.347	0.125	0.133
[L-Lact]-	1	-0.613	0.000	-0.703	0.352	-0.610	0.144	-0.704	0.352	-0.612	0.143
[MeSO3]-	2	-0.280	0.152	-0.212	0.254	-0.281	0.098	-0.211	0.254	-0.280	0.098
[OS]-	3	-0.587	0.126	-0.230	0.216	-0.601	0.101	-0.229	0.215	-0.601	0.101
[PF6]-	4	-0.149	0.085	0.458	0.203	-0.215	0.092	0.458	0.202	-0.215	0.092
[SCN]-	3	-0.272	0.095	0.211	0.254	0.060	0.098	0.212	0.254	0.062	0.098
[TCB]-	4	-0.143	0.093	-0.053	0.218	-0.042	0.084	-0.051	0.218	-0.040	0.084
[TCM]-	6	-0.145	0.117	0.156	0.218	0.060	0.085	0.157	0.218	0.061	0.084
[TDI]-	2	0.013	0.000	0.212	0.296	-0.002	0.115	0.198	0.296	-0.015	0.114
[TFA]-	1	-0.078	0.783	-0.040	0.350	#N/A	#N/A	-0.038	0.350	#N/A	#N/A
[Trif]-	3	-0.175	0.102	0.062	0.240	-0.101	0.093	0.070	0.240	-0.092	0.092

Table D.33: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter l for log K.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		l (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)
[+CS]-	1	0.131	0.000	0.069	0.036	0.121	0.021	0.069	0.036	0.121	0.021
[BETI]-	1	-0.279	0.017	-0.122	0.035	-0.120	0.019	-0.122	0.035	-0.120	0.019
[BF4]-	6	-0.075	0.009	-0.118	0.018	-0.101	0.012	-0.118	0.018	-0.101	0.012
[DCA]-	12	-0.055	0.015	-0.084	0.017	-0.066	0.009	-0.084	0.017	-0.066	0.009
[DEP]-	2	0.061	0.037	0.018	0.036	0.043	0.019	0.018	0.036	0.043	0.019
[EtSO4]-	1	-0.066	0.017	-0.108	0.036	-0.083	0.019	-0.108	0.036	-0.083	0.019

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		l (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)	*l* (ion)	*l* (SD)
[FAP]-	10	-0.039	0.009	-0.052	0.016	-0.043	0.009	-0.052	0.016	-0.043	0.009
[FSI]-	2	0.003	0.014	-0.029	0.035	-0.021	0.019	-0.029	0.035	-0.021	0.019
[L-Lact]-	1	0.003	0.000	-0.059	0.036	-0.007	0.021	-0.059	0.036	-0.007	0.021
[MeSO3]-	2	-0.023	0.023	-0.075	0.026	-0.061	0.014	-0.075	0.026	-0.061	0.014
[OS]-	3	0.108	0.017	0.075	0.022	0.068	0.014	0.075	0.022	0.068	0.014
[PF6]-	4	-0.096	0.010	-0.100	0.021	-0.097	0.013	-0.100	0.021	-0.097	0.013
[SCN]-	3	-0.040	0.013	-0.072	0.026	-0.066	0.014	-0.072	0.026	-0.066	0.014
[TCB]-	4	-0.012	0.013	-0.045	0.022	-0.032	0.012	-0.045	0.022	-0.032	0.012
[TCM]-	6	0.005	0.021	-0.047	0.022	-0.041	0.012	-0.047	0.022	-0.041	0.012
[TDI]-	2	0.049	0.000	0.022	0.030	0.025	0.016	0.022	0.030	0.025	0.016
[TFA]-	1	0.014	0.020	-0.027	0.036	#N/A	#N/A	-0.027	0.036	#N/A	#N/A
[Trif]-	3	-0.002	0.012	-0.040	0.024	-0.035	0.013	-0.040	0.024	-0.035	0.013

Table D.34: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter c for log P.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[+Cs]-	1	-0.049	0.000	0.028	0.140	0.246	0.093	0.031	0.141	0.281	0.091
[BETI]-	1	0.071	0.103	0.258	0.137	0.129	0.086	0.188	0.137	0.079	0.084
[BF4]-	5	-0.084	0.045	0.250	0.079	0.040	0.061	0.268	0.075	0.114	0.060
[DCA]-	11	-0.257	0.087	-0.199	0.066	-0.193	0.042	-0.205	0.066	-0.186	0.041
[DEP]-	2	0.071	0.171	0.152	0.139	0.139	0.088	0.144	0.140	0.134	0.086
[EtSO4]-	1	-0.029	0.099	0.051	0.139	0.038	0.088	0.144	0.140	0.134	0.086
[FAP]-	9	0.198	0.049	0.196	0.062	0.179	0.039	0.130	0.062	0.118	0.038
[FSI]-	2	-0.092	0.086	-0.108	0.138	-0.156	0.087	-0.132	0.139	-0.165	0.085
[L-Lact]-	1	-0.049	0.000	0.028	0.140	0.246	0.093	0.031	0.141	0.281	0.091
[MeSO3]-	2	-0.646	0.158	-0.464	0.101	-0.535	0.064	-0.481	0.101	-0.540	0.062
[OS]-	3	-0.040	0.106	0.197	0.086	0.220	0.066	0.121	0.086	0.180	0.064
[PF6]-	4	0.007	0.047	0.043	0.081	0.001	0.060	0.012	0.081	-0.024	0.059
[SCN]-	3	-0.534	0.091	-0.449	0.101	-0.537	0.064	-0.484	0.101	-0.555	0.062

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		c (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)	*c* (ion)	*c* (SD)
[TCB]-	4	0.072	0.069	0.002	0.087	-0.023	0.055	0.017	0.087	0.000	0.053
[TCM]-	6	-0.079	0.109	-0.326	0.093	-0.442	0.055	-0.378	0.087	-0.451	0.054
[TDI]-	2	-0.043	0.000	0.107	0.118	-0.010	0.075	0.079	0.118	-0.019	0.073
[TFA]-	1	-0.286	0.098	0.001	0.139	#N/A	#N/A	0.015	0.140	#N/A	#N/A
[Trif]-	3	-0.228	0.061	-0.111	0.096	-0.205	0.061	-0.139	0.096	-0.216	0.059

Table D.35: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter e for log P.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		e (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)	*e* (ion)	*e* (SD)
[+Cs]-	1	-0.166	0.000	0.532	0.256	0.155	0.113	0.621	0.263	0.149	0.112
[BETI]-	1	-0.245	0.146	-0.257	0.250	-0.050	0.104	-0.242	0.257	-0.105	0.103
[BF4]-	5	0.129	0.077	-0.192	0.145	0.337	0.074	-0.042	0.141	0.347	0.073
[DCA]-	11	0.164	0.111	0.278	0.121	0.263	0.050	0.343	0.124	0.272	0.050
[DEP]-	2	0.073	0.192	0.099	0.254	0.105	0.106	0.136	0.262	0.091	0.105
[EtSO4]-	1	-0.245	0.171	-0.211	0.254	-0.205	0.106	-0.153	0.262	-0.198	0.105
[FAP]-	9	0.049	0.061	0.092	0.114	0.102	0.047	0.091	0.117	0.073	0.047
[FSI]-	2	-0.038	0.080	-0.048	0.253	0.041	0.104	0.024	0.260	0.051	0.103
[L-Lact]-	1	-0.166	0.000	0.532	0.256	0.155	0.113	0.621	0.263	0.149	0.112
[MeSO3]-	2	0.347	0.164	0.153	0.185	0.259	0.077	0.221	0.190	0.267	0.076
[OS]-	3	-0.043	0.107	0.101	0.158	0.071	0.079	0.201	0.161	0.121	0.079
[PF6]-	4	-0.230	0.077	0.109	0.149	-0.064	0.072	0.226	0.152	0.037	0.072
[SCN]-	3	0.187	0.093	0.065	0.186	0.213	0.077	0.122	0.190	0.204	0.076
[TCB]-	4	-0.075	0.092	-0.076	0.159	-0.039	0.066	0.026	0.163	0.017	0.065
[TCM]-	6	0.056	0.116	0.249	0.170	0.537	0.067	0.442	0.163	0.553	0.066
[TDI]-	2	-0.019	0.000	-0.060	0.216	0.129	0.090	-0.069	0.221	0.053	0.089
[TFA]-	1	-0.697	0.278	-1.441	0.254	#N/A	#N/A	-1.404	0.262	#N/A	#N/A
[Trif]-	3	-0.088	0.096	-0.088	0.176	0.068	0.073	0.000	0.180	0.090	0.072

Table D.36: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter s for log P.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		s (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)	*s* (ion)	*s* (SD)
[+Cs]-	1	0.363	0.000	0.123	0.392	0.456	0.204	0.053	0.397	0.409	0.208
[BETI]-	1	0.038	0.146	-0.224	0.383	-0.345	0.189	-0.298	0.387	-0.332	0.193
[BF4]-	5	0.240	0.090	0.440	0.222	-0.295	0.134	0.305	0.212	-0.286	0.136
[DCA]-	11	0.446	0.120	0.201	0.186	0.209	0.091	0.153	0.187	0.203	0.093
[DEP]-	2	0.006	0.239	0.096	0.389	0.000	0.193	0.061	0.395	0.006	0.197
[EtSO4]-	1	0.129	0.199	0.216	0.389	0.120	0.193	0.181	0.395	0.126	0.197
[FAP]-	9	-0.214	0.071	-0.195	0.174	-0.208	0.085	-0.228	0.176	-0.211	0.087
[FSI]-	2	0.406	0.095	0.610	0.387	0.533	0.189	0.549	0.392	0.536	0.193
[L-Lact]-	1	-0.134	0.000	-0.106	0.392	0.227	0.204	-0.176	0.397	0.180	0.208
[MeSO3]-	2	0.315	0.173	0.399	0.283	0.291	0.139	0.344	0.286	0.300	0.142
[OS]-	3	0.002	0.127	-0.516	0.242	-0.260	0.144	-0.576	0.243	-0.367	0.147
[PF6]-	4	0.417	0.088	-0.278	0.228	0.118	0.131	-0.346	0.228	0.126	0.134
[SCN]-	3	0.644	0.112	0.862	0.285	0.763	0.140	0.794	0.287	0.771	0.143
[TCB]-	4	0.347	0.109	0.528	0.243	0.462	0.119	0.488	0.246	0.464	0.122
[TCM]-	6	0.276	0.128	1.080	0.261	0.814	0.121	0.912	0.246	0.820	0.124
[TDI]-	2	0.104	0.000	-0.074	0.331	-0.189	0.163	-0.147	0.334	-0.178	0.166
[TFA]-	1	0.859	0.443	2.018	0.389	#N/A	#N/A	1.983	0.395	#N/A	#N/A
[Trif]-	3	0.367	0.114	0.238	0.269	0.135	0.132	0.169	0.271	0.144	0.135

Table D.37: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter a for log P.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[+Cs]-	1	5.498	0.000	5.443	0.580	4.505	0.275	5.448	0.580	4.506	0.277
[BETI]-	1	-0.318	0.196	-0.764	0.566	-0.455	0.255	-0.757	0.566	-0.450	0.256
[BF4]-	5	1.108	0.111	0.925	0.328	0.489	0.180	0.932	0.310	0.491	0.181
[DCA]-	11	2.217	0.157	2.423	0.274	2.287	0.123	2.425	0.273	2.287	0.124
[DEP]-	2	5.089	0.297	5.315	0.575	5.229	0.260	5.317	0.577	5.229	0.262
[EtSO4]-	1	2.792	0.248	3.010	0.575	2.924	0.260	3.012	0.577	2.924	0.262

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		a (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)	*a* (ion)	*a* (SD)
[FAP]-	9	-1.344	0.079	-1.215	0.257	-1.244	0.115	-1.215	0.257	-1.244	0.116
[FSI]-	2	0.082	0.118	0.216	0.572	0.253	0.255	0.215	0.572	0.249	0.257
[L-Lact]-	1	1.885	0.000	5.935	0.580	4.997	0.275	5.940	0.580	4.998	0.277
[MeSO3]-	2	3.997	0.275	4.135	0.419	4.247	0.188	4.140	0.418	4.249	0.189
[OS]-	3	2.583	0.204	2.747	0.357	2.611	0.194	2.751	0.356	2.613	0.195
[PF6]-	4	0.131	0.102	0.290	0.337	0.051	0.177	0.294	0.334	0.054	0.178
[SCN]-	3	2.801	0.128	2.456	0.421	2.629	0.188	2.458	0.419	2.629	0.190
[TCB]-	4	0.312	0.123	0.445	0.359	0.423	0.161	0.446	0.359	0.422	0.162
[TCM]-	6	1.223	0.161	2.523	0.385	2.602	0.163	2.530	0.360	2.603	0.164
[TDI]-	2	0.996	0.000	0.546	0.489	0.816	0.220	0.542	0.488	0.810	0.221
[TFA]-	1	2.284	0.893	2.408	0.575	#N/A	#N/A	2.410	0.577	#N/A	#N/A
[Trif]-	3	1.560	0.136	1.434	0.398	1.627	0.178	1.409	0.396	1.599	0.180

Table D.38: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter b for log P.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[+Cs]-	1	-0.568	0.000	-0.767	0.796	-0.666	0.741	-0.614	0.810	-0.666	0.744
[BETI]-	1	0.101	0.157	-0.196	0.777	-0.110	0.685	-0.019	0.790	-0.110	0.688
[BF4]-	5	-0.401	0.101	-1.280	0.451	-0.823	0.485	-0.958	0.433	-0.823	0.487
[DCA]-	11	-0.256	0.120	-0.211	0.377	-0.123	0.331	-0.097	0.381	-0.123	0.332
[DEP]-	2	-0.832	0.224	-0.945	0.789	-0.804	0.700	-0.853	0.806	-0.804	0.702
[EtSO4]-	1	-0.745	0.230	-0.848	0.789	-0.707	0.700	-0.756	0.806	-0.707	0.702
[FAP]-	9	0.449	0.078	0.696	0.353	0.719	0.310	0.763	0.360	0.719	0.312
[FSI]-	2	-0.074	0.092	0.574	0.785	0.686	0.687	0.718	0.800	0.686	0.690
[L-Lact]-	1	-0.554	0.000	-0.753	0.796	-0.652	0.741	-0.600	0.810	-0.652	0.744
[MeSO3]-	2	-0.336	0.183	-0.626	0.575	-0.512	0.506	-0.491	0.585	-0.512	0.508
[OS]-	3	-0.577	0.153	-0.593	0.490	-0.689	0.522	-0.452	0.497	-0.689	0.524
[PF6]-	4	-0.120	0.104	0.111	0.462	-0.412	0.476	0.268	0.466	-0.412	0.478
[SCN]-	3	-0.315	0.121	-0.110	0.577	-0.011	0.507	0.051	0.585	-0.011	0.509

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		b (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)	*b* (ion)	*b* (SD)
[TCB]-	4	-0.121	0.115	0.082	0.493	0.180	0.433	0.179	0.501	0.180	0.435
[TCM]-	6	-0.070	0.143	3.604	0.529	3.982	0.439	4.011	0.503	3.982	0.441
[TDI]-	2	0.146	0.000	-0.076	0.671	0.014	0.592	0.097	0.681	0.014	0.594
[TFA]-	1	0.475	0.948	-0.377	0.789	#N/A	#N/A	-0.285	0.806	#N/A	#N/A
[Trif]-	3	-0.091	0.125	0.020	0.546	0.117	0.480	0.183	0.553	0.117	0.482

Table D.39: Comparison of anion literature values and their errors and the values from methods 1, 2, 3, and 4 and their respective errors for ABSM parameter *v* for *log* P.

Anion	# of Inst	Lit. Values		Method 1		Method 2		Method 3		Method 4	
		v (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)	*v* (ion)	*v* (SD)
[+Cs]-	1	0.510	0.000	0.375	0.402	0.474	0.412	0.366	0.403	0.474	0.414
[BETI]-	1	-0.349	0.089	-0.429	0.393	-0.401	0.381	-0.440	0.392	-0.401	0.382
[BF4]-	5	-0.296	0.044	-0.491	0.228	-0.443	0.269	-0.511	0.215	-0.443	0.270
[DCA]-	11	-0.243	0.079	-0.349	0.190	-0.307	0.184	-0.356	0.189	-0.307	0.185
[DEP]-	2	0.184	0.162	0.118	0.399	0.182	0.389	0.112	0.400	0.182	0.390
[EtSO4]-	1	-0.264	0.078	-0.333	0.399	-0.269	0.389	-0.339	0.400	-0.269	0.390
[FAP]-	9	-0.109	0.043	-0.114	0.179	-0.095	0.172	-0.118	0.179	-0.095	0.173
[FSI]-	2	-0.051	0.075	-0.198	0.397	-0.176	0.382	-0.207	0.397	-0.176	0.383
[L-Lact]-	1	0.113	0.000	-0.022	0.402	0.077	0.412	-0.031	0.403	0.077	0.414
[MeSO3]-	2	-0.242	0.128	-0.261	0.291	-0.215	0.281	-0.269	0.290	-0.215	0.282
[OS]-	3	0.424	0.095	0.287	0.248	0.261	0.290	0.279	0.247	0.261	0.291
[PF6]-	4	-0.297	0.047	-0.336	0.234	-0.355	0.265	-0.346	0.232	-0.355	0.266
[SCN]-	3	-0.130	0.061	-0.249	0.292	-0.224	0.282	-0.259	0.291	-0.224	0.283
[TCB]-	4	0.061	0.061	-0.183	0.249	-0.148	0.241	-0.189	0.249	-0.148	0.242
[TCM]-	6	-0.008	0.094	-0.426	0.267	-0.416	0.244	-0.451	0.250	-0.416	0.245
[TDI]-	2	0.128	0.000	0.050	0.339	0.076	0.329	0.039	0.338	0.076	0.330
[TFA]-	1	0.056	0.099	-0.184	0.399	#N/A	#N/A	-0.190	0.400	#N/A	#N/A
[Trif]-	3	-0.047	0.057	-0.179	0.276	-0.154	0.267	-0.189	0.275	-0.154	0.268

Table D.40: Comparison of cation log *K* ABSM parameters for cations with more than one instance and their literature values and from methods 1, 2, 3, and 4.

	c	*e*	*s*	*a*	*b*	*l*		*c*	*e*	*s*	*a*	*b*	*l*
[(Hexom)2Im]+							[HM2iPam]+						
Lit. value	-0.314	-0.479	2.076	2.376	0.287	0.835	Lit. value	-0.531	-0.124	2.232	2.297	0.344	0.736
Method 1	-0.314	-0.479	2.076	2.376	0.287	0.835	Method 1	-0.531	-0.124	2.232	2.297	0.344	0.736
Method 2	-0.314	-0.479	2.076	2.376	0.287	0.835	Method 2	-0.531	-0.124	2.232	2.297	0.344	0.736
Method 3	-0.314	-0.479	2.076	2.376	0.287	0.835	Method 3	-0.531	-0.124	2.232	2.297	0.344	0.736
Method 4	-0.314	-0.479	2.076	2.376	0.287	0.835	Method 4	-0.531	-0.124	2.232	2.297	0.344	0.736
[(Meo)2Im]+							[HMIM]+						
Lit. value	-0.762	-0.013	2.557	2.427	1.154	0.584	Lit. value	-0.379	-0.103	2.081	2.298	0.533	0.751
Method 1	-0.762	-0.013	2.557	2.427	1.157	0.584	Method 1	-0.428	-0.147	2.164	2.279	0.476	0.753
Method 2	-0.762	-0.013	2.557	2.427	1.157	0.584	Method 2	-0.412	-0.133	2.167	2.31	0.479	0.745
Method 3	-0.762	0	2.557	2.427	1.157	0.584	Method 3	-0.429	-0.112	2.164	2.279	0.475	0.753
Method 4	-0.762	0	2.557	2.427	1.157	0.584	Method 4	-0.412	-0.098	2.167	2.31	0.478	0.745
[1-PrOHPy]+							[HMPip]+						
Lit. value	-0.713	0.151	2.663	2.874	1.311	0.611	Lit. value	-0.404	-0.245	2.469	2.348	0.075	0.775
Method 1	-0.897	0.639	1.593	2.414	2.447	0.673	Method 1	-0.404	-0.245	2.469	2.348	0.075	0.775
Method 2	-0.913	0.705	1.559	2.593	2.468	0.655	Method 2	-0.404	-0.245	2.469	2.348	0.075	0.775
Method 3	-0.897	0.619	1.592	2.414	2.441	0.673	Method 3	-0.404	-0.245	2.469	2.348	0.075	0.775
Method 4	-0.913	0.685	1.559	2.593	2.463	0.655	Method 4	-0.404	-0.245	2.469	2.348	0.075	0.775
[3-MBPy]+							[HMPyrr]+						
Lit. value	-0.338	0.035	2.325	2.289	0.189	0.714	Lit. value	-0.533	-0.11	2.146	2.278	0.65	0.767
Method 1	-0.408	-0.033	2.502	2.594	0.045	0.745	Method 1	-0.533	-0.11	2.146	2.278	0.65	0.767
Method 2	-0.328	0.004	2.346	2.325	0.233	0.741	Method 2	-0.533	-0.11	2.146	2.278	0.65	0.767
Method 3	-0.407	-0.097	2.503	2.594	0.072	0.745	Method 3	-0.533	-0.11	2.146	2.278	0.65	0.767
Method 4	-0.329	-0.063	2.346	2.325	0.26	0.741	Method 4	-0.533	-0.11	2.146	2.278	0.65	0.767
[AllMIm]+							[HxomMIm]+						
Lit. value	-0.432	0.135	2.368	2.324	0.624	0.606	Lit. value	-0.463	-0.394	2.478	2.428	0.337	0.786
Method 1	-0.431	0.087	2.477	2.242	0.583	0.62	Method 1	-0.462	0	2.073	2.022	0.637	0.684
Method 2	-0.439	0.12	2.46	2.331	0.594	0.612	Method 2	-0.462	0	2.073	2.022	0.637	0.684
Method 3	-0.431	0.077	2.477	2.242	0.58	0.62	Method 3	-0.462	0	2.073	2.022	0.637	0.684
Method 4	-0.439	0.11	2.46	2.331	0.591	0.612	Method 4	-0.462	0	2.073	2.022	0.637	0.684
[B3EP]+							[M2EIm]+						

	c	*e*	*s*	*a*	*b*	*l*
Lit. value	-0.45	-0.331	1.731	0.788	0.774	0.783
Method 1	-0.543	-0.372	1.664	0.693	0.865	0.826
Method 2	-0.524	-0.357	1.778	0.875	0.765	0.801
Method 3	-0.543	-0.406	1.663	0.693	0.863	0.826
Method 4	-0.524	-0.393	1.778	0.875	0.672	0.801
[BMIm]+						
Lit. value	-0.421	0.033	2.134	2.281	0.603	0.712
Method 1	-0.512	-0.017	2.384	2.651	0.383	0.735
Method 2	-0.414	0.024	2.186	2.29	0.621	0.733
Method 3	-0.51	-0.045	2.385	2.651	0.383	0.735
Method 4	-0.415	-0.008	2.186	2.29	0.621	0.733
[BMMOR]+						
Lit. value	-0.676	0.277	2.472	2.369	0.597	0.638
Method 1	-0.58	0.141	2.625	2.961	0.296	0.69
Method 2	-0.503	0.16	2.546	2.828	0.392	0.684
Method 3	-0.578	0.144	2.626	2.961	0.295	0.69
Method 4	-0.502	0.16	2.546	2.828	0.391	0.684
[BMPip]+						
Lit. value	-0.364	0.134	2.271	2.467	0.327	0.679
Method 1	-0.347	0.111	2.241	2.472	0.294	0.687
Method 2	-0.347	0.111	2.241	2.472	0.294	0.687
Method 3	-0.347	0	2.241	2.472	0.294	0.687
Method 4	-0.347	0	2.241	2.472	0.294	0.687
[BMPy]+						
Lit. value	-0.449	0.157	2.27	2.416	0.566	0.714
Method 1	-0.543	0.018	2.512	2.231	0.514	0.734
Method 2	-0.446	0.004	2.524	2.235	0.501	0.727
Method 3	-0.54	-0.016	2.513	2.231	0.514	0.734
Method 4	-0.441	-0.031	2.524	2.235	0.5	0.727
[BMPyrr]+						
Lit. value	-0.363	0.119	2.207	2.363	0.388	0.679
Method 1	-0.372	-0.025	2.381	2.59	0.172	0.711
Method 2	-0.336	0.004	2.328	2.55	0.234	0.703

	c	*e*	*s*	*a*	*b*	*l*
Lit. value	-0.611	0.188	2.38	2.101	0.899	0.667
Method 1	-0.565	0.214	2.347	2.075	0.896	0.655
Method 2	-0.565	0.214	2.347	2.075	0.896	0.655
Method 3	-0.565	0.214	2.347	2.075	0.896	0.655
Method 4	-0.565	0.214	2.347	2.075	0.896	0.655
[M3BAm]+						
Lit. value	-0.457	-0.005	2.188	2.375	0.663	0.668
Method 1	-0.457	0	2.188	2.375	0.663	0.668
Method 2	-0.457	0	2.188	2.375	0.663	0.668
Method 3	-0.457	0	2.188	2.375	0.663	0.668
Method 4	-0.457	0	2.188	2.375	0.663	0.668
[MDIm]+						
Lit. value	-0.391	-0.162	2.036	2.054	0.524	0.786
Method 1	-0.412	-0.277	2.049	2.111	0.425	0.817
Method 2	-0.388	-0.257	2.071	2.169	0.414	0.804
Method 3	-0.412	-0.27	2.049	2.111	0.423	0.817
Method 4	-0.388	-0.252	2.071	2.169	0.412	0.804
[MeoeMim]+						
Lit. value	-0.507	-0.015	2.644	2.378	0.413	0.602
Method 1	-0.509	0.065	2.476	2.271	0.671	0.603
Method 2	-0.509	0.065	2.476	2.271	0.671	0.603
Method 3	-0.509	0.065	2.476	2.271	0.671	0.603
Method 4	-0.509	0.065	2.476	2.271	0.671	0.603
[MeoeMMorp]+						
Lit. value	-0.675	0.021	2.823	2.588	0.542	0.644
Method 1	-0.655	0.074	2.764	2.536	0.501	0.63
Method 2	-0.642	0.087	2.758	2.554	0.511	0.626
Method 3	-0.655	0.07	2.764	2.536	0.5	0.63
Method 4	-0.642	0.082	2.758	2.554	0.51	0.626
[MeoeMPip]+						
Lit. value	-0.44	0.065	2.484	2.537	0.241	0.688
Method 1	-0.464	0.041	2.483	2.531	0.171	0.689
Method 2	-0.451	0.053	2.477	2.549	0.181	0.685

	c	*e*	*s*	*a*	*b*	*l*
Method 3	-0.372	-0.043	2.381	2.59	0.169	0.711
Method 4	-0.336	-0.016	2.328	2.55	0.231	0.703
[BzmIm]+						
Lit. value	-0.535	0	2.523	2.333	0.575	0.668
Method 1	-0.535	0	2.523	2.333	0.575	0.668
Method 2	-0.535	0	2.523	2.333	0.575	0.668
Method 3	-0.535	0	2.523	2.333	0.575	0.668
Method 4	-0.535	0	2.523	2.333	0.575	0.668
[BzmPyrr]+						
Lit. value	-0.652	0.154	2.371	2.285	0.531	0.691
Method 1	-0.652	0.154	2.371	2.285	0.531	0.691
Method 2	-0.652	0.154	2.371	2.285	0.531	0.691
Method 3	-0.652	0.154	2.371	2.285	0.531	0.691
Method 4	-0.652	0.154	2.371	2.285	0.531	0.691
[BzPy]+						
Lit. value	-0.83	0	2.617	2.452	0.526	0.711
Method 1	-0.83	0	2.617	2.452	0.526	0.711
Method 2	-0.83	0	2.617	2.452	0.526	0.711
Method 3	-0.83	0	2.617	2.452	0.526	0.711
Method 4	-0.83	0	2.617	2.452	0.526	0.711
[C1,9(M2iPAm)2]2+						
Lit. value	*-0.894*	*0.175*	*2.533*	*2.544*	*0.492*	*0.69*
Method 1	-0.894	0.175	2.533	2.544	0.492	0.69
Method 2	-0.894	0.175	2.533	2.544	0.492	0.69
Method 3	-0.894	0.175	2.533	2.544	0.492	0.69
Method 4	-0.894	0.175	2.533	2.544	0.492	0.69
[C3MPyrr]+						
Lit. value	-0.466	2.562	0	2.505	0.271	0.682
Method 1	-0.466	2.562	0	2.505	0.271	0.682
Method 2	-0.466	2.562	0	2.505	0.271	0.682
Method 3	-0.466	2.562	0	2.505	0.271	0.682
Method 4	-0.466	2.562	0	2.505	0.271	0.682
[C5MPyrr]+						

	c	*e*	*s*	*a*	*b*	*l*
Method 3	-0.464	-0.001	2.483	2.531	0.17	0.689
Method 4	-0.451	0.011	2.477	2.549	0.18	0.685
[MeoeMPyrr]+						
Lit. value	-0.38	0.018	2.497	2.534	0.162	0.671
Method 1	-0.443	0.006	2.495	2.525	0.044	0.681
Method 2	-0.416	0.032	2.483	2.562	0.063	0.672
Method 3	-0.444	-0.002	2.496	2.525	0.043	0.681
Method 4	-0.417	0.022	2.483	2.562	0.062	0.672
[MOIm]+						
Lit. value	-0.197	-0.216	1.301	2.021	0.994	0.837
Method 1	-0.297	-0.335	1.511	1.773	0.732	0.862
Method 2	-0.073	-0.175	1.17	1.959	1.186	0.84
Method 3	-0.254	-0.299	1.515	1.773	0.732	0.862
Method 4	-0.018	-0.121	1.17	1.959	1.185	0.84
[N112N113]+						
Lit. value	-1.338	0.044	2.865	3.28	1.041	0.762
Method 1	-1.338	0.044	2.865	3.28	1.041	0.762
Method 2	-1.338	0.044	2.865	3.28	1.041	0.762
Method 3	-1.338	0	2.865	3.28	1.041	0.762
Method 4	-1.338	0	2.865	3.28	1.041	0.762
[N112N114]+						
Lit. value	-0.725	0.053	2.522	2.863	0.751	0.656
Method 1	-0.725	0.053	2.522	2.863	0.751	0.656
Method 2	-0.725	0.053	2.522	2.863	0.751	0.656
Method 3	-0.725	0	2.522	2.863	0.751	0.656
Method 4	-0.725	0	2.522	2.863	0.751	0.656
[N112O2N113]+						
Lit. value	-0.613	-0.225	2.44	2.608	0.42	0.748
Method 1	-0.613	-0.225	2.44	2.608	0.42	0.748
Method 2	-0.613	-0.225	2.44	2.608	0.42	0.748
Method 3	-0.613	-0.225	2.44	2.608	0.42	0.748
Method 4	-0.613	-0.225	2.44	2.608	0.42	0.748
[N112O2N114]+						

	c	*e*	*s*	*a*	*b*	*l*
Lit. value	-0.549	0	2.317	2.425	0.385	0.747
Method 1	-0.549	0	2.317	2.425	0.385	0.747
Method 2	-0.549	0	2.317	2.425	0.385	0.747
Method 3	-0.549	0	2.317	2.425	0.385	0.747
Method 4	-0.549	0	2.317	2.425	0.385	0.747
[ChxmIm]+						
Lit. value	-0.513	-0.203	2.418	2.688	0.334	0.745
Method 1	-0.513	-0.203	2.418	2.688	0.334	0.745
Method 2	-0.513	-0.203	2.418	2.688	0.334	0.745
Method 3	-0.513	-0.203	2.418	2.688	0.334	0.745
Method 4	-0.513	-0.203	2.418	2.688	0.334	0.745
[ChxmPyrr]+						
Lit. value	0.545	-0.124	2.406	2.411	0.274	0.771
Method 1	0.545	-0.124	2.406	2.411	0.274	0.771
Method 2	0.545	-0.124	2.406	2.411	0.274	0.771
Method 3	0.545	-0.124	2.406	2.411	0.274	0.771
Method 4	0.545	-0.124	2.406	2.411	0.274	0.771
[ChxPy]+						
Lit. value	-0.556	0	2.37	2.496	0.412	0.755
Method 1	-0.556	0	2.37	2.496	0.412	0.755
Method 2	-0.556	0	2.37	2.496	0.412	0.755
Method 3	-0.556	0	2.37	2.496	0.412	0.755
Method 4	-0.556	0	2.37	2.496	0.412	0.755
[CNMeM2iPam]+						
Lit. value	-1.344	-0.14	3.283	3.118	0.819	0.735
Method 1	-1.344	-0.14	3.283	3.118	0.819	0.735
Method 2	-1.344	-0.14	3.283	3.118	0.819	0.735
Method 3	-1.344	-0.14	3.283	3.118	0.819	0.735
Method 4	-1.344	-0.14	3.283	3.118	0.819	0.735
[CNPrMIm]+						
Lit. value	-1.119	0.073	2.617	2.543	0.816	0.699
Method 1	-1.116	-0.859	2.832	2.371	0.743	0.728
Method 2	-1.132	-0.793	2.798	2.55	0.764	0.71

	c	*e*	*s*	*a*	*b*	*l*
Lit. value	-0.436	-0.108	2.279	2.505	0.435	0.707
Method 1	-0.436	-0.108	2.279	2.505	0.435	0.707
Method 2	-0.436	-0.108	2.279	2.505	0.435	0.707
Method 3	-0.436	-0.108	2.279	2.505	0.435	0.707
Method 4	-0.436	-0.108	2.279	2.505	0.435	0.707
[N2,2,2,8]+						
Lit. value	-0.347	-0.063	2.034	2.317	0.179	0.787
Method 1	-0.29	-0.182	2.101	2.435	-0.016	0.807
Method 2	-0.254	-0.153	2.048	2.395	0.046	0.799
Method 3	-0.29	-0.2	2.101	2.435	-0.019	0.807
Method 4	-0.254	-0.173	2.048	2.395	0.043	0.799
[O4AM]+						
Lit. value	0	-0.287	1.478	1.845	0.189	0.816
Method 1	0	-0.287	1.478	1.845	0.189	0.816
Method 2	0	-0.287	1.478	1.845	0.189	0.816
Method 3	0	-0.287	1.478	1.845	0.189	0.816
Method 4	0	-0.287	1.478	1.845	0.189	0.816
[OM3AM]+						
Lit. value	-0.426	-0.338	2.242	2.195	0.684	0.779
Method 1	-0.426	-0.338	2.242	2.195	0.684	0.779
Method 2	-0.426	-0.338	2.242	2.195	0.684	0.779
Method 3	-0.426	-0.338	2.242	2.195	0.684	0.779
Method 4	-0.426	-0.338	2.242	2.195	0.684	0.779
[Ompyrr]+						
Lit. value	-0.587	-0.064	2.08	2.176	0.486	0.822
Method 1	-0.587	-0.064	2.08	2.176	0.486	0.822
Method 2	-0.587	-0.064	2.08	2.176	0.486	0.822
Method 3	-0.587	0	2.08	2.176	0.486	0.822
Method 4	-0.587	0	2.08	2.176	0.486	0.822
[PDMIM]+						
Lit. value	-0.822	0.78	2.357	3.432	0.926	0.526
Method 1	-1.083	0.302	2.67	2.227	0.697	0.716
Method 2	-0.733	0.759	2.444	3.562	0.847	0.559

	c	*e*	*s*	*a*	*b*	*l*
Method 3	-1.116	-0.879	2.831	2.371	0.737	0.728
Method 4	-1.132	-0.813	2.798	2.55	0.759	0.71
[D2MIM]+						
Lit. value	-0.252	-0.269	1.603	1.946	0.354	0.856
Method 1	-0.252	-0.269	1.603	1.946	0.354	0.856
Method 2	-0.252	-0.269	1.603	1.946	0.354	0.856
Method 3	-0.252	-0.269	1.603	1.946	0.354	0.856
Method 4	-0.252	-0.269	1.603	1.946	0.354	0.856
[DM3AM]+						
Lit. value	-0.363	-0.339	1.986	2.144	0.422	0.809
Method 1	-0.363	-0.339	1.986	2.144	0.422	0.809
Method 2	-0.363	-0.339	1.986	2.144	0.422	0.809
Method 3	-0.363	-0.339	1.986	2.144	0.422	0.809
Method 4	-0.363	-0.339	1.986	2.144	0.422	0.809
[DMPyrr]+						
Lit. value	-0.395	-0.241	1.991	2.112	0.268	0.822
Method 1	-0.395	-0.241	1.991	2.112	0.268	0.822
Method 2	-0.395	-0.241	1.991	2.112	0.268	0.822
Method 3	-0.395	-0.241	1.991	2.112	0.268	0.822
Method 4	-0.395	-0.241	1.991	2.112	0.268	0.822
[E3S]+						
Lit. value	-0.606	-0.196	2.992	2.444	0.355	0.69
Method 1	-0.606	-0.196	2.992	2.444	0.355	0.69
Method 2	-0.606	-0.196	2.992	2.444	0.355	0.69
Method 3	-0.606	-0.196	2.992	2.444	0.355	0.69
Method 4	-0.606	-0.196	2.992	2.444	0.355	0.69
[EMIM]+						
Lit. value	-0.505	0.088	2.305	2.381	0.683	0.654
Method 1	-0.598	0.047	2.238	2.266	0.774	0.696
Method 2	-0.579	0.062	2.352	2.448	0.674	0.671
Method 3	-0.598	0.013	2.237	2.266	0.772	0.696
Method 4	-0.579	0.026	2.352	2.448	0.672	0.671
[EtOHM2iPAm]+						

	c	*e*	*s*	*a*	*b*	*l*
Method 3	-1.08	0.293	2.67	2.227	0.696	0.716
Method 4	-0.719	0.741	2.444	3.562	0.846	0.559
[PEMPip]+						
Lit. value	-0.477	-0.186	2.639	2.45	0.103	0.761
Method 1	-0.477	-0.186	2.639	2.45	0.103	0.761
Method 2	-0.477	-0.186	2.639	2.45	0.103	0.761
Method 3	-0.477	-0.186	2.639	2.45	0.103	0.761
Method 4	-0.477	-0.186	2.639	2.45	0.103	0.761
[PeMPyrr]+						
Lit. value	-0.549	0	2.317	2.425	0.385	0.747
Method 1	-0.549	0	2.317	2.425	0.385	0.747
Method 2	-0.549	0	2.317	2.425	0.385	0.747
Method 3	-0.549	0	2.317	2.425	0.385	0.747
Method 4	-0.549	0	2.317	2.425	0.385	0.747
[PM2iPAm]+						
Lit. value	-0.702	0	2.532	2.578	0.331	0.682
Method 1	-0.702	0	2.532	2.578	0.331	0.682
Method 2	-0.702	0	2.532	2.578	0.331	0.682
Method 3	-0.702	0	2.532	2.578	0.331	0.682
Method 4	-0.702	0	2.532	2.578	0.331	0.682
[PMPip]+						
Lit. value	-0.435	0.149	2.281	2.476	0.41	0.675
Method 1	-0.432	0.145	2.287	2.489	0.402	0.674
Method 2	-0.432	0.145	2.287	2.489	0.402	0.674
Method 3	-0.432	0.145	2.287	2.489	0.402	0.674
Method 4	-0.432	0.145	2.287	2.489	0.402	0.674
[PMPyrr]+						
Lit. value	-0.466	0	2.562	2.505	0.271	0.682
Method 1	-0.466	0	2.562	2.505	0.271	0.682
Method 2	-0.466	0	2.562	2.505	0.271	0.682
Method 3	-0.466	0	2.562	2.505	0.271	0.682
Method 4	-0.466	0	2.562	2.505	0.271	0.682
[sec-BMIm]+						

	c	*e*	*s*	*a*	*b*	*l*
Lit. value	-0.934	0.2	2.361	2.695	1.532	0.641
Method 1	-0.934	0.2	2.361	2.695	1.532	0.641
Method 2	-0.934	0.2	2.361	2.695	1.532	0.641
Method 3	-0.934	0.2	2.361	2.695	1.532	0.641
Method 4	-0.934	0.2	2.361	2.695	1.532	0.641
[EtOHMIm]+						
Lit. value	-0.843	0.095	2.462	2.694	1.331	0.58
Method 1	-0.946	-0.091	2.728	2.686	1.276	0.6
Method 2	-0.87	-0.011	2.596	2.715	1.415	0.593
Method 3	-0.95	-0.099	2.732	2.686	1.276	0.6
Method 4	-0.872	-0.02	2.596	2.715	1.415	0.593
[HexM3Am]+						
Lit. value	-0.469	-0.056	2.083	2.176	0.62	0.689
Method 1	-0.469	-0.058	2.085	2.185	0.617	0.617
Method 2	-0.469	-0.058	2.085	2.185	0.617	0.617
Method 3	-0.469	0	2.085	2.185	0.617	0.617
Method 4	-0.469	0	2.085	2.185	0.617	0.617

	c	*e*	*s*	*a*	*b*	*l*
Lit. value	-0.558	-0.097	2.519	2.497	0.456	0.705
Method 1	-0.558	-0.097	2.519	2.497	0.456	0.705
Method 2	-0.558	-0.097	2.519	2.497	0.456	0.705
Method 3	-0.558	-0.097	2.519	2.497	0.456	0.705
Method 4	-0.558	-0.097	2.519	2.497	0.456	0.705
[tert-BMIm]+						
Lit. value	-0.621	-0.118	2.603	2.689	0.41	0.693
Method 1	-0.621	-0.118	2.603	2.689	0.41	0.693
Method 2	-0.621	-0.118	2.603	2.689	0.41	0.693
Method 3	-0.621	-0.118	2.603	2.689	0.41	0.693
Method 4	-0.621	-0.118	2.603	2.689	0.41	0.693

Table D.41: Comparison of cation log *P* ABSM parameters for cations with more than one instance and their literature values and from methods 1, 2, 3, and 4.

	c	*e*	*s*	*a*	*b*	*v*
[(Hexom)2Im]+						
Lit. value	0.074	-0.541	0.642	-1.419	-4.748	3.787
Method 1	0.107	-0.628	0.747	-1.441	-4.808	3.750
Method 2	0.107	-0.628	0.747	-1.441	-4.808	3.750
Method 3	0.107	-0.628	0.747	-1.441	-4.808	3.750
Method 4	0.107	-0.628	0.747	-1.441	-4.808	3.750
[(Meo)2Im]+						
Lit. value	-0.414	-0.103	0.764	-1.120	-3.781	3.056
Method 1	-0.412	-0.104	0.761	-1.124	-3.776	3.055
Method 2	-0.412	-0.104	0.761	-1.124	-3.776	3.055
Method 3	-0.412	0.000	0.761	-1.124	-3.776	3.055
Method 4	-0.412	0.000	0.761	-1.124	-3.776	3.055

	c	*e*	*s*	*a*	*b*	*v*
[HexM3Am]+						
Lit. value	-0.404	0.344	0.945	0.987	-4.526	2.957
Method 1	-0.322	0.242	0.287	-1.383	-4.265	3.513
Method 2	-0.404	0.344	0.945	0.987	-4.526	2.957
Method 3	-0.322	0.242	0.287	-1.383	-4.265	3.513
Method 4	-0.404	0.344	0.945	0.987	-4.526	2.957
[HM2iPam]+						
Lit. value	-0.340	0.000	0.582	-1.194	-4.631	3.640
Method 1	-0.340	0.000	0.582	-1.194	-4.631	3.640
Method 2	-0.340	0.000	0.582	-1.194	-4.631	3.640
Method 3	-0.340	0.000	0.582	-1.194	-4.631	3.640
Method 4	-0.340	0.000	0.582	-1.194	-4.631	3.640

	c	e	s	a	b	v
[3-MBPy]+						
Lit. value	0.040	0.087	0.657	-1.197	-4.970	3.435
Method 1	-0.073	0.158	0.751	-1.241	-4.824	3.512
Method 2	0.033	-0.015	0.859	-1.473	-4.918	3.487
Method 3	0.030	0.173	0.822	-1.227	-4.993	3.523
Method 4	0.118	0.067	0.850	-1.456	-4.918	3.487
[AllMIm]+						
Lit. value	0.028	0.127	0.519	-1.365	-4.282	3.102
Method 1	-0.002	0.070	0.641	-1.467	-4.304	3.065
Method 2	-0.004	0.078	0.637	-1.399	-4.348	3.043
Method 3	0.002	0.008	0.665	-1.468	-4.360	3.068
Method 4	-0.008	0.044	0.640	-1.399	-4.348	3.043
[B3EP]+						
Lit. value	0.049	-0.315	0.303	-3.190	-4.153	3.539
Method 1	-0.032	-0.341	0.213	-3.416	-4.400	3.605
Method 2	-0.019	-0.347	0.309	-3.330	-4.541	3.541
Method 3	-0.144	-0.378	0.248	-3.418	-4.492	3.611
Method 4	-0.134	-0.333	0.303	-3.330	-4.541	3.541
[BMIm]+						
Lit. value	-0.048	0.328	0.296	-1.382	-4.337	3.390
Method 1	-0.235	0.340	0.558	-0.937	-4.040	3.470
Method 2	-0.106	0.133	0.679	-1.246	-4.126	3.442
Method 3	-0.188	0.242	0.632	-0.944	-4.217	3.481
Method 4	-0.079	0.105	0.666	-1.251	-4.126	3.442
[BMMOR]+						
Lit. value	-0.239	0.318	0.675	-1.223	-4.414	3.130
Method 1	0.008	0.125	-0.129	-2.523	-8.088	3.548
Method 2	0.124	-0.163	0.137	-2.602	-8.466	3.538
Method 3	0.060	-0.068	0.039	-2.530	-8.495	3.573
Method 4	0.133	-0.179	0.131	-2.603	-8.466	3.538
[BMPip]+						
Lit. value	-0.115	0.448	0.322	-1.108	-4.452	3.390
Method 1	-0.129	0.494	0.235	-1.165	-4.385	3.422

	c	e	s	a	b	v
[HMIM]+						
Lit. value	-0.083	0.098	0.348	-1.275	-4.426	3.585
Method 1	-0.065	0.088	0.304	-1.440	-4.512	3.573
Method 2	-0.051	0.072	0.330	-1.423	-4.552	3.555
Method 3	-0.049	0.001	0.328	-1.440	-4.567	3.576
Method 4	-0.039	0.010	0.330	-1.422	-4.552	3.555
[HMPyrr]+						
Lit. value	-0.226	-0.083	0.560	-1.301	-4.501	3.673
Method 1	-0.226	-0.083	0.560	-1.301	-4.501	3.673
Method 2	-0.226	-0.083	0.560	-1.301	-4.501	3.673
Method 3	-0.226	0.000	0.560	-1.301	-4.501	3.673
Method 4	-0.226	0.000	0.560	-1.301	-4.501	3.673
[HxomMIm]+						
Lit. value	-0.071	-0.558	1.080	-1.351	-4.718	3.646
Method 1	-0.275	0.000	0.407	-1.478	4.320	3.510
Method 2	-0.275	0.000	0.407	-1.478	4.320	3.510
Method 3	-0.275	0.000	0.407	-1.478	4.320	3.510
Method 4	-0.275	0.000	0.407	-1.478	4.320	3.510
[M2EIm]+						
Lit. value	-0.095	0.292	0.443	-1.681	-4.024	3.174
Method 1	-0.095	0.299	0.360	-1.906	-3.805	3.177
Method 2	-0.095	0.299	0.360	-1.906	-3.805	3.177
Method 3	0.000	0.299	0.360	-1.906	-3.805	3.177
Method 4	0.000	0.299	0.360	-1.906	-3.805	3.177
[M3BAm]+						
Lit. value	0.047	-0.021	0.356	-1.262	-4.400	3.209
Method 1	0.047	-0.051	0.356	-1.262	-4.400	3.209
Method 2	0.047	-0.051	0.356	-1.262	-4.400	3.209
Method 3	0.000	0.000	0.356	-1.262	-4.400	3.209
Method 4	0.000	0.000	0.356	-1.262	-4.400	3.209
[MDIm]+						
Lit. value	0.036	-0.064	0.395	-1.611	-4.546	3.587
Method 1	0.106	-0.062	0.214	-1.724	-4.749	3.709

	c	*e*	*s*	*a*	*b*	*v*
Method 2	-0.129	0.494	0.235	-1.165	-4.385	3.422
Method 3	0.000	0.494	0.235	-1.165	-4.385	3.422
Method 4	0.000	0.494	0.235	-1.165	-4.385	3.422
[BMPy]+						
Lit. value	-0.090	0.238	0.549	-1.246	-4.417	3.433
Method 1	-0.378	0.671	0.523	-0.985	-2.460	3.426
Method 2	-0.207	0.102	1.124	-0.878	-3.394	3.446
Method 3	-0.294	0.260	0.892	-1.002	-3.359	3.480
Method 4	-0.219	0.093	1.119	-0.879	-3.394	3.446
[BMPyrr]+						
Lit. value	-0.340	0.380	0.308	-1.276	-4.474	3.330
Method 1	-0.034	0.313	0.207	-1.365	-5.166	3.485
Method 2	0.014	0.224	0.284	-1.402	-5.278	3.463
Method 3	-0.010	0.241	0.268	-1.364	-5.310	3.494
Method 4	0.023	0.214	0.281	-1.398	-5.278	3.463
[BzmIm]+						
Lit. value	-0.187	0.000	0.768	-1.284	-4.378	3.310
Method 1	-0.187	0.000	0.768	-1.284	-4.378	3.310
Method 2	-0.187	0.000	0.768	-1.284	-4.378	3.310
Method 3	-0.187	0.000	0.768	-1.284	-4.378	3.310
Method 4	-0.187	0.000	0.768	-1.284	-4.378	3.310
[BzmPyrr]+						
Lit. value	-0.387	0.197	0.658	-1.275	-4.401	3.449
Method 1	-0.387	0.197	0.658	-1.275	-4.401	3.449
Method 2	-0.387	0.197	0.658	-1.275	-4.401	3.449
Method 3	-0.387	0.197	0.658	-1.275	-4.401	3.449
Method 4	-0.387	0.197	0.658	-1.275	-4.401	3.449
[BzPy]+						
Lit. value	-0.516	0.092	0.865	-1.143	-4.432	3.485
Method 1	-0.516	0.092	0.865	-1.143	-4.432	3.485
Method 2	-0.516	0.092	0.865	-1.143	-4.432	3.485
Method 3	-0.516	0.000	0.865	-1.143	-4.432	3.485
Method 4	-0.516	0.000	0.865	-1.143	-4.432	3.485

	c	*e*	*s*	*a*	*b*	*v*
Method 2	0.131	-0.099	0.280	-1.702	-4.847	3.674
Method 3	-0.017	-0.164	0.254	-1.725	-4.846	3.715
Method 4	0.000	-0.155	0.278	-1.701	-4.847	3.674
[MeoeMim]+						
Lit. value	-0.150	0.012	0.653	-1.289	-4.263	3.116
Method 1	-0.150	0.012	0.818	-1.289	-4.263	3.116
Method 2	-0.150	0.012	0.818	-1.289	-4.263	3.116
Method 3	-0.150	0.000	0.818	-1.289	-4.263	3.116
Method 4	-0.150	0.000	0.818	-1.289	-4.263	3.116
[MeoeMMorp]+						
Lit. value	-0.264	0.067	0.995	-1.058	-4.381	3.168
Method 1	-0.192	0.001	0.972	-1.163	-4.532	3.110
Method 2	-0.183	-0.004	0.978	-1.149	-4.544	3.101
Method 3	-0.159	-0.045	0.988	-1.163	-4.565	3.112
Method 4	-0.153	-0.037	0.980	-1.149	-4.544	3.101
[MeoeMPip]+						
Lit. value	-0.102	0.191	0.660	-1.094	-4.665	3.360
Method 1	-0.075	0.147	0.656	-1.177	-4.792	3.335
Method 2	-0.066	0.142	0.663	-1.163	-4.803	3.326
Method 3	-0.065	0.148	0.673	-1.177	-4.825	3.337
Method 4	-0.059	0.156	0.664	-1.163	-4.803	3.326
[MeoeMPyrr]+						
Lit. value	-0.068	0.119	0.691	-1.140	-4.694	3.324
Method 1	-0.066	0.076	0.672	-1.268	-4.941	3.329
Method 2	-0.049	0.066	0.685	-1.239	-4.964	3.310
Method 3	-0.130	0.077	0.705	-1.268	-5.008	3.333
Method 4	-0.118	0.095	0.688	-1.239	-4.964	3.310
[MOIm]+						
Lit. value	-0.011	0.009	-0.150	-1.641	-3.980	3.872
Method 1	-0.188	-0.249	0.508	-1.842	-4.551	4.030
Method 2	-0.036	-0.093	0.088	-1.153	-3.595	3.962
Method 3	-0.166	-0.326	0.603	-1.845	-4.772	4.043
Method 4	-0.045	-0.087	0.080	-1.156	-3.595	3.962

	c	e	s	a	b	v		c	e	s	a	b	v
[C1,9(M2iPAm)2]2+							[N112N113]+						
Lit. value	-0.606	0.225	0.798	-1.034	-4.438	3.429	Lit. value	-1.042	0.143	1.160	-0.335	-3.910	3.643
Method 1	-0.606	0.225	0.798	-1.034	-4.438	3.429	Method 1	-1.042	0.143	1.160	-0.335	-3.910	3.643
Method 2	-0.606	0.225	0.798	-1.034	-4.438	3.429	Method 2	-1.042	0.143	1.160	-0.335	-3.910	3.643
Method 3	-0.606	0.225	0.798	-1.034	-4.438	3.429	Method 3	-1.042	0.143	1.160	-0.335	-3.910	3.643
Method 4	-0.606	0.225	0.798	-1.034	-4.438	3.429	Method 4	-1.042	0.143	1.160	-0.335	-3.910	3.643
[C3MPyrr]+							[N112N114]+						
Lit. value	-0.236	0.000	0.908	-1.015	-4.691	3.446	Lit. value	-0.397	0.000	0.779	0.712	-4.181	3.291
Method 1	-0.236	0.000	0.908	-1.015	-4.691	3.446	Method 1	-0.397	0.000	0.779	0.712	-4.181	3.291
Method 2	-0.236	0.000	0.908	-1.015	-4.691	3.446	Method 2	-0.397	0.000	0.779	0.712	-4.181	3.291
Method 3	-0.236	0.000	0.908	-1.015	-4.691	3.446	Method 3	-0.397	0.000	0.779	0.712	-4.181	3.291
Method 4	-0.236	0.000	0.908	-1.015	-4.691	3.446	Method 4	-0.397	0.000	0.779	0.712	-4.181	3.291
[C5MPyrr]+							[N112O2N113]+						
Lit. value	-0.303	0.000	0.727	-1.107	-4.622	3.630	Lit. value	-0.339	-0.149	0.748	-0.945	-4.542	3.605
Method 1	-0.303	0.000	0.727	-1.107	-4.622	3.630	Method 1	-0.339	-0.149	0.748	-0.945	-4.542	3.605
Method 2	-0.303	0.000	0.727	-1.107	-4.622	3.630	Method 2	-0.339	-0.149	0.748	-0.945	-4.542	3.605
Method 3	-0.303	0.000	0.727	-1.107	-4.622	3.630	Method 3	-0.339	-0.149	0.748	-0.945	-4.542	3.605
Method 4	-0.303	0.000	0.727	-1.107	-4.622	3.630	Method 4	-0.339	-0.149	0.748	-0.945	-4.542	3.605
[ChxmIm]+							[N112O2N114]+						
Lit. value	-0.299	-0.094	0.754	-0.851	-4.618	3.653	Lit. value	-0.205	-0.053	0.584	-1.037	-4.475	3.508
Method 1	-0.299	-0.094	0.754	-0.851	-4.618	3.653	Method 1	-0.205	-0.053	0.584	-1.037	-4.475	3.508
Method 2	-0.299	-0.094	0.754	-0.851	-4.618	3.653	Method 2	-0.205	-0.053	0.584	-1.037	-4.475	3.508
Method 3	-0.299	0.000	0.754	-0.851	-4.618	3.653	Method 3	-0.205	0.000	0.584	-1.037	-4.475	3.508
Method 4	-0.299	0.000	0.754	-0.851	-4.618	3.653	Method 4	-0.205	0.000	0.584	-1.037	-4.475	3.508
[ChxmPyrr]+							[N2,2,2,8]+						
Lit. value	-0.297	0.073	0.697	-1.157	-4.687	3.709	Lit. value	-0.003	0.192	0.294	-1.339	-4.769	3.663
Method 1	-0.297	0.073	0.697	-1.157	-4.687	3.709	Method 1	-0.001	0.279	-0.014	-1.517	-5.372	3.802
Method 2	-0.297	0.073	0.697	-1.157	-4.687	3.709	Method 2	0.047	0.190	0.063	-1.554	-5.484	3.780
Method 3	-0.297	0.000	0.697	-1.157	-4.687	3.709	Method 3	0.132	0.207	0.047	-1.516	-5.516	3.811
Method 4	-0.297	0.000	0.697	-1.157	-4.687	3.709	Method 4	0.165	0.180	0.060	-1.550	-5.484	3.780
[ChxPy]+							[O4AM]+						
Lit. value	-0.344	0.146	0.703	-1.047	-4.535	3.681	Lit. value	0.226	0.000	-0.212	-1.756	-4.739	3.825
Method 1	-0.344	0.146	0.703	-1.047	-4.535	3.681	Method 1	0.226	0.000	-0.212	-1.756	-4.739	3.825

	c	*e*	*s*	*a*	*b*	*v*
Method 2	-0.344	0.146	0.703	-1.047	-4.535	3.681
Method 3	-0.344	0.146	0.703	-1.047	-4.535	3.681
Method 4	-0.344	0.146	0.703	-1.047	-4.535	3.681
[CNMeM2iPam]+						
Lit. value	-1.001	0.000	1.512	-0.459	-4.191	3.529
Method 1	-1.001	0.000	1.512	-0.459	-4.191	3.529
Method 2	-1.001	0.000	1.512	-0.459	-4.191	3.529
Method 3	-1.001	0.000	1.512	-0.459	-4.191	3.529
Method 4	-1.001	0.000	1.512	-0.459	-4.191	3.529
[CNPrMIm]+						
Lit. value	-0.680	0.206	0.782	-1.167	-4.055	3.301
Method 1	-0.729	0.095	1.023	-1.381	-4.096	3.395
Method 2	-0.735	0.110	1.015	-1.245	-4.184	3.353
Method 3	-0.723	0.030	1.071	-1.383	-4.210	3.402
Method 4	-0.742	0.101	1.021	-1.245	-4.184	3.353
[D2MIM]+						
Lit. value	-0.093	-0.052	0.040	-1.620	-4.667	4.034
Method 1	-0.093	-0.052	0.040	-1.620	-4.667	4.034
Method 2	-0.093	-0.052	0.040	-1.620	-4.667	4.034
Method 3	0.000	0.000	0.000	-1.620	-4.667	4.034
Method 4	0.000	0.000	0.000	-1.620	-4.667	4.034
[DM3AM]+						
Lit. value	-0.128	-0.131	0.329	-1.458	-4.550	3.816
Method 1	-0.128	-0.131	0.329	-1.458	-4.550	3.816
Method 2	-0.128	-0.131	0.329	-1.458	-4.550	3.816
Method 3	0.000	0.000	0.329	-1.458	-4.550	3.816
Method 4	0.000	0.000	0.329	-1.458	-4.550	3.816
[DMPyrr]+						
Lit. value	-0.083	-0.142	0.419	-1.467	-4.859	3.824
Method 1	-0.083	-0.142	0.419	-1.467	-4.859	3.824
Method 2	-0.083	-0.142	0.419	-1.467	-4.859	3.824
Method 3	0.000	-0.142	0.419	-1.467	-4.859	3.824
Method 4	0.000	-0.142	0.419	-1.467	-4.859	3.824

	c	*e*	*s*	*a*	*b*	*v*
Method 2	0.226	0.000	-0.212	-1.756	-4.739	3.825
Method 3	0.226	0.000	-0.212	-1.756	-4.739	3.825
Method 4	0.226	0.000	-0.212	-1.756	-4.739	3.825
[OM3AM]+						
Lit. value	-0.165	-0.181	0.569	-1.419	-4.677	3.711
Method 1	-0.165	-0.181	0.569	-1.419	-4.677	3.711
Method 2	-0.165	-0.181	0.569	-1.419	-4.677	3.711
Method 3	-0.165	-0.181	0.569	-1.419	-4.677	3.711
Method 4	-0.165	-0.181	0.569	-1.419	-4.677	3.711
[Ompyrr]+						
Lit. value	-0.253	0.000	0.520	-1.460	-4.696	3.815
Method 1	-0.253	0.000	0.520	-1.460	-4.696	3.815
Method 2	-0.253	0.000	0.520	-1.460	-4.696	3.815
Method 3	-0.253	0.000	0.520	-1.460	-4.696	3.815
Method 4	-0.253	0.000	0.520	-1.460	-4.696	3.815
[PDMIM]+						
Lit. value	-0.499	0.685	0.568	-0.238	-4.006	2.907
Method 1	-0.864	0.555	0.715	-1.147	-3.735	3.528
Method 2	-0.643	0.462	1.119	0.394	-3.594	3.079
Method 3	-0.873	0.480	0.783	-1.150	-3.897	3.538
Method 4	-0.717	0.452	1.110	0.392	-3.594	3.079
[PeMPyrr]+						
Lit. value	-0.303	0.000	0.727	-1.107	-4.622	3.630
Method 1	-0.303	0.000	0.727	-1.107	-4.622	3.630
Method 2	-0.303	0.000	0.727	-1.107	-4.622	3.630
Method 3	-0.303	0.000	0.727	-1.107	-4.622	3.630
Method 4	-0.303	0.000	0.727	-1.107	-4.622	3.630
[PM2iPAm]+						
Lit. value	-0.378	0.115	0.723	-1.061	-4.594	3.388
Method 1	-0.378	0.115	0.723	-1.061	-4.594	3.388
Method 2	-0.378	0.115	0.723	-1.061	-4.594	3.388
Method 3	-0.378	0.115	0.723	-1.061	-4.594	3.388
Method 4	-0.378	0.115	0.723	-1.061	-4.594	3.388

	c	*e*	*s*	*a*	*b*	*v*		*c*	*e*	*s*	*a*	*b*	*v*
[E3S]+							[PMPip]+						
Lit. value	-0.062	-1.347	2.716	-1.550	-5.274	3.242	Lit. value	-0.230	0.458	0.342	-1.259	-4.296	3.409
Method 1	-0.062	-1.347	2.716	1.350	-5.274	3.242	Method 1	-0.231	0.453	0.352	-1.263	-4.290	3.401
Method 2	-0.062	-1.347	2.716	1.350	-5.274	3.242	Method 2	-0.231	0.453	0.352	-1.263	-4.290	3.401
Method 3	0.000	-1.347	2.716	1.350	-5.274	3.242	Method 3	-0.231	0.453	0.352	-1.263	-4.290	3.401
Method 4	0.000	-1.347	2.716	1.350	-5.274	3.242	Method 4	-0.231	0.453	0.352	-1.263	-4.290	3.401
[EMIM]+							[PMPyrr]+						
Lit. value	-0.049	0.215	0.428	-1.294	-4.209	3.163	Lit. value	-0.236	0.000	0.908	-1.015	-4.691	3.446
Method 1	-0.130	0.190	0.338	-1.519	-4.096	3.228	Method 1	-0.236	0.000	0.908	-1.015	-4.691	3.446
Method 2	-0.117	0.184	0.434	-1.433	-4.237	3.164	Method 2	-0.236	0.000	0.908	-1.015	-4.691	3.446
Method 3	-0.144	0.153	0.373	-1.521	-4.188	3.234	Method 3	-0.236	0.000	0.908	-1.015	-4.691	3.446
Method 4	-0.134	0.198	0.428	-1.433	-4.237	3.164	Method 4	-0.236	0.000	0.908	-1.015	-4.691	3.446
[EtOHM2iPAm]+							[sec-BMIm]+						
Lit. value	-0.669	0.236	0.617	-0.850	-3.356	3.270	Lit. value	-0.215	0.000	0.740	-1.119	-4.496	3.436
Method 1	-0.669	0.236	0.617	-0.850	-3.356	3.270	Method 1	-0.215	0.000	0.740	-1.119	-4.496	3.436
Method 2	-0.669	0.236	0.617	-0.850	-3.356	3.270	Method 2	-0.215	0.000	0.740	-1.119	-4.496	3.436
Method 3	-0.669	0.236	0.617	-0.850	-3.356	3.270	Method 3	-0.215	0.000	0.740	-1.119	-4.496	3.436
Method 4	-0.669	0.236	0.617	-0.850	-3.356	3.270	Method 4	-0.215	0.000	0.740	-1.119	-4.496	3.436
[EtOHMIm]+							[tert-BMIm]+						
Lit. value	-0.404	0.229	0.517	-1.026	-3.493	2.931	Lit. value	-0.275	0.000	0.796	-0.926	-4.526	3.395
Method 1	-0.394	0.023	0.845	-1.045	-3.508	3.003	Method 1	-0.275	0.000	0.796	-0.926	-4.526	3.395
Method 2	-0.374	0.077	0.717	-0.956	-3.341	3.003	Method 2	-0.275	0.000	0.796	-0.926	-4.526	3.395
Method 3	-0.362	-0.004	0.879	-1.047	-3.583	3.007	Method 3	-0.275	0.000	0.796	-0.926	-4.526	3.395
Method 4	-0.346	0.065	0.716	-0.957	-3.341	3.003	Method 4	-0.275	0.000	0.796	-0.926	-4.526	3.395

Table D.42: Comparison of anion log *K* ABSM parameters for anions with more than one instance and their literature values and from methods 1, 2, 3, and 4.

	c	*e*	*s*	*a*	*b*	*l*		*c*	*e*	*s*	*a*	*b*	*l*
[+CS]-							[NTf2]-						
Lit. value	0.157	0.058	0.229	4.084	-0.522	0.131	Lit. value	0.000	0.000	0.000	0.000	0.000	0.000
Method 1	0.086	0.324	0.312	5.578	-0.612	0.069	Method 1	0.000	0.000	0.000	0.000	0.000	0.000
Method 2	0.317	0.075	0.345	4.468	-0.519	0.121	Method 2	0.000	0.000	0.000	0.000	0.000	0.000
Method 3	0.089	0.343	0.318	5.578	-0.613	0.069	Method 3	0.000	0.000	0.000	0.000	0.000	0.000

	c	*e*	*s*	*a*	*b*	*l*
Method 4	0.318	0.090	0.345	4.468	-0.521	0.121
[BETI]-						
Lit. value	0.068	-0.334	0.217	-0.196	-0.238	-0.279
Method 1	0.052	0.158	-0.178	-0.671	0.313	-0.122
Method 2	-0.046	0.117	0.020	-0.310	0.075	-0.120
Method 3	0.050	0.186	-0.179	-0.671	0.313	-0.122
Method 4	-0.045	0.149	0.020	-0.310	0.075	-0.120
[BF4]-						
Lit. value	-0.192	0.227	0.343	0.978	-0.287	-0.075
Method 1	-0.078	0.176	0.397	1.108	-0.465	-0.118
Method 2	-0.292	0.238	0.284	0.963	-0.329	-0.101
Method 3	-0.085	0.195	0.396	1.108	-0.465	-0.118
Method 4	-0.306	0.256	0.284	0.963	-0.328	-0.101
[DCA]-						
Lit. value	-0.372	0.345	0.476	2.270	-0.198	-0.055
Method 1	-0.373	0.441	0.257	2.436	-0.117	-0.084
Method 2	-0.357	0.375	0.291	2.257	-0.138	-0.066
Method 3	-0.373	0.461	0.258	2.436	-0.111	-0.084
Method 4	-0.357	0.395	0.291	2.257	-0.133	-0.066
[DEP]-						
Lit. value	0.093	0.107	-0.068	5.071	-0.774	0.061
Method 1	0.186	0.148	-0.001	5.166	-0.865	0.018
Method 2	0.167	0.133	-0.115	4.984	-0.765	0.043
Method 3	0.186	0.182	0.000	5.166	-0.863	0.018
Method 4	0.167	0.169	-0.115	4.984	-0.672	0.043
[EtSO4]-						
Lit. value	-0.173	-0.072	0.239	2.931	-0.668	-0.066
Method 1	-0.069	-0.047	0.319	3.061	-0.774	-0.108
Method 2	-0.088	-0.062	0.205	2.879	-0.674	-0.083
Method 3	-0.069	-0.013	0.320	3.061	-0.772	-0.108
Method 4	-0.088	-0.026	0.205	2.879	-0.672	-0.083
[FAP]-						
Lit. value	0.229	-0.049	-0.114	-1.277	0.341	-0.039

	c	*e*	*s*	*a*	*b*	*l*
Method 4	0.000	0.000	0.000	0.000	0.000	0.000
[OS]-						
Lit. value	0.057	-0.126	-0.077	2.575	-0.587	0.108
Method 1	0.195	0.103	-0.568	2.722	-0.230	0.075
Method 2	0.262	-0.074	-0.133	2.711	-0.601	0.068
Method 3	0.195	0.130	-0.567	2.722	-0.229	0.075
Method 4	0.262	-0.051	-0.133	2.711	-0.601	0.068
[PF6]-						
Lit. value	-0.016	-0.158	0.529	0.035	-0.149	-0.096
Method 1	-0.021	0.292	-0.155	0.109	0.458	-0.100
Method 2	-0.088	-0.067	0.474	0.175	-0.215	-0.097
Method 3	-0.001	0.340	-0.167	0.109	0.458	-0.100
Method 4	-0.066	-0.014	0.474	0.175	-0.215	-0.097
[SCN]-						
Lit. value	-0.566	0.431	0.534	2.806	-0.272	-0.040
Method 1	-0.520	0.723	0.144	2.464	0.211	-0.072
Method 2	-0.587	0.688	0.270	2.665	0.060	-0.066
Method 3	-0.521	0.746	0.143	2.464	0.212	-0.072
Method 4	-0.586	0.714	0.270	2.665	0.062	-0.066
[TCB]-						
Lit. value	0.048	-0.009	0.345	0.371	-0.143	-0.012
Method 1	0.077	0.101	0.339	0.310	-0.053	-0.045
Method 2	0.053	0.081	0.317	0.252	-0.042	-0.032
Method 3	0.077	0.094	0.339	0.310	-0.051	-0.045
Method 4	0.053	0.076	0.317	0.252	-0.040	-0.032
[TCM]-						
Lit. value	-0.098	0.094	0.290	1.338	-0.145	0.005
Method 1	-0.194	0.230	0.137	0.746	0.156	-0.047
Method 2	-0.271	0.211	0.216	0.879	0.060	-0.041
Method 3	-0.196	0.227	0.136	0.746	0.157	-0.047
Method 4	-0.272	0.211	0.216	0.879	0.061	-0.041
[TDI]-						
Lit. value	-0.046	0.013	0.088	1.132	0.013	0.049

	c	*e*	*s*	*a*	*b*	*l*
Method 1	0.298	-0.006	-0.135	-1.277	0.479	-0.052
Method 2	0.271	-0.032	-0.123	-1.314	0.460	-0.043
Method 3	0.299	0.002	-0.136	-1.277	0.480	-0.052
Method 4	0.272	-0.022	-0.123	-1.314	0.461	-0.043
[FSI]-						
Lit. value	-0.147	0.134	0.295	0.133	-0.021	0.003
Method 1	-0.171	0.266	0.175	-0.040	0.184	-0.029
Method 2	-0.207	0.237	0.228	0.000	0.122	-0.021
Method 3	-0.171	0.284	0.175	-0.040	0.187	-0.029
Method 4	-0.207	0.257	0.228	0.000	0.125	-0.021
[L-Lact]-						
Lit. value	0.197	0.113	0.124	4.370	-0.613	0.003
Method 1	0.096	0.379	0.207	5.864	-0.703	-0.059
Method 2	0.327	0.130	0.240	4.754	-0.610	-0.007
Method 3	0.099	0.398	0.213	5.864	-0.704	-0.059
Method 4	0.328	0.145	0.240	4.754	-0.612	-0.007
[MeSO3]-						
Lit. value	-0.827	0.463	0.417	4.083	-0.280	-0.023
Method 1	-0.585	0.422	0.317	4.047	-0.212	-0.075
Method 2	-0.644	0.394	0.359	4.136	-0.281	-0.061
Method 3	-0.586	0.452	0.316	4.047	-0.211	-0.075
Method 4	-0.643	0.428	0.359	4.136	-0.280	-0.061

	c	*e*	*s*	*a*	*b*	*l*
Method 1	0.035	0.055	-0.126	0.794	0.212	0.022
Method 2	-0.054	0.016	0.052	1.109	-0.002	0.025
Method 3	0.033	0.123	-0.127	0.794	0.198	0.022
Method 4	-0.053	0.087	0.052	1.109	-0.015	0.025
[TFA]-						
Lit. value	-0.295	-0.186	0.545	3.113	-0.078	0.014
Method 1	-0.212	-0.047	0.456	3.196	-0.040	-0.027
Method 2	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
Method 3	-0.212	-0.013	0.457	3.196	-0.038	-0.027
Method 4	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
[Trif]-						
Lit. value	-0.275	0.035	0.323	1.709	-0.175	-0.002
Method 1	-0.201	0.150	0.087	1.361	0.062	-0.040
Method 2	-0.272	0.115	0.223	1.585	-0.101	-0.035
Method 3	-0.202	0.175	0.086	1.361	0.070	-0.040
Method 4	-0.271	0.142	0.223	1.585	-0.092	-0.035

Table D.43: Comparison of anion log *P* ABSM parameters for anions with more than one instance and their literature values and from methods 1, 2, 3, and 4.

	c	*e*	*s*	*a*	*b*	*v*
[+CS]-						
Lit. value	-0.049	-0.166	0.363	5.498	-0.568	0.510
Method 1	0.028	0.532	0.123	5.443	-0.767	0.375
Method 2	0.246	0.155	0.456	4.505	-0.666	0.474
Method 3	0.031	0.621	0.053	5.448	-0.614	0.366
Method 4	0.281	0.149	0.409	4.506	-0.666	0.474

	c	*e*	*s*	*a*	*b*	*v*
[NTf2]-						
Lit. value	0.000	0.000	0.000	0.000	0.000	0.000
Method 1	0.000	0.000	0.000	0.000	0.000	0.000
Method 2	0.000	0.000	0.000	0.000	0.000	0.000
Method 3	0.000	0.000	0.000	0.000	0.000	0.000
Method 4	0.000	0.000	0.000	0.000	0.000	0.000

	c	*e*	*s*	*a*	*b*	*v*		*c*	*e*	*s*	*a*	*b*	*v*
[BETI]-							[OS]-						
Lit. value	0.071	-0.245	0.038	-0.318	0.101	-0.349	Lit. value	-0.040	-0.043	0.002	2.583	-0.577	0.424
Method 1	0.258	-0.257	-0.224	-0.764	-0.196	-0.429	Method 1	0.197	0.101	-0.516	2.747	-0.593	0.287
Method 2	0.129	-0.050	-0.345	-0.455	-0.110	-0.401	Method 2	0.220	0.071	-0.260	2.611	-0.689	0.261
Method 3	0.188	-0.242	-0.298	-0.757	-0.019	-0.440	Method 3	0.121	0.201	-0.576	2.751	-0.452	0.279
Method 4	0.079	-0.105	-0.332	-0.450	-0.110	-0.401	Method 4	0.180	0.121	-0.367	2.613	-0.689	0.261
[BF4]-							[PF6]-						
Lit. value	-0.084	0.129	0.240	1.108	-0.401	-0.296	Lit. value	0.007	-0.230	0.417	0.131	-0.120	-0.297
Method 1	0.250	-0.192	0.440	0.925	-1.280	-0.491	Method 1	0.043	0.109	-0.278	0.290	0.111	-0.336
Method 2	0.040	0.337	-0.295	0.489	-0.823	-0.443	Method 2	0.001	-0.064	0.118	0.051	-0.412	-0.355
Method 3	0.268	-0.042	0.305	0.932	-0.958	-0.511	Method 3	0.012	0.226	-0.346	0.294	0.268	-0.346
Method 4	0.114	0.347	-0.286	0.491	-0.823	-0.443	Method 4	-0.024	0.037	0.126	0.054	-0.412	-0.355
[DCA]-							[SCN]-						
Lit. value	-0.257	0.164	0.446	2.217	-0.256	-0.243	Lit. value	-0.534	0.187	0.644	2.801	-0.315	-0.130
Method 1	-0.199	0.278	0.201	2.423	-0.211	-0.349	Method 1	-0.449	0.065	0.862	2.456	-0.110	-0.249
Method 2	-0.193	0.263	0.209	2.287	-0.123	-0.307	Method 2	-0.537	0.213	0.763	2.629	-0.011	-0.224
Method 3	-0.205	0.343	0.153	2.425	-0.097	-0.356	Method 3	-0.484	0.122	0.794	2.458	0.051	-0.259
Method 4	-0.186	0.272	0.203	2.287	-0.123	-0.307	Method 4	-0.555	0.204	0.771	2.629	-0.011	-0.224
[DEP]-							[TCB]-						
Lit. value	0.071	0.073	0.006	5.089	-0.832	0.184	Lit. value	0.072	-0.075	0.347	0.312	-0.121	0.061
Method 1	0.152	0.099	0.096	5.315	-0.945	0.118	Method 1	0.002	-0.076	0.528	0.445	0.082	-0.183
Method 2	0.139	0.105	0.000	5.229	-0.804	0.182	Method 2	-0.023	-0.039	0.462	0.423	0.180	-0.148
Method 3	0.144	0.136	0.061	5.317	-0.853	0.112	Method 3	0.017	0.026	0.488	0.446	0.179	-0.189
Method 4	0.134	0.091	0.006	5.229	-0.804	0.182	Method 4	0.000	0.017	0.464	0.422	0.180	-0.148
[EtSO4]-							[TCM]-						
Lit. value	-0.029	-0.245	0.129	2.792	-0.745	-0.264	Lit. value	-0.079	0.056	0.276	1.223	-0.070	-0.008
Method 1	0.051	-0.211	0.216	3.010	-0.848	-0.333	Method 1	-0.326	0.249	1.080	2.523	3.604	-0.426
Method 2	0.038	-0.205	0.120	2.924	-0.707	-0.269	Method 2	-0.442	0.537	0.814	2.602	3.982	-0.416
Method 3	0.144	-0.153	0.181	3.012	-0.756	-0.339	Method 3	-0.378	0.442	0.912	2.530	4.011	-0.451
Method 4	0.134	-0.198	0.126	2.924	-0.707	-0.269	Method 4	-0.451	0.553	0.820	2.603	3.982	-0.416
[FAP]-							[TDI]-						
Lit. value	0.198	0.049	-0.214	-1.344	0.449	-0.109	Lit. value	-0.043	-0.019	0.104	0.996	0.146	0.128
Method 1	0.196	0.092	-0.195	-1.215	0.696	-0.114	Method 1	0.107	-0.060	-0.074	0.546	-0.076	0.050

	c	*e*	*s*	*a*	*b*	*v*
Method 2	0.179	0.102	-0.208	-1.244	0.719	-0.095
Method 3	0.130	0.091	-0.228	-1.215	0.763	-0.118
Method 4	0.118	0.073	-0.211	-1.244	0.719	-0.095
[FSI]-						
Lit. value	-0.092	-0.038	0.406	0.082	-0.074	-0.051
Method 1	-0.108	-0.048	0.610	0.216	0.574	-0.198
Method 2	-0.156	0.041	0.533	0.253	0.686	-0.176
Method 3	-0.132	0.024	0.549	0.215	0.718	-0.207
Method 4	-0.165	0.051	0.536	0.249	0.686	-0.176
[L-Lact]-						
Lit. value	-0.049	-0.166	-0.134	1.885	-0.554	0.113
Method 1	0.028	0.532	-0.106	5.935	-0.753	-0.022
Method 2	0.246	0.155	0.227	4.997	-0.652	0.077
Method 3	0.031	0.621	-0.176	5.940	-0.600	-0.031
Method 4	0.281	0.149	0.180	4.998	-0.652	0.077
[MeSO3]-						
Lit. value	-0.646	0.347	0.315	3.997	-0.336	-0.242
Method 1	-0.464	0.153	0.399	4.135	-0.626	-0.261
Method 2	-0.535	0.259	0.291	4.247	-0.512	-0.215
Method 3	-0.481	0.221	0.344	4.140	-0.491	-0.269
Method 4	-0.540	0.267	0.300	4.249	-0.512	-0.215

	c	*e*	*s*	*a*	*b*	*v*
Method 2	-0.010	0.129	-0.189	0.816	0.014	0.076
Method 3	0.079	-0.069	-0.147	0.542	0.097	0.039
Method 4	-0.019	0.053	-0.178	0.810	0.014	0.076
[TFA]-						
Lit. value	-0.286	-0.697	0.859	2.284	0.475	0.056
Method 1	0.001	-1.441	2.018	2.408	-0.377	-0.184
Method 2	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
Method 3	0.015	-1.404	1.983	2.410	-0.285	-0.190
Method 4	#N/A	#N/A	#N/A	#N/A	#N/A	#N/A
[Trif]-						
Lit. value	-0.228	-0.088	0.367	1.560	-0.091	-0.047
Method 1	-0.111	-0.088	0.238	1.434	0.020	-0.179
Method 2	-0.205	0.068	0.135	1.627	0.117	-0.154
Method 3	-0.139	0.000	0.169	1.409	0.183	-0.189
Method 4	-0.216	0.090	0.144	1.599	0.117	-0.154

Table D.44: Calculated $[EMIM]^+[FAP]^-$/dichloromethane partitioning from water (log *P*) and from gas (log *K*).

	log *P*	log *K*	Δ from literature log *P*	Δ from literature log *K*
IL Specific	1.356	2.347	0.000	0.000
Lit (cation + anion)	1.432	2.391	-0.076	-0.044
Method 1	1.353	2.376	0.003	-0.030
Method 2	1.376	2.412	-0.020	-0.065
Method 3	1.259	2.366	0.097	-0.019
Method 4	1.287	2.403	0.069	-0.056

Table D.45: Calculated [Bmpyrr]$^+$[DCA]$^-$/dichloromethane partitioning from water (log *P*) and from gas (log *K*).

	log *P*	log *K*	Δ from literature log *P*	Δ from literature log *K*
IL Specific	2.018	2.861	0.000	0.000
Lit (cation + anion)	1.428	2.708	0.590	0.153
Method 1	1.617	2.692	0.401	0.169
Method 2	1.670	2.719	0.348	0.142
Method 3	1.640	2.694	0.379	0.167
Method 4	1.681	2.719	0.337	0.142

Table D.46: Calculated [Bmpyrr]$^+$[Trif]$^-$/dichloromethane partitioning from water (log *P*) and from gas (log *K*).

	log *P*	log *K*	Δ from literature log *P*	Δ from literature log *K*
IL Specific	1.624	2.633	0.000	0.000
Lit (cation + anion)	1.354	2.649	0.270	-0.015
Method 1	1.580	2.644	0.044	-0.011
Method 2	1.562	2.661	0.062	-0.028
Method 3	1.576	2.645	0.048	-0.012
Method 4	1.565	2.665	0.058	-0.032

Table D.47: Calculated [HMIM]$^+$[NTf2]$^-$/dichloromethane partitioning from water (log *P*) and from gas (log *K*).

	log *P*	log *K*	Δ from literature log *P*	Δ from literature log *K*
IL Specific	1.497	2.501	0.000	0.000
Lit (cation + anion)	1.577	2.540	-0.080	-0.038
Method 1	1.539	2.520	-0.042	-0.019
Method 2	1.553	2.530	-0.056	-0.029
Method 3	1.534	2.533	-0.037	-0.031
Method 4	1.540	2.544	-0.044	-0.043

Table D.48: Comparison of $[BMIM]^+[DCA]^-$ log K and log P values for IL specific parameters, literature cation + anion parameters, and parameters from Methods 1, 2, 3, and 4 for all the solutes listed Table D.1.

	CAS	IL Specific		Lit (cation + anion)		Method 1		Method 2		Method 3		Method 4	
		log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*
(E)-Hept-2-ene	14686-13-6	1.277	2.520	1.336	2.568	1.279	2.497	1.289	2.495	1.278	2.480	1.288	2.487
(E)-Hex-2-enal	6728-26-3	3.753	1.177	3.776	1.242	3.597	1.019	3.651	1.069	3.593	1.009	3.646	1.058
(E)-Oct-2-enal	2548-87-0	4.309	2.024	4.312	2.091	4.156	1.866	4.200	1.907	4.153	1.855	4.196	1.896
(Z)-1,2-Dichloroethene	156-59-2	2.986	1.964	3.007	2.001	2.808	1.795	2.888	1.847	2.802	1.780	2.882	1.840
(Z)-Pent-2-ene	627-20-3	0.687	1.708	0.764	1.753	0.696	1.695	0.712	1.699	0.694	1.679	0.710	1.691
1,1,1,2,3,3-Hexafluoropropane	431-63-0	0.491	1.425	0.524	1.422	0.364	1.258	0.449	1.286	0.373	1.220	0.459	1.260
1,1,1,2-Tetrachloroethane	630-20-6	3.788	2.705	3.794	2.754	3.615	2.543	3.681	2.587	3.608	2.530	3.673	2.582
1,1,1,2-Tetrafluoroethane	811-97-2	0.359	0.951	0.409	0.957	0.270	0.832	0.340	0.855	0.275	0.799	0.346	0.834
1,1,1-Trichloroethane	71-55-6	2.055	1.956	2.104	2.003	1.964	1.859	2.011	1.891	1.959	1.845	2.005	1.885
1,1,1-Trifluoroethane	420-46-2	-0.585	0.488	-0.499	0.505	-0.619	0.417	-0.566	0.438	-0.614	0.388	-0.561	0.419
1,1,2,2-Tetrachloroethane	79-34-5	4.589	2.717	4.577	2.767	4.377	2.523	4.453	2.574	4.369	2.511	4.444	2.569
1,1,2-Trichloroethane	79-00-5	3.844	2.410	3.845	2.453	3.647	2.226	3.725	2.277	3.640	2.212	3.717	2.271
1,1,2-TrichloroTrifluoroethane	76-13-1	0.752	2.147	0.813	2.179	0.711	2.080	0.749	2.094	0.711	2.058	0.749	2.083
1,1-Dibromoethane	557-91-5	3.497	1.982	3.525	2.040	3.355	1.853	3.411	1.895	3.346	1.846	3.402	1.892
1,1-Dichloro-1-fluoroethane	1717-00-6	1.532	1.766	1.574	1.793	1.396	1.614	1.471	1.658	1.395	1.591	1.470	1.645
1,1-Dichloroethane	75-34-3	2.492	1.705	2.525	1.744	2.361	1.573	2.424	1.612	2.357	1.557	2.419	1.604
1,1-Difluoroethane	75-37-6	0.842	0.973	0.883	0.978	0.663	0.768	0.768	0.826	0.666	0.736	0.772	0.805
1,1-Difluoroethylene	75-38-7	-0.859	0.523	-0.752	0.551	-0.840	0.511	-0.808	0.521	-0.838	0.489	-0.806	0.509
1,1-Dimethylcyclohexane	590-66-9	1.599	3.114	1.651	3.164	1.588	3.082	1.600	3.082	1.584	3.067	1.596	3.076
1,1-Dimethylcyclopentane	1638-26-2	1.246	2.695	1.306	2.741	1.235	2.663	1.253	2.666	1.232	2.646	1.249	2.660
1,2,3,4-Tetrachlorobenzene	634-66-2	5.914	4.394	5.889	4.467	5.677	4.191	5.745	4.255	5.660	4.191	5.726	4.261
1,2,3,4-Tetrahydronaphthalene	119-64-2	4.501	3.182	4.515	3.261	4.381	3.078	4.410	3.111	4.369	3.077	4.396	3.114
1,2,3,5-Tetrachlorobenzene	634-90-2	5.552	4.324	5.536	4.398	5.340	4.144	5.400	4.201	5.324	4.144	5.382	4.207
1,2,3-Trichlorobenzene	87-61-6	5.221	3.935	5.207	4.000	4.994	3.736	5.066	3.799	4.979	3.733	5.049	3.803
1,2,3-Trimethylbenzene	526-73-8	3.940	2.909	3.962	2.982	3.826	2.803	3.859	2.835	3.816	2.798	3.848	2.834
1,2,4,5-Tetrachlorobenzene	95-94-3	5.583	4.333	5.567	4.407	5.367	4.149	5.429	4.207	5.351	4.150	5.411	4.213
1,2,4-Trichlorobenzene	120-82-1	4.952	3.874	4.944	3.937	4.740	3.686	4.808	3.745	4.726	3.682	4.792	3.748
1,2,4-Trimethylbenzene	95-63-6	3.701	2.847	3.727	2.919	3.601	2.752	3.630	2.780	3.592	2.747	3.620	2.779
1,2-Dibromoethane	106-93-4	4.120	2.078	4.135	2.138	3.943	1.921	4.008	1.973	3.933	1.916	3.997	1.972
1,2-Dichlorobenzene	95-50-1	4.391	3.273	4.395	3.334	4.191	3.094	4.261	3.152	4.179	3.088	4.247	3.153
1,2-Dichloroethane	107-06-2	3.125	1.828	3.144	1.868	2.948	1.658	3.025	1.710	2.942	1.643	3.019	1.702
1,2-Dichloropropane	78-87-5	2.786	1.846	2.816	1.892	2.629	1.686	2.698	1.737	2.624	1.671	2.692	1.728
1,2-Dichlorotetrafluoroethane	76-14-2	-0.038	1.705	0.035	1.727	-0.066	1.642	-0.024	1.654	-0.063	1.615	-0.021	1.639
1,3,5-Trichlorobenzene	108-70-3	4.597	3.801	4.599	3.868	4.416	3.643	4.474	3.693	4.402	3.640	4.458	3.697
1,3-Butadiene	106-99-0	0.788	1.233	0.874	1.282	0.769	1.202	0.799	1.220	0.765	1.189	0.794	1.214
1,3-Cyclohexadiene	592-57-4	2.116	1.846	2.176	1.905	2.059	1.789	2.090	1.813	2.053	1.780	2.082	1.811
1,3-Dichloro-2-propanol	96-23-1	5.545	0.570	5.539	0.652	5.447	0.499	5.461	0.507	5.441	0.498	5.454	0.502
1,3-Dichlorobenzene	541-73-1	4.164	3.312	4.172	3.372	3.977	3.143	4.044	3.198	3.965	3.137	4.030	3.199
1,3-Dichloropropane	142-28-9	3.281	1.959	3.298	2.003	3.085	1.764	3.166	1.825	3.080	1.749	3.160	1.816
1,3-Dimethylnaphthalene	575-41-7	6.118	4.023	6.116	4.124	5.951	3.892	5.983	3.937	5.932	3.902	5.961	3.948
1,4-Dichlorobutane	110-56-5	4.133	2.559	4.122	2.598	3.854	2.283	3.963	2.363	3.849	2.265	3.957	2.351
1,4-Dimethylnaphthalene	571-58-4	6.157	4.017	6.154	4.119	5.994	3.891	6.023	3.935	5.975	3.902	6.001	3.946
1,4-Dioxane	123-91-1	3.349	-0.468	3.394	-0.395	3.252	-0.566	3.283	-0.525	3.250	-0.573	3.280	-0.536

	CAS	IL Specific		Lit (cation + anion)		Method 1		Method 2		Method 3		Method 4	
		log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*
1,4-Hexadiene	592-45-0	1.370	1.998	1.434	2.048	1.348	1.959	1.369	1.970	1.345	1.945	1.366	1.963
1,6-Heptadiene	3070-53-9	1.568	2.391	1.624	2.440	1.540	2.342	1.561	2.350	1.537	2.326	1.558	2.342
1-Bromo-2-methylpropane	78-77-3	2.081	2.034	2.130	2.084	2.008	1.952	2.046	1.977	2.004	1.938	2.041	1.971
1-Bromobutane	109-65-9	2.265	2.067	2.309	2.118	2.182	1.977	2.221	2.005	2.177	1.964	2.216	1.999
1-Bromoheptane	629-04-9	3.218	3.288	3.234	3.345	3.126	3.185	3.155	3.204	3.121	3.171	3.150	3.197
1-Bromohexane	111-25-1	2.893	2.883	2.919	2.937	2.804	2.784	2.837	2.806	2.800	2.770	2.832	2.799
1-Bromooctane	111-83-1	3.426	3.698	3.436	3.756	3.332	3.591	3.359	3.607	3.327	3.576	3.354	3.600
1-Bromopentane	110-53-2	2.577	2.477	2.612	2.529	2.491	2.383	2.527	2.408	2.487	2.370	2.522	2.401
1-Bromopropane	106-94-5	1.969	1.662	2.023	1.710	1.890	1.576	1.932	1.607	1.885	1.563	1.927	1.601
1-Butanol	71-36-3	3.882	0.413	3.898	0.477	3.831	0.372	3.842	0.370	3.830	0.362	3.840	0.360
1-Butene	106-98-9	0.251	1.286	0.339	1.327	0.259	1.271	0.282	1.279	0.258	1.254	0.280	1.270
1-Butyne	107-00-6	1.364	1.081	1.428	1.125	1.331	1.038	1.362	1.050	1.329	1.023	1.360	1.042
1-Chloro-1,1-difluoroethane	75-68-3	0.650	1.239	0.711	1.262	0.572	1.137	0.632	1.164	0.573	1.112	0.633	1.150
1-Chloroanthraquinone	82-44-0	10.784	4.125	10.694	4.255	10.409	3.824	10.479	3.923	10.385	3.845	10.451	3.935
1-Chlorobutane	109-69-3	1.963	1.957	2.005	1.997	1.861	1.842	1.913	1.875	1.859	1.824	1.910	1.865
1-Chloroheptane	629-06-1	2.918	3.178	2.931	3.224	2.806	3.049	2.848	3.074	2.804	3.031	2.846	3.064
1-Chlorohexane	544-10-5	2.610	2.772	2.633	2.816	2.502	2.648	2.547	2.676	2.499	2.630	2.544	2.666
1-Chloropentane	543-59-9	2.272	2.366	2.305	2.408	2.168	2.247	2.216	2.278	2.165	2.229	2.213	2.268
1-Chloroprop-2-ene	107-05-1	2.070	1.834	2.111	1.869	1.911	1.670	1.991	1.724	1.906	1.653	1.986	1.715
1-Cyanobutane	110-59-8	3.739	1.315	3.740	1.356	3.501	1.070	3.595	1.142	3.500	1.051	3.593	1.125
1-Cyanopropane	109-74-0	3.398	0.909	3.409	0.948	3.163	0.669	3.260	0.744	3.162	0.650	3.258	0.728
1-Decanol	112-30-1	5.738	2.858	5.698	2.934	5.669	2.792	5.660	2.772	5.668	2.780	5.659	2.761
1-Decene	872-05-9	2.101	3.737	2.134	3.791	2.093	3.700	2.095	3.689	2.092	3.682	2.094	3.681
1-Decyne	764-93-2	2.969	3.704	2.980	3.756	2.912	3.627	2.929	3.625	2.910	3.609	2.927	3.616
1-Dodecene	112-41-4	2.707	4.556	2.722	4.614	2.694	4.511	2.689	4.495	2.693	4.493	2.688	4.486
1-Ethylnaphthalene	1127-76-0	5.905	3.971	5.908	4.073	5.755	3.856	5.782	3.896	5.736	3.866	5.760	3.907
1H-1,2,4-Triazole	288-88-0	10.425	1.641	10.260	1.676	9.939	1.239	10.090	1.318	9.931	1.227	10.081	1.305
1-Heptanol	111-70-6	4.812	1.637	4.801	1.707	4.753	1.584	4.754	1.573	4.752	1.574	4.752	1.563
1-Heptene	592-76-7	1.194	2.510	1.253	2.557	1.193	2.483	1.205	2.482	1.192	2.465	1.204	2.473
1-Heptyne	628-71-7	2.249	2.529	2.282	2.575	2.194	2.461	2.222	2.467	2.192	2.444	2.220	2.458
1-Hexadecene	629-73-2	3.928	6.189	3.907	6.256	3.904	6.129	3.885	6.100	3.903	6.110	3.884	6.091
1-Hexanol	111-27-3	4.501	1.228	4.498	1.296	4.444	1.178	4.448	1.170	4.443	1.168	4.446	1.160
1-Hexene	592-41-6	0.887	2.098	0.955	2.142	0.888	2.073	0.904	2.075	0.887	2.055	0.903	2.066
1-Hexyne	693-02-7	1.950	2.123	1.993	2.168	1.899	2.060	1.930	2.069	1.897	2.043	1.928	2.060
1-Iodobutane	542-69-8	2.702	2.261	2.754	2.329	2.653	2.214	2.672	2.233	2.645	2.209	2.662	2.233
1-Iodoheptane	4282-40-0	3.599	3.527	3.622	3.601	3.538	3.465	3.548	3.475	3.530	3.458	3.539	3.475
1-Iodohexane	638-45-9	3.311	3.076	3.344	3.148	3.256	3.021	3.268	3.034	3.247	3.015	3.258	3.033
1-Iodopentane	628-17-1	3.008	2.667	3.050	2.737	2.956	2.615	2.971	2.631	2.948	2.609	2.962	2.631
1-Iodopropane	107-08-4	2.395	1.852	2.456	1.918	2.349	1.808	2.371	1.830	2.340	1.803	2.361	1.830
1-Methyl-3-propylbenzene	1074-43-7	3.667	3.228	3.691	3.300	3.580	3.141	3.602	3.161	3.572	3.134	3.593	3.159
1-Methyl-4-propylbenzene	1074-55-1	3.682	3.228	3.705	3.300	3.595	3.141	3.617	3.161	3.587	3.134	3.608	3.159
1-Methylcyclohexene	591-49-1	1.925	2.265	1.983	2.325	1.916	2.246	1.924	2.252	1.911	2.236	1.918	2.249
1-Methylnaphthalene	90-12-0	5.898	3.525	5.899	3.622	5.724	3.388	5.762	3.438	5.706	3.397	5.741	3.447
1-Naphthol	90-15-3	9.469	3.333	9.390	3.440	9.253	3.200	9.280	3.221	9.234	3.216	9.257	3.233
1-Naphthylamine	134-32-7	8.474	2.401	8.444	2.529	8.274	2.270	8.297	2.318	8.253	2.291	8.272	2.332

	CAS	IL Specific		Lit (cation + anion)		Method 1		Method 2		Method 3		Method 4	
		log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*
1-Nitrobutane	627-05-4	4.062	1.751	4.051	1.788	3.792	1.478	3.897	1.557	3.790	1.458	3.894	1.541
1-Nitropentane	628-05-7	4.377	2.154	4.355	2.192	4.102	1.875	4.205	1.951	4.101	1.854	4.202	1.934
1-Nitropropane	108-03-2	3.753	1.254	3.753	1.291	3.491	0.991	3.597	1.072	3.489	0.972	3.594	1.056
1-Nonanol	143-08-8	5.427	2.449	5.396	2.523	5.361	2.386	5.355	2.369	5.360	2.375	5.354	2.358
1-Nonene	124-11-8	1.817	3.328	1.858	3.380	1.811	3.294	1.816	3.287	1.810	3.276	1.815	3.278
1-Nonyne	3452-09-3'	2.653	3.298	2.674	3.349	2.600	3.226	2.620	3.227	2.598	3.209	2.617	3.218
1-Octanol	111-87-5	5.119	2.043	5.098	2.115	5.056	1.985	5.054	1.971	5.056	1.974	5.052	1.961
1-Octene	111-66-0	1.505	2.919	1.556	2.968	1.502	2.889	1.511	2.884	1.501	2.871	1.510	2.875
1-Octyne	629-05-0	2.570	2.939	2.594	2.987	2.513	2.867	2.537	2.869	2.511	2.849	2.535	2.860
1-Pentadecene	13360-61-7	3.623	5.780	3.611	5.845	3.601	5.724	3.587	5.698	3.600	5.704	3.585	5.689
1-Pentanol	71-41-0	4.193	0.822	4.200	0.888	4.140	0.777	4.147	0.772	4.139	0.768	4.145	0.762
1-Pentene	109-67-1	0.567	1.692	0.645	1.734	0.571	1.672	0.591	1.677	0.570	1.654	0.589	1.668
1-Pentyne	627-19-0	1.642	1.714	1.693	1.756	1.593	1.655	1.627	1.666	1.591	1.638	1.625	1.657
1-Propanal	123-38-6	2.267	-0.127	2.323	-0.074	2.155	-0.248	2.209	-0.202	2.154	-0.262	2.207	-0.215
1-Propanol	71-23-8	3.538	0.010	3.565	0.073	3.492	-0.025	3.506	-0.024	3.491	-0.033	3.503	-0.033
1-Tetradecene	1120-36-1	3.323	5.374	3.320	5.437	3.304	5.323	3.293	5.300	3.303	5.304	3.291	5.291
1-Tridecene	2437-56-1	3.018	4.965	3.024	5.026	3.003	4.917	2.994	4.897	3.002	4.898	2.993	4.888
1-Undecene	821-95-4	2.403	4.147	2.427	4.203	2.393	4.106	2.391	4.092	2.392	4.087	2.390	4.083
2,2,2-Trifluoroethanol	75-89-8	4.336	1.078	4.306	1.102	4.129	0.888	4.215	0.916	4.130	0.866	4.215	0.900
2,2,3,3-Tetramethylpentane	7154-79-2	1.404	3.669	1.447	3.714	1.404	3.635	1.411	3.623	1.404	3.613	1.411	3.613
2,2,3-Trimethylbutane	464-06-2	0.810	2.851	0.871	2.891	0.815	2.823	0.829	2.818	0.815	2.802	0.829	2.808
2,2,3-Trimethylpentane	564-02-3	1.062	3.260	1.115	3.303	1.064	3.229	1.076	3.221	1.064	3.208	1.076	3.211
2,2,4,4-Tetramethylpentane	1070-87-7	1.177	3.669	1.227	3.714	1.178	3.635	1.189	3.623	1.178	3.613	1.189	3.613
2,2,4-Trimethylpentane	540-84-1	0.926	3.260	0.983	3.303	0.930	3.229	0.943	3.221	0.930	3.208	0.943	3.211
2,2,5-Trimethylhexane	3522-94-9	1.211	3.669	1.260	3.714	1.212	3.635	1.222	3.623	1.212	3.613	1.222	3.613
2,2-Dichloro-1,1,1-trifluoroethane	306-83-2	2.232	2.187	2.235	2.196	2.052	1.992	2.143	2.030	2.054	1.962	2.145	2.012
2,2-Dimethyl-3-ethylpentane	16747-32-3	1.318	3.669	1.363	3.714	1.318	3.635	1.327	3.623	1.318	3.613	1.327	3.613
2,2-Dimethylbutane	75-83-2	0.461	2.441	0.532	2.480	0.468	2.418	0.487	2.416	0.468	2.397	0.487	2.406
2,2-Dimethylhexane	590-73-8	1.022	3.260	1.076	3.303	1.025	3.229	1.037	3.221	1.025	3.208	1.037	3.211
2,2-Dimethyloctane	15869-87-1	1.617	4.078	1.654	4.125	1.615	4.040	1.620	4.026	1.615	4.019	1.620	4.016
2,2-Dimethylpentane	590-35-2	0.735	2.851	0.798	2.891	0.740	2.823	0.756	2.818	0.740	2.802	0.756	2.808
2,2-Dimethylpropane	630-18-2	3.387	0.975	3.401	1.020	3.183	0.761	3.264	0.824	3.182	0.742	3.263	0.807
2,3,3-Trimethyl-1-butene	594-56-9	1.111	2.162	1.180	2.216	1.129	2.153	1.133	2.148	1.128	2.138	1.132	2.140
2,3,3-Trimethylpentane	560-21-4	1.125	3.260	1.176	3.303	1.127	3.229	1.138	3.221	1.127	3.208	1.138	3.211
2,3,4-Trimethylpentane	565-75-3	1.158	3.260	1.208	3.303	1.159	3.229	1.170	3.221	1.159	3.208	1.170	3.211
2,3-Butanediol	513-85-9	7.114	-0.506	7.067	-0.425	6.951	-0.634	6.979	-0.620	6.949	-0.638	6.976	-0.633
2,3-Dimethyl-1,3-butaDiene	513-81-5	1.524	1.879	1.593	1.937	1.512	1.855	1.527	1.864	1.508	1.844	1.522	1.859
2,3-Dimethyl-1-butene	563-78-0	0.838	1.839	0.916	1.892	0.865	1.842	0.870	1.838	0.863	1.827	0.868	1.831
2,3-Dimethyl-1-hexene	16746-86-4	1.414	2.699	1.472	2.753	1.425	2.683	1.428	2.675	1.424	2.666	1.427	2.667
2,3-Dimethyl-2-butene	563-79-1	1.129	1.877	1.203	1.932	1.153	1.881	1.156	1.878	1.151	1.867	1.153	1.871
2,3-Dimethylbutane	79-29-8	0.549	2.441	0.618	2.480	0.556	2.418	0.573	2.416	0.556	2.397	0.573	2.406
2,3-Dimethylhexane	584-94-1	1.139	3.260	1.190	3.303	1.141	3.229	1.152	3.221	1.141	3.208	1.152	3.211
2,3-Dimethylnaphthalene	581-40-8	6.254	4.063	6.249	4.165	6.079	3.927	6.113	3.974	6.059	3.938	6.091	3.986
2,3-Dimethylpentane	565-59-3	0.871	2.851	0.930	2.891	0.875	2.823	0.889	2.818	0.875	2.802	0.889	2.808
2,3-Dimethylphenol	526-75-0	7.410	2.614	7.350	2.692	7.224	2.477	7.259	2.493	7.213	2.477	7.246	2.493

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2,3-Dimethylpyridine	583-61-9	4.235	0.551	4.274	0.644	4.155	0.480	4.167	0.511	4.148	0.481	4.158	0.507
2,4,4-Trimethyl-1-pentene	107-39-1	1.304	2.910	1.361	2.960	1.306	2.883	1.316	2.878	1.305	2.865	1.314	2.869
2,4,4-Trimethyl-2-pentene	107-40-4	1.328	2.935	1.386	2.987	1.331	2.912	1.340	2.907	1.330	2.895	1.338	2.899
2,4-Dichlorotoluene	95-73-8	4.557	3.708	4.559	3.774	4.374	3.544	4.433	3.595	4.361	3.540	4.419	3.597
2,4-Dimethyl-3-ethylpentane	1068-87-7	1.372	3.669	1.416	3.714	1.372	3.635	1.380	3.623	1.372	3.613	1.380	3.613
2,4-Dimethylhexane	589-43-5	1.058	3.260	1.111	3.303	1.060	3.229	1.072	3.221	1.060	3.208	1.072	3.211
2,4-Dimethylpentan-3-one	565-80-0	3.079	1.149	3.108	1.211	2.978	1.028	3.013	1.056	2.979	1.012	3.013	1.041
2,4-Dimethylpentane	108-08-7	0.743	2.851	0.806	2.891	0.748	2.823	0.763	2.818	0.748	2.802	0.763	2.808
2,4-Dimethylphenol	105-67-9	7.278	2.465	7.223	2.546	7.102	2.338	7.134	2.352	7.092	2.338	7.122	2.351
2,4-Dimethylpyridine	108-47-4	4.175	0.486	4.214	0.579	4.098	0.418	4.109	0.448	4.092	0.418	4.101	0.443
2,5-Dimethylhexane	592-13-2	1.051	3.260	1.104	3.303	1.053	3.229	1.065	3.221	1.053	3.208	1.065	3.211
2,5-Dimethylphenol	95-87-4	7.329	2.589	7.278	2.673	7.163	2.474	7.190	2.486	7.151	2.477	7.176	2.488
2,5-Dimethylpyridine	589-93-5	4.100	0.514	4.142	0.606	4.030	0.450	4.039	0.479	4.023	0.451	4.031	0.474
2,5-Dimethyltetrahydrofuran	1003-38-9	2.263	0.074	2.333	0.152	2.280	0.074	2.270	0.078	2.279	0.067	2.268	0.068
2,6-Dimethylaniline	87-62-7	6.195	2.083	6.183	2.176	6.043	1.965	6.070	1.998	6.031	1.970	6.056	2.000
2,6-Dimethylheptane	1072-05-5	1.342	3.669	1.387	3.714	1.342	3.635	1.351	3.623	1.342	3.613	1.351	3.613
2,6-Dimethylnaphthalene	581-42-0	5.781	3.692	5.791	3.798	5.659	3.604	5.674	3.637	5.641	3.615	5.653	3.648
2,6-Dimethylphenol	576-26-1	6.531	2.332	6.499	2.415	6.374	2.215	6.403	2.235	6.363	2.216	6.391	2.235
2,6-Dimethylpyridine	108-48-5	3.838	0.471	3.887	0.563	3.782	0.419	3.788	0.444	3.776	0.420	3.780	0.440
2-Bromo-2-chloro-1,1,1-trifluoroethane	151-67-7	2.216	2.204	2.239	2.232	2.083	2.062	2.151	2.093	2.082	2.040	2.149	2.081
2-Bromo-2-methylpropane	507-19-7	1.521	1.824	1.587	1.879	1.497	1.787	1.518	1.799	1.493	1.775	1.513	1.794
2-Bromopropane	75-26-3	1.677	1.512	1.739	1.562	1.618	1.445	1.654	1.470	1.614	1.432	1.649	1.463
2-Butanol	78-92-2	3.389	-0.042	3.426	0.030	3.385	-0.041	3.379	-0.052	3.384	-0.048	3.377	-0.061
2-Butoxyethanol	111-76-2	4.660	-0.186	4.678	-0.094	4.659	-0.185	4.632	-0.201	4.660	-0.189	4.631	-0.212
2-Chloro-1,1,1,2-Tetrafluoroethane	2837-89-0	0.452	1.198	0.506	1.213	0.376	1.091	0.437	1.113	0.381	1.062	0.442	1.094
2-Chloro-2-methylpropane	507-20-0	1.201	1.707	1.265	1.750	1.157	1.642	1.192	1.660	1.155	1.625	1.190	1.651
2-Chloroaniline	95-51-2	6.262	2.395	6.240	2.476	6.067	2.242	6.116	2.285	6.054	2.245	6.100	2.288
2-Chlorobutane	78-86-4	1.708	1.814	1.758	1.856	1.628	1.719	1.673	1.747	1.626	1.702	1.670	1.737
2-Chlorophenol	95-57-8	6.107	2.246	6.080	2.317	5.905	2.081	5.961	2.122	5.894	2.079	5.948	2.121
2-Chloropropane	75-29-6	1.352	1.401	1.413	1.441	1.275	1.309	1.324	1.340	1.273	1.292	1.321	1.330
2-Chloropyridine	109-09-1	4.804	1.485	4.808	1.552	4.575	1.275	4.652	1.349	4.566	1.270	4.642	1.344
2-Chlorotoluene	95-49-8	3.774	3.037	3.793	3.098	3.621	2.896	3.676	2.941	3.611	2.889	3.664	2.941
2-Decanone	693-54-9	4.461	2.462	4.451	2.530	4.324	2.307	4.356	2.333	4.325	2.291	4.356	2.318
2-Ethoxyethanol	110-80-5	4.064	-0.992	4.101	-0.901	4.072	-0.978	4.050	-0.988	4.072	-0.980	4.048	-0.998
2-Ethoxyethyl acetate	111-15-9	3.968	-0.008	3.991	0.069	3.861	-0.129	3.886	-0.096	3.863	-0.140	3.887	-0.113
2-Ethyl-1-butanol	97-95-0	4.368	1.207	4.371	1.277	4.325	1.172	4.325	1.160	4.324	1.162	4.323	1.151
2-Ethyl-1-butene	760-21-4	0.946	2.072	1.017	2.120	0.955	2.058	0.967	2.058	0.954	2.042	0.965	2.050
2-Ethyl-1-hexanol	104-76-7	4.922	2.019	4.908	2.093	4.873	1.973	4.867	1.956	4.872	1.964	4.865	1.946
2-Ethyl-1-pentene	3404-71-5	1.215	2.423	1.278	2.474	1.226	2.410	1.233	2.406	1.225	2.394	1.231	2.398
2-Ethyl-p-xylene	1758-88-9	3.912	3.250	3.933	3.325	3.815	3.157	3.840	3.181	3.806	3.152	3.829	3.180
2-Ethylpyrazine	13925-00-3	4.345	0.255	4.381	0.346	4.246	0.165	4.266	0.203	4.240	0.166	4.258	0.197
2-Ethylpyridine	100-71-0	3.877	0.607	3.923	0.697	3.813	0.548	3.823	0.575	3.807	0.548	3.815	0.570
2-Ethyltoluene	611-14-3	3.609	2.883	3.638	2.955	3.511	2.790	3.541	2.817	3.502	2.785	3.530	2.816
2-Fluorophenol	367-12-4	6.409	2.204	6.359	2.264	6.225	2.066	6.275	2.081	6.217	2.060	6.265	2.078
2-Heptanone	110-43-0	3.549	1.238	3.566	1.300	3.420	1.095	3.462	1.130	3.421	1.079	3.461	1.115

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2-Hexanone	591-78-6	3.264	0.835	3.290	0.896	3.140	0.698	3.184	0.737	3.140	0.684	3.183	0.722
2-Hexyne	764-35-2	1.734	1.862	1.790	1.912	1.685	1.798	1.715	1.816	1.683	1.783	1.712	1.808
2-Hydroxybenzoic acid	69-72-7	8.370	2.614	8.286	2.692	8.160	2.468	8.200	2.479	8.149	2.469	8.186	2.479
2-Iodophenol	533-58-4	7.531	2.808	7.496	2.907	7.336	2.676	7.374	2.709	7.319	2.687	7.353	2.718
2-Isobutylpyrazine	29460-92-2	5.048	1.191	5.061	1.285	4.928	1.079	4.947	1.115	4.922	1.078	4.939	1.108
2-Methoxyaniline	90-04-0	6.636	1.824	6.614	1.915	6.441	1.668	6.484	1.713	6.429	1.673	6.470	1.714
2-Methoxybenzoic acid	579-75-9	9.305	2.136	9.204	2.218	8.959	1.846	9.043	1.912	8.949	1.845	9.031	1.906
2-Methoxyethanol	109-86-4	3.879	-1.436	3.925	-1.346	3.895	-1.412	3.872	-1.421	3.894	-1.413	3.870	-1.430
2-Methoxyphenol	90-05-1	5.967	1.447	5.958	1.535	5.808	1.320	5.842	1.356	5.799	1.322	5.830	1.354
2-Methyl-1-butanol	137-32-6	4.037	0.785	4.047	0.851	3.993	0.747	3.998	0.740	3.992	0.737	3.996	0.729
2-Methyl-1-butene	563-46-2	0.638	1.711	0.715	1.754	0.641	1.691	0.661	1.696	0.640	1.674	0.659	1.688
2-Methyl-1-hexene	6094-02-6	1.225	2.466	1.281	2.511	1.214	2.427	1.230	2.429	1.213	2.408	1.230	2.418
2-Methyl-1-pentene	763-29-1	0.901	2.101	0.969	2.146	0.902	2.078	0.918	2.079	0.901	2.060	0.917	2.070
2-Methyl-2-butanol	75-85-4	3.306	0.103	3.348	0.181	3.332	0.128	3.311	0.107	3.331	0.121	3.310	0.098
2-Methyl-2-butene	513-35-9	0.704	1.714	0.782	1.761	0.715	1.705	0.730	1.708	0.713	1.689	0.727	1.701
2-Methyl-2-pentene	625-27-4	0.988	2.124	1.058	2.172	0.997	2.110	1.009	2.110	0.995	2.094	1.006	2.103
2-Methyl-3-ethylpentane	609-26-7	1.144	3.260	1.195	3.303	1.146	3.229	1.157	3.221	1.146	3.208	1.157	3.211
2-Methylbenzoic acid	118-90-1	6.788	2.182	6.743	2.260	6.607	2.038	6.645	2.061	6.599	2.036	6.634	2.058
2-Methylbuta-1,3-diene	78-79-5	1.128	1.639	1.204	1.689	1.106	1.603	1.132	1.618	1.102	1.590	1.127	1.612
2-Methylbutane	78-78-4	0.252	2.032	0.329	2.068	0.261	2.012	0.282	2.013	0.261	1.991	0.282	2.003
2-Methylheptane	592-27-8	1.157	3.260	1.208	3.303	1.159	3.229	1.169	3.221	1.159	3.208	1.169	3.211
2-Methylhexane	591-76-4	0.862	2.851	0.921	2.891	0.866	2.823	0.880	2.818	0.866	2.802	0.880	2.808
2-Methylnonane	871-83-0	1.758	4.078	1.790	4.125	1.754	4.040	1.758	4.026	1.754	4.019	1.758	4.016
2-Methyloctane	3221-61-2	1.457	3.669	1.499	3.714	1.456	3.635	1.463	3.623	1.456	3.613	1.463	3.613
2-Methylpentan-2-ol	590-36-3	3.577	0.505	3.609	0.585	3.598	0.524	3.575	0.501	3.598	0.517	3.574	0.491
2-Methylpentan-3-ol	565-67-3	3.855	0.746	3.879	0.823	3.857	0.749	3.841	0.730	3.857	0.742	3.839	0.720
2-Methylpentane	107-83-5	0.554	2.441	0.622	2.480	0.561	2.418	0.578	2.416	0.561	2.397	0.578	2.406
2-Methylpropan-1-ol	78-83-1	3.679	0.386	3.702	0.451	3.641	0.356	3.649	0.350	3.640	0.346	3.647	0.341
2-Methylpropanal	78-84-2	2.346	0.235	2.396	0.288	2.237	0.113	2.288	0.155	2.237	0.098	2.287	0.140
2-Methylpropane	75-28-5	-0.121	1.623	-0.033	1.657	-0.109	1.606	-0.084	1.610	-0.109	1.586	-0.084	1.600
2-Methylpyrazine	109-08-0	4.015	-0.133	4.062	-0.044	3.914	-0.225	3.940	-0.182	3.908	-0.224	3.932	-0.188
2-Methylpyridine	109-06-8	3.749	0.331	3.795	0.415	3.662	0.251	3.684	0.287	3.656	0.250	3.676	0.282
2-Methyltetrahydrofuran	96-47-9	2.446	-0.004	2.508	0.067	2.418	-0.043	2.428	-0.024	2.417	-0.052	2.425	-0.035
2-Methylthiophene	554-14-3	2.993	1.950	3.038	2.014	2.893	1.858	2.933	1.895	2.884	1.853	2.922	1.894
2-Naphthol	135-19-3	9.612	3.224	9.530	3.332	9.391	3.087	9.418	3.110	9.371	3.103	9.395	3.122
2-Naphthylamine	91-59-8	8.650	2.529	8.613	2.654	8.436	2.385	8.463	2.436	8.415	2.406	8.438	2.449
2-Nitroaniline	88-74-4	8.463	2.823	8.384	2.900	8.114	2.534	8.209	2.615	8.099	2.536	8.192	2.615
2-Nitrophenol	88-75-5	5.753	2.082	5.748	2.164	5.538	1.899	5.598	1.963	5.525	1.901	5.583	1.964
2-Nitropropane	79-46-9	3.451	1.175	3.459	1.213	3.203	0.923	3.306	1.000	3.201	0.903	3.303	0.984
2-Nitrotoluene	88-72-2	5.664	2.688	5.644	2.756	5.392	2.440	5.479	2.519	5.381	2.435	5.466	2.516
2-Octanol	123-96-6	4.601	1.575	4.599	1.653	4.580	1.553	4.563	1.532	4.580	1.544	4.562	1.521
2-Octanone	111-13-7	3.851	1.644	3.859	1.707	3.720	1.495	3.758	1.528	3.720	1.480	3.758	1.513
2-Pentanol	6032-29-7	3.691	0.361	3.718	0.434	3.682	0.355	3.674	0.342	3.682	0.347	3.672	0.332
2-Pentanone	107-87-9	2.936	0.426	2.972	0.484	2.815	0.293	2.863	0.334	2.815	0.278	2.862	0.319
2-Phenylethanol	60-12-8	6.266	1.032	6.257	1.131	6.157	0.955	6.164	0.971	6.149	0.959	6.153	0.968

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2-Propoxyethanol	2807-30-9	4.358	-0.592	4.385	-0.501	4.361	-0.586	4.336	-0.599	4.361	-0.589	4.335	-0.610
3,3,5-Trimethylheptane	7154-80-5	1.635	4.078	1.671	4.125	1.632	4.040	1.638	4.026	1.632	4.019	1.638	4.016
3,3-Diethylpentane	1067-20-5	2.181	3.878	2.198	3.915	2.091	3.758	2.131	3.771	2.091	3.734	2.131	3.758
3,3-Dimethyl-1-butene	558-37-2	0.553	1.776	0.633	1.824	0.581	1.774	0.588	1.770	0.581	1.757	0.588	1.760
3,3-Dimethylbutan-2-one	75-97-8	2.859	0.771	2.896	0.832	2.757	0.652	2.796	0.685	2.757	0.637	2.795	0.670
3,3-Dimethylhexane	563-16-6	1.083	3.260	1.135	3.303	1.085	3.229	1.096	3.221	1.085	3.208	1.096	3.211
3,3-Dimethylpentane	562-49-2	0.828	2.851	0.888	2.891	0.832	2.823	0.846	2.818	0.832	2.802	0.846	2.808
3,4-Dimethylhexane	583-48-2	1.206	3.260	1.255	3.303	1.207	3.229	1.217	3.221	1.207	3.208	1.217	3.211
3,4-Dimethylphenol	95-65-8	7.720	2.544	7.651	2.622	7.517	2.392	7.556	2.411	7.507	2.392	7.544	2.410
3,4-Dimethylpyridine	583-58-4	4.636	0.675	4.663	0.766	4.524	0.576	4.546	0.615	4.517	0.576	4.537	0.611
3,5-Dimethylphenol	108-68-9	7.617	2.669	7.549	2.744	7.413	2.515	7.455	2.533	7.403	2.514	7.443	2.532
3,5-Dimethylpyridine	591-22-0	4.388	0.660	4.421	0.750	4.295	0.577	4.311	0.611	4.288	0.577	4.303	0.607
3,5-Dinitrobenzoic acid	99-34-3	12.088	3.252	11.923	3.342	11.659	2.912	11.753	2.979	11.644	2.917	11.735	2.979
3-Acetylpyridine	350-03-8	6.073	-0.266	6.083	-0.158	5.916	-0.400	5.941	-0.345	5.909	-0.394	5.931	-0.350
3-Chloroaniline	108-42-9	7.168	2.657	7.118	2.731	6.898	2.437	6.972	2.496	6.884	2.437	6.956	2.497
3-Chlorobenzoic acid	535-80-8	8.423	3.004	8.327	3.073	8.162	2.802	8.222	2.831	8.152	2.799	8.209	2.829
3-Chlorophenol	108-43-0	8.720	3.500	8.606	3.553	8.382	3.230	8.478	3.278	8.370	3.224	8.464	3.276
3-Chloropyridine	626-60-8	4.184	1.119	4.212	1.195	4.041	0.991	4.085	1.041	4.032	0.989	4.075	1.038
3-Cyanophenol	873-62-1	10.828	3.530	10.656	3.577	10.325	3.109	10.474	3.196	10.313	3.100	10.460	3.188
3-Cyanopyridine	100-54-9	5.753	0.656	5.747	0.735	5.494	0.420	5.573	0.504	5.486	0.418	5.563	0.496
3-Ethyl-1-pentene	4038-04-4'	1.098	2.465	1.161	2.512	1.100	2.440	1.113	2.438	1.100	2.422	1.112	2.429
3-Ethylhexane	619-99-8	1.181	3.260	1.231	3.303	1.183	3.229	1.193	3.221	1.183	3.208	1.193	3.211
3-Ethyl-o-xylene	933-98-2	4.179	3.321	4.195	3.397	4.064	3.213	4.094	3.242	4.054	3.209	4.083	3.241
3-Ethylpentane	617-78-7	0.917	2.851	0.975	2.891	0.921	2.823	0.934	2.818	0.921	2.802	0.934	2.808
3-Ethylphenol	620-17-7	7.653	2.665	7.582	2.738	7.425	2.487	7.477	2.513	7.416	2.485	7.466	2.511
3-Ethylpyridine	536-78-7	4.293	0.789	4.325	0.877	4.192	0.697	4.213	0.733	4.185	0.696	4.205	0.729
3-Formylpyridine	500-22-1	5.609	-0.042	5.623	0.054	5.429	-0.198	5.472	-0.134	5.420	-0.195	5.461	-0.140
3-Hexanol	623-37-0	4.001	0.770	4.020	0.846	3.990	0.761	3.978	0.744	3.990	0.753	3.977	0.735
3-Hexanone	589-38-8	3.197	0.817	3.226	0.878	3.081	0.687	3.122	0.724	3.081	0.673	3.121	0.709
3-Hydroxybenzaldehyde	100-83-4	10.146	2.819	10.010	2.884	9.747	2.498	9.854	2.561	9.735	2.495	9.840	2.557
3-Methoxyaniline	536-90-3	7.442	1.802	7.400	1.892	7.186	1.592	7.249	1.653	7.174	1.596	7.234	1.652
3-Methoxyphenol	150-19-6	8.662	2.677	8.563	2.744	8.341	2.416	8.426	2.467	8.330	2.413	8.413	2.464
3-Methyl-1-butanol	123-51-3	4.037	0.785	4.047	0.851	3.993	0.747	3.998	0.740	3.992	0.737	3.996	0.729
3-Methyl-1-butene	563-45-1	0.471	1.682	0.550	1.723	0.473	1.658	0.495	1.663	0.472	1.639	0.494	1.654
3-Methyl-1-hexene	3404-61-3	1.063	2.501	1.126	2.548	1.067	2.478	1.079	2.475	1.066	2.460	1.077	2.467
3-Methyl-3-ethylpentane	1067-08-9	1.171	3.260	1.221	3.303	1.172	3.229	1.183	3.221	1.172	3.208	1.183	3.211
3-Methylbenzoic acid	99-04-7	7.865	2.577	7.785	2.648	7.639	2.400	7.688	2.421	7.630	2.397	7.678	2.418
3-Methylbutan-2-one	563-80-4	2.807	0.396	2.847	0.454	2.697	0.272	2.741	0.310	2.697	0.257	2.740	0.296
3-Methylbutanoic acid	503-74-2	5.741	1.115	5.700	1.173	5.610	1.006	5.640	1.005	5.610	0.994	5.638	0.992
3-Methylheptane	589-81-1	1.176	3.260	1.225	3.303	1.177	3.229	1.188	3.221	1.177	3.208	1.188	3.211
3-Methylhexane	589-34-4	0.888	2.851	0.946	2.891	0.892	2.823	0.906	2.818	0.892	2.802	0.906	2.808
3-Methylnonane	5911-04-6'	1.778	4.078	1.810	4.125	1.774	4.040	1.778	4.026	1.774	4.019	1.778	4.016
3-Methyloctane	2216-33-3	1.477	3.669	1.518	3.714	1.476	3.635	1.483	3.623	1.476	3.613	1.483	3.613
3-Methylpentane	96-14-0	0.602	2.441	0.669	2.480	0.609	2.418	0.626	2.416	0.609	2.397	0.626	2.406
3-Methylpyridine	108-99-6	4.049	0.531	4.085	0.613	3.934	0.426	3.966	0.470	3.928	0.425	3.958	0.465

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3-Methylthiophene	616-44-4	3.125	2.104	3.164	2.165	3.010	1.998	3.055	2.039	3.000	1.992	3.045	2.038
3-Methyl-trans-2-pentene	616-12-6	1.038	2.078	1.107	2.127	1.048	2.067	1.058	2.067	1.046	2.051	1.056	2.060
3-Nitroaniline	99-09-2	10.081	3.277	9.950	3.342	9.590	2.860	9.735	2.971	9.575	2.858	9.717	2.968
3-Nitrobenzoic acid	121-92-6	9.954	2.598	9.836	2.682	9.658	2.375	9.717	2.407	9.646	2.377	9.703	2.406
3-Nitrophenol	554-84-7	11.322	3.890	11.139	3.938	10.808	3.465	10.956	3.553	10.794	3.458	10.940	3.548
3-Nitrophthalic acid	603-11-2	16.236	2.857	15.975	2.958	15.696	2.446	15.801	2.509	15.681	2.456	15.782	2.507
3-Nitrotoluene	99-08-1	5.770	2.679	5.748	2.747	5.501	2.435	5.585	2.512	5.490	2.430	5.572	2.509
3-Pentanol	584-02-1	3.711	0.367	3.739	0.442	3.704	0.364	3.695	0.351	3.704	0.357	3.693	0.342
3-Pentanone	96-22-0	2.917	0.411	2.955	0.471	2.804	0.286	2.848	0.326	2.804	0.272	2.847	0.311
3-Phenylpropanol	122-97-4	6.828	1.473	6.804	1.574	6.696	1.374	6.706	1.392	6.687	1.379	6.694	1.390
4-Acetylpyridine	1122-54-9	5.785	-0.039	5.798	0.063	5.628	-0.177	5.657	-0.122	5.620	-0.172	5.647	-0.128
4-Bromophenol	106-41-2	9.250	3.563	9.133	3.626	8.900	3.287	8.994	3.340	8.885	3.285	8.978	3.340
4-Bromotoluene	106-38-7	4.342	3.220	4.353	3.287	4.171	3.066	4.227	3.116	4.159	3.062	4.213	3.117
4-Chloro-3-methylphenol	59-50-7	8.770	3.476	8.661	3.539	8.468	3.238	8.544	3.276	8.456	3.234	8.530	3.275
4-Chloroaniline	106-47-8	7.250	2.642	7.199	2.717	6.972	2.414	7.049	2.477	6.958	2.415	7.033	2.477
4-Chlorobenzoic acid	74-11-3	8.449	3.295	8.348	3.358	8.151	3.055	8.229	3.094	8.140	3.050	8.216	3.091
4-Chlorophenol	106-48-9	8.712	3.231	8.603	3.288	8.383	2.969	8.474	3.016	8.371	2.964	8.460	3.015
4-Cyanophenol	767-00-0	11.314	3.534	11.129	3.580	10.783	3.088	10.940	3.181	10.771	3.079	10.926	3.173
4-Cyanopyridine	100-48-1	5.516	0.747	5.515	0.825	5.270	0.523	5.346	0.602	5.262	0.520	5.336	0.595
4-Ethyl-m-xylene	874-41-9	3.925	3.250	3.946	3.325	3.829	3.157	3.853	3.181	3.820	3.152	3.842	3.180
4-Ethyl-o-xylene	934-80-5	3.971	3.260	3.990	3.334	3.870	3.163	3.896	3.187	3.861	3.157	3.885	3.186
4-Ethylphenol	123-07-9	7.613	2.698	7.542	2.770	7.387	2.520	7.439	2.546	7.377	2.518	7.427	2.544
4-Ethylpyridine	536-75-4	4.337	0.795	4.367	0.882	4.231	0.698	4.254	0.735	4.224	0.696	4.246	0.730
4-Ethyltoluene	622-96-8	3.440	2.831	3.471	2.901	3.352	2.745	3.379	2.769	3.344	2.739	3.369	2.768
4-Fluorophenol	371-41-5	7.543	2.617	7.455	2.665	7.242	2.369	7.334	2.413	7.234	2.359	7.324	2.407
4-Formylpyridine	872-85-5	5.689	0.006	5.698	0.101	5.515	-0.143	5.553	-0.082	5.507	-0.140	5.543	-0.087
4-Heptanone	123-19-3	3.453	1.217	3.473	1.278	3.332	1.079	3.371	1.113	3.332	1.064	3.371	1.098
4-Hydroxyacetanilide	103-90-2	13.416	1.969	13.221	2.064	13.003	1.657	13.080	1.700	12.992	1.663	13.065	1.695
4-Hydroxybenzaldehyde	123-08-0	10.711	2.699	10.563	2.767	10.311	2.382	10.412	2.443	10.298	2.380	10.397	2.439
4-Hydroxybenzoic acid	99-96-7	9.072	1.882	8.983	1.972	8.883	1.763	8.905	1.764	8.873	1.769	8.892	1.765
4-Isopropyltoluene	99-87-6	3.564	3.170	3.591	3.243	3.483	3.087	3.504	3.106	3.475	3.081	3.495	3.104
4-Methoxyacetophenone	100-06-1	7.794	2.525	7.727	2.601	7.400	2.164	7.517	2.273	7.390	2.160	7.504	2.266
4-Methoxyaniline	104-94-9	7.247	1.490	7.217	1.587	7.021	1.309	7.071	1.363	7.009	1.315	7.056	1.363
4-Methoxybenzoic acid	100-09-4	9.681	2.604	9.564	2.681	9.357	2.344	9.430	2.390	9.347	2.343	9.417	2.386
4-Methyl-1-pentene	691-37-2	0.776	2.230	0.844	2.272	0.769	2.197	0.790	2.201	0.768	2.178	0.789	2.192
4-Methylacetophenone	122-00-9	5.562	1.847	5.563	1.937	5.385	1.688	5.426	1.741	5.375	1.689	5.414	1.738
4-Methylbenzaldehyde	104-87-0	5.226	1.898	5.231	1.979	5.030	1.723	5.086	1.783	5.020	1.722	5.074	1.781
4-Methyl-cis-2-pentene	691-38-3	0.820	2.059	0.892	2.105	0.826	2.039	0.841	2.040	0.825	2.022	0.839	2.031
4-Methylheptane	589-53-7	1.159	3.260	1.209	3.303	1.161	3.229	1.171	3.221	1.161	3.208	1.171	3.211
4-Methylnonane	17301-94-9	1.750	4.078	1.783	4.125	1.747	4.040	1.751	4.026	1.747	4.019	1.751	4.016
4-Methyloctane	2216-34-4	1.454	3.669	1.496	3.714	1.453	3.635	1.460	3.623	1.453	3.613	1.460	3.613
4-Methylpentan-2-ol	108-11-2	3.802	0.733	3.825	0.808	3.800	0.730	3.787	0.712	3.800	0.722	3.786	0.702
4-Methylpentan-2-one	108-10-1	3.044	0.798	3.076	0.858	2.930	0.668	2.972	0.704	2.930	0.653	2.972	0.689
4-Methylpyridine	108-89-4	4.088	0.495	4.123	0.577	3.971	0.389	4.004	0.433	3.965	0.387	3.995	0.427
4-Nitroaniline	100-01-6	11.058	3.348	10.900	3.409	10.496	2.866	10.663	2.995	10.481	2.863	10.644	2.990

	CAS	IL Specific		Lit (cation + anion)		Method 1		Method 2		Method 3		Method 4	
		log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*
4-Nitrobenzoic acid	62-23-7	10.748	3.405	10.592	3.469	10.296	3.029	10.419	3.106	10.284	3.025	10.404	3.101
4-Nitrobenzyl chloride	100-14-1	2.845	3.055	2.888	3.120	2.746	2.951	2.787	2.979	2.738	2.943	2.778	2.976
4-Nitrophenol	100-02-7	12.031	3.925	11.829	3.971	11.465	3.453	11.630	3.553	11.451	3.446	11.614	3.547
4-n-Propylphenol	645-56-7	7.833	3.040	7.756	3.116	7.613	2.867	7.658	2.888	7.603	2.865	7.647	2.885
4-tert-Butylphenol	98-54-4	7.974	3.384	7.896	3.463	7.756	3.210	7.799	3.227	7.746	3.209	7.787	3.225
5-Ethylidene-2-norbornene	16219-75-3	2.604	2.863	2.652	2.931	2.581	2.839	2.587	2.846	2.573	2.832	2.578	2.846
5-Methyl-2-hexanone	110-12-3	3.524	1.144	3.543	1.207	3.400	1.004	3.440	1.039	3.400	0.988	3.440	1.023
5-Methylnonane	15869-85-9	1.745	4.078	1.778	4.125	1.741	4.040	1.745	4.026	1.741	4.019	1.745	4.016
Acenaphthene	83-32-9	6.724	3.803	6.717	3.911	6.533	3.662	6.570	3.717	6.512	3.676	6.545	3.731
Acetaldehyde	75-07-0	1.968	-0.515	2.032	-0.464	1.852	-0.639	1.912	-0.587	1.850	-0.652	1.910	-0.600
Acetic acid	64-19-7	5.175	0.226	5.151	0.275	5.017	0.099	5.070	0.116	5.015	0.088	5.067	0.104
Acetonitrile	75-05-8	3.096	0.280	3.118	0.315	2.861	0.047	2.965	0.126	2.859	0.029	2.962	0.111
Acetophenone	98-86-2	5.209	1.622	5.216	1.705	5.019	1.451	5.072	1.510	5.010	1.450	5.060	1.507
Acetylene (ethyne)	74-86-2	1.075	0.929	1.137	0.953	0.934	0.783	1.023	0.831	0.932	0.763	1.020	0.820
Acetylsalicylic acid	50-78-2	11.729	2.822	11.549	2.891	11.248	2.411	11.370	2.490	11.239	2.404	11.360	2.478
Acrolein	107-02-8	2.166	-0.295	2.234	-0.234	2.085	-0.381	2.126	-0.340	2.082	-0.390	2.122	-0.350
Ammonia	7664-41-7	1.422	-2.044	1.516	-1.978	1.452	-2.019	1.453	-2.011	1.453	-2.026	1.452	-2.022
Aniline	62-53-3	5.984	1.608	5.973	1.690	5.792	1.457	5.844	1.503	5.780	1.459	5.830	1.503
Anthracene	120-12-7	8.524	4.588	8.510	4.730	8.305	4.446	8.335	4.510	8.274	4.478	8.299	4.536
Argon	7440-37-1	-1.414	0.223	-1.289	0.249	-1.392	0.218	-1.352	0.233	-1.392	0.198	-1.352	0.223
Benzaldehyde	100-52-7	4.838	1.612	4.849	1.687	4.633	1.427	4.699	1.493	4.623	1.425	4.687	1.490
Benzamide	55-21-0	9.892	1.598	9.782	1.682	9.528	1.301	9.615	1.374	9.517	1.303	9.601	1.368
Benzene	71-43-2	2.517	1.787	2.570	1.846	2.421	1.696	2.466	1.733	2.413	1.689	2.456	1.731
Benzil	134-81-6	9.096	3.529	9.032	3.646	8.769	3.250	8.837	3.335	8.751	3.262	8.816	3.340
Benzoic acid	65-85-0	7.746	2.167	7.670	2.236	7.518	1.991	7.570	2.017	7.509	1.987	7.559	2.013
Benzonitrile	100-47-0	5.118	1.953	5.110	2.015	4.848	1.702	4.942	1.784	4.839	1.695	4.931	1.778
Benzotrifluoride	98-08-8	2.307	2.372	2.339	2.413	2.176	2.228	2.238	2.266	2.173	2.209	2.234	2.256
Benzyl alcohol	100-51-6	6.239	1.148	6.224	1.236	6.093	1.038	6.120	1.064	6.084	1.040	6.108	1.062
Benzyl chloride	100-44-7	4.542	2.930	4.545	2.992	4.331	2.736	4.404	2.798	4.320	2.730	4.391	2.797
Benzyl ethyl ether	539-30-0	4.304	1.639	4.332	1.729	4.218	1.557	4.232	1.583	4.211	1.556	4.223	1.579
Betulin	473-98-3	20.405	8.889	20.067	9.073	19.924	8.507	19.923	8.529	19.903	8.531	19.898	8.534
Bicyclohexyl	92-51-3	4.251	4.663	4.241	4.726	4.133	4.540	4.160	4.558	4.125	4.528	4.152	4.554
Biotin	58-85-5	17.738	2.279	17.458	2.404	17.124	1.783	17.235	1.878	17.110	1.796	17.217	1.869
Biphenyl	92-52-4	6.197	3.679	6.194	3.780	6.014	3.534	6.053	3.584	5.996	3.543	6.032	3.594
Bromobenzene	108-86-1	3.977	2.801	3.998	2.867	3.812	2.655	3.871	2.707	3.800	2.651	3.857	2.709
Bromoethane	74-96-4	1.661	1.252	1.724	1.299	1.584	1.171	1.630	1.205	1.579	1.158	1.624	1.198
Bromomethane	74-83-9	1.448	0.971	1.517	1.014	1.360	0.881	1.415	0.922	1.355	0.869	1.409	0.916
Bromotrichloromethane	75-62-7	2.610	2.597	2.652	2.650	2.505	2.498	2.552	2.534	2.496	2.489	2.542	2.533
Bromotrifluoromethane	75-63-8	-0.521	1.004	-0.418	1.038	-0.492	1.006	-0.469	1.011	-0.493	0.987	-0.469	1.002
But-1-en-3-yne	689-97-4	1.655	1.715	1.710	1.754	1.589	1.649	1.635	1.667	1.585	1.635	1.630	1.661
Butane	106-97-8	0.006	1.623	0.090	1.657	0.017	1.606	0.041	1.610	0.017	1.586	0.041	1.600
Butanethiol	109-79-5	2.183	1.450	2.241	1.513	2.149	1.410	2.166	1.426	2.145	1.400	2.161	1.421
Butanoic acid	107-92-6	5.684	0.988	5.642	1.040	5.527	0.857	5.571	0.866	5.526	0.844	5.569	0.853
Butanone	78-93-3	2.716	0.045	2.761	0.102	2.593	-0.088	2.645	-0.042	2.593	-0.102	2.644	-0.057
Butyl acetate	123-86-4	3.023	1.183	3.049	1.239	2.908	1.050	2.950	1.083	2.909	1.033	2.950	1.068

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Butyl acrylate	141-32-2	3.379	1.657	3.399	1.718	3.259	1.523	3.299	1.556	3.258	1.508	3.298	1.542
Butyl ethyl ether	628-81-9	1.767	0.799	1.831	0.864	1.783	0.788	1.779	0.787	1.784	0.774	1.780	0.774
Butyl formate	592-84-7	2.855	1.135	2.883	1.185	2.719	0.985	2.775	1.028	2.719	0.968	2.774	1.013
Butylamine	109-73-9	2.740	-0.317	2.800	-0.238	2.765	-0.297	2.749	-0.304	2.764	-0.303	2.747	-0.313
Butylbenzene	104-51-8	3.688	3.366	3.707	3.435	3.588	3.266	3.616	3.289	3.580	3.258	3.607	3.287
butylcyclohexane	1678-93-9	2.736	4.057	2.754	4.108	2.671	3.973	2.693	3.980	2.667	3.956	2.689	3.973
Butyraldehyde	123-72-8	2.544	0.278	2.591	0.334	2.428	0.153	2.480	0.196	2.428	0.139	2.478	0.183
Caprolactam	105-60-2	9.355	1.167	9.236	1.229	8.895	0.754	9.031	0.860	8.890	0.744	9.023	0.842
Carbon dioxide	124-38-9	0.134	0.334	0.217	0.359	0.064	0.245	0.128	0.279	0.064	0.223	0.128	0.266
Carbon monoxide	630-08-0	-1.489	0.135	-1.358	0.164	-1.456	0.138	-1.420	0.150	-1.456	0.119	-1.420	0.140
Carbon tetrachloride	56-23-5	2.021	2.313	2.070	2.359	1.929	2.219	1.977	2.252	1.923	2.206	1.970	2.248
Chlorobenzene	108-90-7	3.441	2.615	3.467	2.672	3.286	2.472	3.347	2.521	3.276	2.464	3.335	2.520
Chlorodifluoromethane	75-45-6	0.721	0.990	0.779	1.006	0.592	0.841	0.676	0.887	0.593	0.815	0.677	0.871
Chloroethane	75-00-3	1.327	1.145	1.389	1.182	1.232	1.040	1.291	1.079	1.229	1.023	1.287	1.070
Chloroform	67-66-3	2.841	2.097	2.865	2.135	2.698	1.961	2.764	2.000	2.692	1.947	2.757	1.994
Chloromethane	74-87-3	1.094	0.860	1.163	0.893	0.988	0.746	1.056	0.792	0.985	0.729	1.052	0.783
Chloropentafluoroethane	76-15-3	-1.137	1.191	-1.041	1.208	-1.114	1.169	-1.082	1.170	-1.109	1.140	-1.076	1.153
Chlorotrifluoromethane	75-72-9	-1.100	0.778	-0.999	0.797	-1.090	0.751	-1.051	0.760	-1.086	0.724	-1.047	0.745
cis-1,2-Dimethylcyclohexane	2207-01-4	1.746	3.127	1.796	3.179	1.738	3.101	1.747	3.100	1.734	3.087	1.742	3.095
cis-1,2-Dimethylcyclopentane	1192-18-3	1.412	2.708	1.470	2.756	1.404	2.681	1.418	2.684	1.400	2.666	1.414	2.678
cis-1,3-Dimethylcyclohexane	638-04-0	1.554	3.100	1.604	3.149	1.538	3.064	1.553	3.064	1.535	3.047	1.550	3.058
cis-1,3-Dimethylcyclopentane	2532-58-3	1.254	2.682	1.311	2.726	1.237	2.644	1.257	2.648	1.235	2.626	1.254	2.641
cis-1,3-Pentadiene	1574-41-0	1.254	1.652	1.328	1.704	1.235	1.621	1.258	1.636	1.230	1.610	1.253	1.631
cis-1,4-Dimethylcyclohexane	624-29-3	1.967	3.191	2.004	3.236	1.912	3.118	1.940	3.128	1.909	3.099	1.937	3.121
cis-2-Butene	590-18-1	0.386	1.390	0.471	1.431	0.393	1.376	0.414	1.384	0.391	1.359	0.412	1.376
cis-2-Heptene	6443-92-1	1.304	2.526	1.363	2.576	1.307	2.507	1.316	2.504	1.306	2.490	1.314	2.496
cis-2-Hexene	7688-21-3	0.979	2.117	1.048	2.165	0.986	2.101	0.998	2.102	0.984	2.084	0.996	2.094
cis-2-Octene	7642-04-8'	1.595	2.935	1.646	2.987	1.597	2.912	1.602	2.907	1.595	2.895	1.600	2.899
cis-3-Heptene	7642-10-6'	1.258	2.523	1.318	2.572	1.262	2.502	1.271	2.500	1.260	2.485	1.269	2.492
cis-3-Octene	14850-22-7	1.568	2.932	1.619	2.984	1.569	2.908	1.575	2.902	1.567	2.890	1.573	2.894
cis-4-Octene	7642-15-1	1.545	2.932	1.596	2.984	1.546	2.908	1.552	2.902	1.544	2.890	1.550	2.894
Cumene	98-82-8	3.236	2.894	3.269	2.961	3.149	2.806	3.178	2.830	3.141	2.799	3.169	2.828
Cyclohepta-1,3,5-triene	544-25-2	2.822	2.009	2.880	2.084	2.772	1.968	2.791	1.990	2.762	1.966	2.779	1.992
Cycloheptane	291-64-5	1.716	2.740	1.771	2.794	1.716	2.728	1.722	2.729	1.711	2.716	1.717	2.725
Cycloheptanol	502-41-0	5.254	1.028	5.255	1.116	5.208	1.001	5.197	0.995	5.203	0.999	5.190	0.990
Cycloheptene	628-92-2	2.078	2.290	2.133	2.350	2.063	2.267	2.072	2.274	2.057	2.256	2.066	2.271
Cyclohexane	110-82-7	1.244	2.318	1.311	2.367	1.244	2.304	1.257	2.308	1.239	2.290	1.252	2.304
Cyclohexanol	108-93-0	4.831	0.648	4.840	0.731	4.780	0.615	4.777	0.614	4.776	0.612	4.771	0.608
Cyclohexanone	108-94-1	4.214	0.541	4.231	0.611	4.059	0.389	4.106	0.440	4.055	0.380	4.101	0.429
Cyclohexene	110-83-8	1.644	1.859	1.710	1.917	1.638	1.845	1.649	1.854	1.633	1.835	1.643	1.851
Cyclohexylamine	108-91-8	4.100	0.549	4.123	0.626	4.044	0.495	4.049	0.506	4.041	0.489	4.045	0.497
Cyclononane	293-55-0	2.440	3.585	2.480	3.647	2.444	3.577	2.438	3.569	2.438	3.566	2.431	3.568
Cyclooctane	292-64-8	2.124	3.169	2.172	3.228	2.128	3.162	2.127	3.158	2.122	3.151	2.120	3.156
Cyclopentane	287-92-3	0.925	1.893	0.997	1.937	0.921	1.875	0.941	1.883	0.918	1.860	0.936	1.878
Cyclopentanol	96-41-3	4.496	0.275	4.512	0.352	4.442	0.238	4.446	0.242	4.438	0.234	4.440	0.235

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Cyclopentanone	120-92-3	3.833	0.304	3.856	0.367	3.668	0.142	3.726	0.199	3.665	0.131	3.722	0.187
Cyclopentene	142-29-0	1.239	1.431	1.314	1.483	1.230	1.412	1.248	1.424	1.225	1.400	1.243	1.420
Cyclopropane	75-19-4	0.639	1.241	0.727	1.285	0.607	1.204	0.646	1.229	0.601	1.192	0.639	1.225
Decane	124-18-5	1.901	4.078	1.930	4.125	1.897	4.040	1.899	4.026	1.897	4.019	1.899	4.016
Deuterium	7782-39-0	-1.730	-0.014	-1.596	0.011	-1.705	-0.016	-1.662	0.000	-1.705	-0.036	-1.662	-0.010
Dibromomethane	74-95-3	3.510	1.892	3.536	1.945	3.349	1.750	3.415	1.800	3.340	1.743	3.404	1.799
DichloroDifluoromethane	75-71-8	-0.227	1.077	-0.131	1.112	-0.215	1.064	-0.188	1.073	-0.215	1.045	-0.188	1.063
Dichlorofluoromethane	75-43-4	1.939	1.470	1.972	1.496	1.807	1.332	1.878	1.369	1.805	1.311	1.877	1.357
Dichloromethane	75-09-2	2.545	1.618	2.576	1.652	2.380	1.459	2.460	1.510	2.375	1.443	2.454	1.503
Diethyl disulfide	110-81-6	3.366	1.911	3.410	1.990	3.321	1.871	3.328	1.888	3.312	1.869	3.318	1.888
Diethyl ether	60-29-7	1.201	0.045	1.282	0.106	1.218	0.039	1.222	0.045	1.219	0.026	1.222	0.033
Diethyl sulfide	352-93-2	2.295	1.111	2.354	1.178	2.268	1.077	2.279	1.092	2.264	1.068	2.275	1.086
Diethylamine	109-89-7	2.078	-0.778	2.159	-0.695	2.139	-0.731	2.112	-0.741	2.140	-0.736	2.112	-0.751
Difluoromethane	75-10-5	0.633	0.668	0.674	0.665	0.435	0.444	0.553	0.509	0.440	0.410	0.558	0.486
Diisobutyl ketone	108-83-8	3.590	1.961	3.603	2.026	3.483	1.830	3.513	1.853	3.484	1.813	3.513	1.837
Diisopropyl ether	108-20-3	1.344	0.323	1.423	0.392	1.394	0.341	1.379	0.331	1.397	0.327	1.381	0.317
Diisopropyl sulfide	625-80-9	2.434	1.635	2.492	1.710	2.435	1.622	2.430	1.623	2.432	1.614	2.426	1.617
Diisopropylamine	108-18-9	2.187	-0.183	2.261	-0.097	2.265	-0.128	2.227	-0.150	2.267	-0.135	2.229	-0.162
Dimethyl ether	115-10-6	0.753	-0.641	0.842	-0.589	0.758	-0.656	0.775	-0.641	0.760	-0.671	0.776	-0.654
Dimethyl sulfide	75-18-3	1.770	0.575	1.843	0.633	1.721	0.522	1.752	0.551	1.717	0.513	1.747	0.545
Dimethyl sulfoxide	67-68-5	6.723	-0.794	6.686	-0.729	6.319	-1.174	6.454	-1.045	6.315	-1.184	6.449	-1.064
Dimethyl Disulfide	624-92-0	2.979	1.529	3.030	1.596	2.880	1.440	2.920	1.479	2.871	1.436	2.910	1.478
Dimethylacetylene	503-17-3	1.005	0.714	1.089	0.768	1.004	0.700	1.021	0.713	1.001	0.688	1.017	0.707
Dimethylamine	124-40-3	1.594	-1.493	1.690	-1.413	1.659	-1.437	1.638	-1.441	1.659	-1.442	1.637	-1.450
Di-n-butyl ether	142-96-1	2.341	1.614	2.387	1.683	2.350	1.594	2.340	1.587	2.352	1.580	2.341	1.574
Di-n-butylamine	626-23-3	2.715	0.652	2.777	0.745	2.795	0.707	2.748	0.678	2.796	0.701	2.749	0.667
Di-n-propyl ether	111-43-3	1.562	0.818	1.632	0.883	1.587	0.815	1.581	0.811	1.589	0.801	1.583	0.798
Di-n-propyl sulfide	111-47-7	2.918	1.926	2.959	1.997	2.884	1.883	2.890	1.893	2.881	1.874	2.885	1.886
Di-n-propylamine	142-84-7	2.656	0.030	2.718	0.116	2.710	0.066	2.678	0.051	2.711	0.060	2.678	0.040
Diphenyl sulfone	127-63-9	11.289	3.530	11.169	3.641	10.795	3.101	10.914	3.232	10.776	3.111	10.891	3.233
Diuron	330-54-1	12.101	3.541	11.945	3.648	11.718	3.237	11.786	3.295	11.703	3.246	11.767	3.295
Docosane	629-97-0	5.637	8.988	5.556	9.063	5.602	8.908	5.562	8.856	5.602	8.885	5.562	8.846
Dodecane	112-40-3	2.524	4.896	2.535	4.948	2.515	4.851	2.510	4.831	2.515	4.830	2.510	4.821
Eicosane	112-95-8	5.014	8.170	4.952	8.240	4.984	8.097	4.951	8.051	4.984	8.074	4.951	8.041
Ethane	74-84-0	-0.686	0.805	-0.582	0.834	-0.670	0.795	-0.638	0.805	-0.670	0.775	-0.638	0.795
Ethanethiol	75-08-1	1.734	0.880	1.802	0.933	1.671	0.813	1.709	0.845	1.666	0.802	1.704	0.839
Ethanol	64-17-5	3.205	-0.396	3.242	-0.334	3.163	-0.426	3.180	-0.422	3.161	-0.434	3.177	-0.431
Ethene	74-85-1	-0.453	0.489	-0.344	0.525	-0.445	0.475	-0.411	0.491	-0.446	0.458	-0.413	0.482
Ethyl acetate	141-78-6	2.454	0.396	2.499	0.448	2.341	0.268	2.392	0.309	2.342	0.252	2.391	0.294
Ethyl benzoate	93-89-0	5.044	2.104	5.049	2.188	4.895	1.965	4.929	2.006	4.887	1.962	4.919	2.002
Ethyl formate	109-94-4	2.266	0.354	2.313	0.400	2.128	0.204	2.194	0.255	2.127	0.187	2.193	0.241
Ethyl hexanoate	123-66-0	3.508	1.973	3.518	2.033	3.393	1.836	3.427	1.862	3.394	1.818	3.428	1.846
Ethyl oxirane	75-21-8	2.552	0.026	2.591	0.066	2.376	-0.148	2.459	-0.085	2.374	-0.164	2.456	-0.098
Ethyl pentanoate	539-82-2	3.214	1.567	3.234	1.625	3.103	1.435	3.140	1.464	3.104	1.418	3.141	1.448
Ethyl tert-butyl ether	637-92-3	1.468	0.360	1.547	0.432	1.517	0.379	1.501	0.370	1.519	0.367	1.502	0.358

	CAS	IL Specific		Lit (cation + anion)		Method 1		Method 2		Method 3		Method 4	
		log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*
Ethyl fluoride	353-36-6	0.434	0.737	0.512	0.764	0.345	0.627	0.413	0.667	0.345	0.606	0.412	0.654
Ethyl iodide	75-03-6	2.055	1.446	2.126	1.510	2.013	1.407	2.038	1.432	2.004	1.403	2.028	1.432
Ethyl isobutyrate	97-62-1	2.699	1.033	2.734	1.090	2.605	0.918	2.641	0.946	2.606	0.901	2.642	0.930
Ethyl methacrylate	97-63-2	2.695	1.000	2.740	1.066	2.637	0.928	2.657	0.948	2.636	0.916	2.655	0.936
Ethyl n-butyrate	105-54-4	2.915	1.165	2.944	1.221	2.808	1.039	2.848	1.070	2.809	1.022	2.848	1.055
Ethyl n-octyl sulfide	3698-94-0	3.986	3.335	3.998	3.418	3.965	3.298	3.948	3.289	3.962	3.289	3.944	3.283
Ethyl propionate	105-37-3	2.636	0.762	2.675	0.817	2.534	0.643	2.576	0.677	2.534	0.627	2.576	0.662
Ethyl tert-butyl sulfide	14290-92-7	2.369	1.163	2.437	1.246	2.402	1.180	2.383	1.174	2.399	1.175	2.379	1.168
Ethyl vinyl ether	109-92-2	1.421	0.332	1.498	0.390	1.396	0.289	1.418	0.308	1.395	0.276	1.417	0.297
Ethylamine	75-04-7	2.167	-1.129	2.245	-1.054	2.199	-1.099	2.188	-1.100	2.198	-1.104	2.186	-1.109
Ethylbenzene	100-41-4	3.104	2.551	3.141	2.616	3.010	2.459	3.045	2.488	3.002	2.452	3.035	2.486
Ethylcyclohexane	1678-91-7	1.789	3.120	1.836	3.171	1.778	3.092	1.788	3.091	1.774	3.077	1.783	3.086
Ethylcyclopentane	1640-89-7	1.436	2.701	1.492	2.749	1.425	2.672	1.440	2.675	1.422	2.656	1.436	2.669
Ethylene glycol	107-21-1	6.501	-0.906	6.469	-0.832	6.338	-1.030	6.374	-1.007	6.335	-1.034	6.370	-1.019
Ethylenediamine	107-15-3	4.369	-2.589	4.430	-2.475	4.410	-2.531	4.370	-2.541	4.408	-2.523	4.365	-2.548
Ethyleneimine	151-56-4	3.910	-0.103	3.924	-0.055	3.695	-0.303	3.782	-0.236	3.692	-0.315	3.777	-0.249
Ferrocene	102-54-5	5.523	3.231	5.536	3.329	5.381	3.127	5.409	3.170	5.363	3.137	5.388	3.181
Fluoranthene	206-44-0	9.923	5.368	9.868	5.506	9.617	5.149	9.670	5.231	9.585	5.179	9.632	5.257
Fluorene	86-73-7	7.042	3.957	7.027	4.068	6.850	3.815	6.882	3.868	6.829	3.830	6.858	3.882
Fluoro benzene	462-06-6	2.596	2.023	2.635	2.071	2.457	1.886	2.521	1.932	2.451	1.873	2.513	1.927
Formaldehyde	50-00-0	1.699	-0.349	1.762	-0.310	1.546	-0.507	1.629	-0.443	1.545	-0.522	1.626	-0.456
Formic acid	64-18-6	6.031	0.615	5.976	0.652	5.802	0.433	5.882	0.460	5.799	0.419	5.878	0.449
Furan	110-00-9	1.854	1.222	1.910	1.266	1.738	1.103	1.801	1.149	1.734	1.089	1.795	1.141
Haloperidol	52-86-8	15.226	2.218	15.104	2.462	15.168	2.245	15.031	2.208	15.148	2.295	15.005	2.224
Helium	7440-59-7	-2.064	-0.132	-1.920	-0.107	-2.036	-0.133	-1.989	-0.116	-2.036	-0.153	-1.989	-0.126
Heptanal	111-71-7	3.509	1.490	3.525	1.549	3.380	1.346	3.423	1.382	3.380	1.330	3.422	1.367
Heptane	142-82-5	0.968	2.851	1.024	2.891	0.971	2.823	0.984	2.818	0.971	2.802	0.984	2.808
Heptylamine	111-68-2	3.687	0.904	3.718	0.988	3.703	0.910	3.677	0.895	3.702	0.903	3.675	0.885
Hexa-1,5-diene	592-42-7	1.157	1.952	1.228	2.004	1.155	1.932	1.170	1.938	1.152	1.919	1.167	1.931
Hexachlorobenzene	118-74-1	6.986	5.270	6.948	5.360	6.749	5.079	6.803	5.138	6.728	5.086	6.779	5.150
Hexadecane	544-76-3	3.770	6.533	3.744	6.594	3.750	6.474	3.731	6.441	3.750	6.452	3.731	6.431
Hexafluoropropylene	116-15-4	-1.419	0.626	-1.316	0.645	-1.367	0.626	-1.346	0.620	-1.360	0.596	-1.338	0.600
Hexanal	66-25-1	3.200	1.084	3.225	1.141	3.074	0.945	3.120	0.983	3.074	0.930	3.119	0.969
Hexane	110-54-3	0.656	2.441	0.721	2.480	0.662	2.418	0.678	2.416	0.662	2.397	0.678	2.406
Hexanoic acid	142-62-1	6.284	1.775	6.222	1.830	6.125	1.639	6.160	1.640	6.124	1.625	6.159	1.627
Hexyl acetate	142-92-7	3.635	1.998	3.642	2.058	3.514	1.856	3.550	1.884	3.515	1.839	3.550	1.868
Hexylamine	111-26-2	3.372	0.494	3.412	0.577	3.390	0.505	3.367	0.492	3.389	0.498	3.366	0.483
Hexylbenzene	1077-16-3	4.266	4.172	4.268	4.245	4.164	4.067	4.184	4.083	4.156	4.059	4.175	4.081
Hydrogen	74-90-8	4.217	1.414	4.184	1.422	3.890	1.110	4.033	1.188	3.888	1.086	4.030	1.173
Hydroquinone	123-31-9	11.364	1.994	11.212	2.074	11.028	1.755	11.097	1.783	11.015	1.760	11.082	1.782
Indan	496-11-7	4.014	2.726	4.038	2.800	3.902	2.628	3.933	2.663	3.891	2.626	3.921	2.664
Iodobenzene	591-50-4	4.651	3.090	4.674	3.172	4.490	2.959	4.539	3.010	4.474	2.963	4.521	3.018
Iodomethane	74-88-4	1.860	1.168	1.938	1.230	1.808	1.123	1.841	1.154	1.799	1.119	1.831	1.155
Isoamyl acetate	4245-35-6	3.425	2.005	3.441	2.066	3.317	1.878	3.350	1.904	3.317	1.863	3.349	1.890
Isoamyl formate	110-45-2	2.980	1.416	3.005	1.469	2.856	1.274	2.904	1.310	2.856	1.257	2.903	1.295

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Isobutene	115-11-7	0.294	1.247	0.382	1.289	0.306	1.237	0.326	1.244	0.305	1.221	0.324	1.236
Isobutyl acetate	110-19-0	2.819	1.058	2.851	1.116	2.719	0.938	2.757	0.968	2.720	0.921	2.757	0.952
Isobutyl formate	542-55-2	2.665	1.010	2.700	1.062	2.544	0.874	2.595	0.912	2.545	0.856	2.595	0.897
Isobutyl isobutanoate	97-85-8	3.045	1.797	3.069	1.858	2.963	1.688	2.988	1.706	2.965	1.671	2.989	1.690
Isobutyl mercaptan	513-44-0	2.093	1.426	2.153	1.488	2.065	1.390	2.080	1.404	2.061	1.380	2.075	1.399
Isobutylamine	78-81-9	2.562	-0.442	2.628	-0.362	2.602	-0.409	2.581	-0.419	2.602	-0.415	2.580	-0.429
Isobutylbenzene	538-93-2	3.423	3.323	3.449	3.392	3.337	3.235	3.363	3.254	3.330	3.227	3.354	3.252
Isoflurane	26675-46-7	1.852	2.012	1.867	2.024	1.660	1.794	1.758	1.842	1.664	1.762	1.762	1.820
Isopentyl acetate	123-92-2	3.176	1.467	3.198	1.527	3.073	1.344	3.107	1.370	3.074	1.327	3.108	1.355
Isophorone	78-59-1	5.577	2.052	5.555	2.123	5.321	1.803	5.399	1.872	5.316	1.793	5.392	1.861
Isopropanol	67-63-0	3.031	-0.454	3.078	-0.385	3.029	-0.452	3.027	-0.459	3.028	-0.459	3.026	-0.468
Isopropyl acetate	108-21-4	2.443	0.652	2.487	0.708	2.347	0.537	2.389	0.570	2.348	0.521	2.389	0.554
Isopropyl formate	625-55-8	2.316	0.598	2.360	0.647	2.197	0.463	2.253	0.505	2.198	0.446	2.252	0.490
Isopropyl mercaptan	75-33-2	1.743	0.983	1.813	1.041	1.712	0.942	1.734	0.962	1.708	0.932	1.729	0.956
Isopropylamine	75-31-0	2.200	-0.767	2.274	-0.691	2.236	-0.738	2.223	-0.744	2.236	-0.744	2.221	-0.753
Isopropylcyclopentane	3875-51-2	1.770	3.107	1.815	3.156	1.755	3.073	1.766	3.073	1.752	3.057	1.763	3.067
Krypton	7439-90-9'	-1.120	0.385	-1.003	0.412	-1.100	0.379	-1.064	0.393	-1.100	0.359	-1.064	0.383
m-Cresol	108-39-4	7.387	2.387	7.323	2.457	7.166	2.217	7.220	2.244	7.156	2.215	7.208	2.242
m-Cymene	535-77-3	3.547	3.173	3.575	3.246	3.467	3.092	3.488	3.111	3.459	3.086	3.479	3.109
m-Diethylbenzene	141-93-5	3.660	3.234	3.685	3.307	3.575	3.150	3.597	3.170	3.567	3.144	3.587	3.168
Mesitylene	108-67-8	3.514	2.801	3.545	2.873	3.427	2.717	3.452	2.741	3.419	2.711	3.443	2.740
Methane	74-82-8	-1.189	0.396	-1.070	0.423	-1.169	0.389	-1.131	0.403	-1.169	0.369	-1.131	0.393
Methanol	67-56-1	3.239	-0.675	3.277	-0.617	3.188	-0.709	3.211	-0.703	3.186	-0.717	3.208	-0.712
Methoxyflurane	76-38-0	3.584	2.775	3.564	2.796	3.339	2.527	3.442	2.583	3.338	2.502	3.441	2.568
Methyl 4-hydroxybenzoate	99-76-3	10.286	3.096	10.143	3.163	9.893	2.773	9.993	2.833	9.883	2.769	9.980	2.827
Methyl acetate	79-20-9	2.275	0.014	2.326	0.066	2.159	-0.113	2.214	-0.067	2.159	-0.128	2.213	-0.082
Methyl benzoate	93-58-3	4.831	1.708	4.844	1.792	4.687	1.578	4.722	1.622	4.679	1.576	4.712	1.618
Methyl butanoate	623-42-7	2.754	0.787	2.790	0.842	2.646	0.663	2.689	0.699	2.646	0.647	2.689	0.684
Methyl cyclohexyl ketone	823-76-7	5.576	2.276	5.536	2.328	5.257	1.962	5.365	2.048	5.254	1.945	5.360	2.033
Methyl cyclopropyl ketone	765-43-5	4.596	1.205	4.579	1.244	4.274	0.888	4.398	0.986	4.271	0.870	4.394	0.969
Methyl ethyl sulfide	624-89-5	1.784	0.781	1.859	0.846	1.766	0.756	1.782	0.773	1.762	0.748	1.776	0.768
Methyl formate	107-31-3	1.993	-0.024	2.050	0.021	1.854	-0.172	1.925	-0.117	1.853	-0.188	1.923	-0.130
Methyl hexanoate	106-70-7	3.348	1.595	3.365	1.654	3.232	1.460	3.270	1.490	3.232	1.443	3.270	1.475
Methyl pentanoate	624-24-8	3.062	1.196	3.089	1.254	2.951	1.068	2.991	1.101	2.951	1.053	2.991	1.086
Methyl phenyl ether	100-66-3	3.961	1.928	3.987	1.998	3.818	1.796	3.865	1.842	3.809	1.791	3.855	1.840
Methyl propionate	554-12-1	2.477	0.384	2.522	0.438	2.373	0.267	2.419	0.305	2.373	0.252	2.418	0.291
Methyl tert-butyl ether	1634-04-4	1.452	0.012	1.532	0.081	1.481	0.015	1.476	0.015	1.483	0.003	1.477	0.002
Methyl trimethylacetate	598-98-1	2.583	1.122	2.621	1.179	2.491	1.008	2.528	1.036	2.492	0.991	2.529	1.020
Methyl acrylate	96-33-3	2.638	0.489	2.684	0.545	2.518	0.360	2.571	0.405	2.516	0.347	2.568	0.393
Methyl fluoride	593-53-3	0.118	0.379	0.204	0.405	0.030	0.274	0.102	0.317	0.030	0.253	0.102	0.305
Methyl mercaptan	74-93-1	1.952	1.001	2.005	1.040	1.804	0.854	1.881	0.911	1.799	0.839	1.875	0.903
Methyl n-butyl sulfide	628-29-5	2.638	1.439	2.689	1.509	2.609	1.402	2.617	1.414	2.605	1.393	2.612	1.408
Methyl tert-butyl sulfide	6163-64-0	2.062	0.684	2.141	0.767	2.112	0.720	2.089	0.713	2.109	0.716	2.085	0.708
Methyl-2-pyrrolidone	872-50-4	5.637	-0.193	5.629	-0.117	5.376	-0.441	5.456	-0.357	5.372	-0.447	5.450	-0.371
Methylacetylene	74-99-7	1.120	0.694	1.192	0.735	1.083	0.648	1.120	0.665	1.081	0.633	1.117	0.656

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Methylamine	74-89-5	1.925	-1.399	2.009	-1.327	1.953	-1.371	1.948	-1.367	1.952	-1.376	1.946	-1.376
Methylcyclohexane	108-87-2	1.439	2.704	1.495	2.752	1.429	2.677	1.444	2.679	1.426	2.661	1.440	2.674
Methylcyclopentane	96-37-7	1.123	2.292	1.187	2.337	1.114	2.266	1.132	2.272	1.111	2.251	1.129	2.267
Methylpyrrolidine	120-94-5	4.047	1.179	4.048	1.227	3.800	0.932	3.895	1.008	3.797	0.916	3.891	0.993
m-Ethyltoluene	620-14-4	3.431	2.831	3.462	2.901	3.343	2.745	3.370	2.769	3.335	2.739	3.361	2.768
m-Methylstyrene	100-80-1	3.987	2.911	4.015	2.989	3.871	2.809	3.905	2.844	3.860	2.808	3.892	2.846
Monuron	150-68-5	10.771	2.592	10.653	2.700	10.444	2.330	10.500	2.384	10.432	2.338	10.484	2.382
Morpholine	110-91-8	4.148	-1.449	4.197	-1.352	4.103	-1.488	4.100	-1.463	4.100	-1.487	4.096	-1.473
m-Xylene	108-38-3	3.179	2.518	3.215	2.584	3.084	2.426	3.118	2.456	3.076	2.419	3.108	2.454
N,N-Dimethylaniline	121-69-7	4.870	2.029	4.894	2.123	4.746	1.925	4.773	1.965	4.734	1.929	4.759	1.967
N,N-Dimethylformamide	68-12-2	5.188	-0.453	5.181	-0.392	4.899	-0.732	4.999	-0.637	4.897	-0.743	4.995	-0.654
Naphthalene	91-20-3	5.436	3.188	5.450	3.282	5.268	3.057	5.311	3.110	5.250	3.066	5.290	3.119
Naproxen	22204-53-1	14.236	4.693	14.025	4.798	13.702	4.254	13.815	4.346	13.683	4.263	13.793	4.347
n-Butylacetamide	1119-49-9	7.892	1.158	7.803	1.220	7.562	0.856	7.653	0.920	7.560	0.843	7.650	0.902
Neon	7440-01-9'	-1.962	-0.082	-1.820	-0.058	-1.935	-0.084	-1.889	-0.067	-1.935	-0.104	-1.889	-0.077
Neopentane	463-82-1	0.133	2.032	0.213	2.068	0.143	2.012	0.165	2.013	0.143	1.991	0.165	2.003
Nitrobenzene	98-95-3	5.466	2.279	5.452	2.344	5.196	2.035	5.285	2.116	5.185	2.030	5.272	2.113
Nitroethane	79-24-3	3.572	0.783	3.581	0.820	3.319	0.532	3.424	0.613	3.317	0.514	3.421	0.598
Nitrogen	55-63-0	8.920	3.713	8.772	3.736	8.258	3.077	8.486	3.252	8.252	3.050	8.480	3.229
Nitromethane	75-52-5	3.453	0.469	3.467	0.506	3.201	0.224	3.309	0.306	3.198	0.207	3.305	0.292
Nitrous oxide	10024-97-2	0.188	0.374	0.273	0.400	0.102	0.270	0.172	0.313	0.102	0.250	0.172	0.300
N-Methylaniline	100-61-8	5.720	1.785	5.719	1.872	5.560	1.658	5.597	1.698	5.549	1.661	5.583	1.699
N-Methylmorpholine	109-02-4	3.663	-1.129	3.719	-1.033	3.629	-1.167	3.625	-1.145	3.628	-1.169	3.622	-1.156
N-Methylpiperidine	626-67-5	2.460	-0.349	2.541	-0.253	2.531	-0.290	2.492	-0.300	2.530	-0.291	2.489	-0.307
n-Octane	111-65-9	1.279	3.260	1.326	3.303	1.279	3.229	1.289	3.221	1.279	3.208	1.289	3.211
n-Octylamine	111-86-4	3.902	1.310	3.926	1.396	3.914	1.311	3.886	1.293	3.914	1.304	3.885	1.283
Nonadecane	629-92-5	4.702	7.761	4.649	7.828	4.675	7.691	4.646	7.649	4.675	7.668	4.646	7.639
Nonan-2-one	821-55-6	4.150	2.056	4.150	2.122	4.017	1.906	4.052	1.935	4.017	1.890	4.051	1.920
Nonan-5-one	502-56-7	4.062	2.032	4.063	2.097	3.935	1.886	3.968	1.914	3.935	1.870	3.968	1.898
Nonanal	124-19-6	4.124	2.311	4.123	2.376	3.991	2.162	4.027	2.191	3.991	2.146	4.026	2.177
Nonane	111-84-2	1.590	3.669	1.628	3.714	1.588	3.635	1.594	3.623	1.588	3.613	1.594	3.613
o-Cresol	95-48-7	7.028	2.464	6.974	2.535	6.815	2.300	6.869	2.328	6.804	2.298	6.856	2.327
Octadecane	593-45-3	4.391	7.351	4.347	7.417	4.367	7.285	4.341	7.246	4.367	7.263	4.341	7.236
Octafluorocyclobutane	115-25-3	-1.832	0.880	-1.716	0.906	-1.705	0.951	-1.715	0.921	-1.698	0.923	-1.707	0.904
Octanal	124-13-0	3.823	1.905	3.830	1.968	3.693	1.761	3.731	1.793	3.693	1.746	3.730	1.779
o-Cymene	527-84-4	3.722	3.226	3.748	3.300	3.632	3.137	3.656	3.159	3.623	3.132	3.646	3.158
o-Diethylbenzene	135-01-3	3.822	3.287	3.845	3.361	3.727	3.195	3.752	3.218	3.718	3.190	3.742	3.217
o-Methylstyrene	611-15-4	3.992	2.928	4.023	3.008	3.881	2.832	3.913	2.866	3.869	2.832	3.899	2.869
o-Toluidine	95-53-4	6.059	1.775	6.050	1.863	5.893	1.646	5.930	1.684	5.882	1.650	5.916	1.685
Oxygen	7782-44-7	-1.436	0.202	-1.310	0.228	-1.413	0.198	-1.373	0.213	-1.413	0.178	-1.373	0.203
o-Xylene	95-47-6	3.371	2.568	3.403	2.634	3.264	2.466	3.301	2.499	3.255	2.460	3.291	2.498
Ozone	10028-15-6	-0.247	0.548	-0.157	0.570	-0.274	0.502	-0.225	0.522	-0.274	0.481	-0.225	0.510
p-Cresol	106-44-5	7.351	2.468	7.287	2.537	7.129	2.298	7.184	2.325	7.119	2.296	7.172	2.323
p-Diethylbenzene	105-05-5	3.692	3.237	3.717	3.311	3.608	3.155	3.629	3.174	3.600	3.149	3.619	3.173
p-Diisopropylbenzene	100-18-5	3.962	3.928	3.979	4.007	3.888	3.850	3.900	3.859	3.881	3.844	3.891	3.858

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		log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*
Penta-1,4-diene	591-93-5	0.760	1.518	0.840	1.565	0.759	1.498	0.779	1.506	0.757	1.483	0.777	1.499
Pentachloroethane	76-01-7	4.629	3.280	4.616	3.333	4.443	3.112	4.506	3.152	4.434	3.102	4.496	3.149
Pentadecane	629-62-9	3.458	6.124	3.441	6.183	3.441	6.068	3.425	6.039	3.441	6.046	3.425	6.029
Pentafluoroethane	354-33-6	-0.570	0.726	-0.497	0.733	-0.602	0.652	-0.549	0.663	-0.595	0.619	-0.540	0.641
Pentanal	110-62-3	2.891	0.678	2.926	0.734	2.769	0.544	2.818	0.585	2.769	0.529	2.817	0.571
Pentane	109-66-0	0.344	2.032	0.418	2.068	0.352	2.012	0.372	2.013	0.352	1.991	0.372	2.003
Pentanoic acid	109-52-4	5.966	1.379	5.916	1.434	5.814	1.252	5.851	1.256	5.813	1.239	5.849	1.243
Pentyl acetate	628-63-7	3.326	1.592	3.343	1.650	3.208	1.455	3.247	1.486	3.209	1.438	3.247	1.470
Pentyl propanoate	624-54-4	3.503	1.958	3.515	2.019	3.397	1.830	3.427	1.854	3.398	1.813	3.428	1.838
Pentyl mercaptan	110-66-7	2.713	2.065	2.752	2.124	2.638	1.983	2.667	2.006	2.634	1.972	2.662	2.000
Pentylamine	110-58-7	3.057	0.089	3.108	0.169	3.079	0.104	3.060	0.094	3.078	0.097	3.058	0.085
Pentylbenzene	538-68-1	3.992	3.772	4.002	3.843	3.889	3.667	3.914	3.687	3.881	3.659	3.905	3.685
Pentylcyclopentane	3741-00-2	2.162	3.907	2.196	3.962	2.151	3.874	2.155	3.865	2.148	3.857	2.151	3.859
Phenanthrene	85-01-8	8.324	4.558	8.300	4.688	8.094	4.398	8.130	4.462	8.067	4.423	8.098	4.484
Phenetole	103-73-1	4.036	2.145	4.060	2.221	3.914	2.031	3.949	2.068	3.905	2.027	3.939	2.066
Phenol	108-95-2	7.204	2.193	7.141	2.256	6.968	2.012	7.032	2.043	6.958	2.009	7.020	2.041
Phenyl methyl sulfide	100-68-5	5.049	2.640	5.062	2.723	4.869	2.487	4.921	2.543	4.855	2.489	4.905	2.546
Phenyl mercaptan	108-98-5	4.727	2.637	4.739	2.710	4.557	2.496	4.611	2.545	4.543	2.496	4.596	2.548
Phenylhydrazine	100-63-0	7.448	1.598	7.413	1.693	7.241	1.444	7.283	1.488	7.227	1.452	7.266	1.491
Piperidine	110-89-4	3.681	-0.358	3.730	-0.266	3.697	-0.335	3.674	-0.340	3.694	-0.335	3.669	-0.346
p-Methylstyrene	622-97-9	4.002	2.911	4.030	2.989	3.886	2.809	3.920	2.844	3.874	2.808	3.907	2.846
Prop-2-en-1-ol	107-18-6	3.915	0.047	3.937	0.112	3.864	0.016	3.878	0.014	3.862	0.009	3.874	0.007
Propane	74-98-6	-0.342	1.214	-0.248	1.245	-0.328	1.201	-0.301	1.208	-0.328	1.180	-0.301	1.198
Propanoic acid	79-09-4	5.445	0.613	5.411	0.662	5.281	0.477	5.332	0.492	5.280	0.464	5.330	0.479
Propanone	67-64-1	2.539	-0.233	2.587	-0.180	2.411	-0.367	2.470	-0.319	2.411	-0.381	2.468	-0.333
Propanonitrile	107-12-0	3.195	0.508	3.210	0.544	2.957	0.268	3.059	0.345	2.957	0.248	3.058	0.328
Propargyl alcohol	107-19-7	4.140	-0.538	4.167	-0.464	4.080	-0.576	4.094	-0.568	4.077	-0.580	4.089	-0.576
Propene	115-07-1	-0.109	0.877	-0.011	0.915	-0.098	0.865	-0.071	0.876	-0.099	0.848	-0.072	0.867
Propyl acetate	109-60-4	2.701	0.780	2.737	0.835	2.591	0.653	2.636	0.690	2.591	0.637	2.636	0.674
Propyl butanoate	105-66-8	3.165	1.549	3.186	1.607	3.061	1.425	3.096	1.451	3.063	1.407	3.096	1.436
Propyl formate	110-74-7	2.535	0.729	2.573	0.777	2.403	0.584	2.462	0.629	2.403	0.567	2.461	0.615
Propyl chloride	540-54-5	1.646	1.551	1.698	1.589	1.548	1.441	1.603	1.477	1.545	1.423	1.600	1.467
Propyl mercaptan	107-03-9	1.923	1.044	1.990	1.105	1.893	1.009	1.913	1.028	1.889	1.000	1.907	1.023
Propyl propionate	106-36-5	2.898	1.146	2.928	1.204	2.799	1.028	2.835	1.058	2.800	1.012	2.836	1.042
Propylamine	107-10-8	2.449	-0.723	2.518	-0.646	2.478	-0.698	2.465	-0.702	2.477	-0.704	2.463	-0.711
Propylbenzene	103-65-1	3.350	2.948	3.380	3.015	3.257	2.855	3.287	2.880	3.249	2.847	3.278	2.878
Propylcyclohexane	1678-92-8	2.432	3.647	2.459	3.696	2.369	3.568	2.395	3.577	2.366	3.551	2.391	3.570
Propylcyclopentane	2040-96-2	1.732	3.110	1.779	3.160	1.718	3.078	1.730	3.078	1.715	3.062	1.726	3.072
Propyne	80-46-6	8.564	3.657	8.471	3.741	8.348	3.487	8.381	3.499	8.339	3.486	8.369	3.497
p-Toluidine	106-49-0	6.132	1.785	6.118	1.871	5.950	1.639	5.994	1.681	5.939	1.641	5.980	1.681
p-Xylene	106-42-3	3.175	2.515	3.210	2.580	3.079	2.421	3.113	2.451	3.071	2.414	3.104	2.449
Pyrene	129-00-0	10.568	5.472	10.522	5.630	10.256	5.264	10.306	5.352	10.218	5.305	10.261	5.386
Pyridine	110-86-1	3.751	0.240	3.794	0.317	3.623	0.123	3.666	0.174	3.617	0.121	3.658	0.168
Pyrimidine	289-95-2	3.979	-0.485	4.024	-0.402	3.850	-0.602	3.891	-0.549	3.845	-0.603	3.883	-0.556
Pyrrole	109-97-7	5.197	1.276	5.181	1.333	5.020	1.134	5.078	1.167	5.012	1.127	5.069	1.163

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Pyrrolidine	123-75-1	5.003	0.912	4.986	0.963	4.764	0.693	4.849	0.753	4.760	0.681	4.844	0.741
Quinoline	91-22-5	5.879	1.548	5.901	1.661	5.763	1.469	5.774	1.511	5.748	1.483	5.755	1.518
Radon	10043-92-2	-0.449	0.786	-0.352	0.815	-0.434	0.777	-0.405	0.787	-0.434	0.756	-0.405	0.777
Salicylamide	65-45-2	10.726	2.735	10.589	2.812	10.301	2.390	10.410	2.469	10.287	2.392	10.393	2.467
sec-Butyl mercaptan	513-53-1	2.101	1.401	2.160	1.461	2.063	1.353	2.083	1.371	2.059	1.343	2.078	1.365
sec-Butylbenzene	135-98-8	3.467	3.294	3.494	3.364	3.382	3.207	3.407	3.226	3.374	3.199	3.398	3.224
Styrene	100-42-5	3.651	2.586	3.686	2.659	3.531	2.480	3.572	2.519	3.519	2.478	3.559	2.521
Sulfur dioxide	7446-09-5'	2.914	1.205	2.935	1.235	2.715	1.020	2.812	1.073	2.710	1.004	2.806	1.063
Sulfur hexafluoride	2551-62-4	-1.867	0.642	-1.765	0.648	-1.836	0.619	-1.799	0.620	-1.828	0.584	-1.790	0.598
Teflurane	124-72-1	1.391	1.873	1.428	1.893	1.298	1.764	1.358	1.782	1.299	1.739	1.359	1.768
tert-Amyl methyl ether	994-05-8	1.815	0.431	1.886	0.504	1.845	0.435	1.834	0.431	1.846	0.424	1.834	0.419
tert-Butanol	75-65-0	2.891	-0.310	2.944	-0.234	2.919	-0.283	2.903	-0.300	2.918	-0.289	2.902	-0.309
tert-Butyl mercaptan	75-66-1	1.667	1.236	1.737	1.297	1.652	1.207	1.667	1.218	1.649	1.196	1.663	1.211
tert-Butylbenzene	98-06-6	3.446	3.309	3.475	3.380	3.360	3.221	3.386	3.242	3.352	3.215	3.376	3.240
Tetrachloroethylene	127-18-4	2.731	2.710	2.771	2.765	2.633	2.617	2.675	2.650	2.624	2.609	2.665	2.650
Tetracosane	646-31-1	6.265	9.807	6.166	9.885	6.225	9.719	6.178	9.662	6.225	9.696	6.178	9.652
Tetradecane	629-59-4	3.147	5.715	3.139	5.771	3.132	5.663	3.121	5.636	3.132	5.641	3.121	5.626
Tetrafluoroethylene	116-14-3	-1.426	0.693	-1.319	0.710	-1.402	0.676	-1.366	0.682	-1.398	0.648	-1.361	0.666
Tetrafluoromethane	75-73-0	-2.463	0.176	-2.341	0.182	-2.403	0.182	-2.371	0.179	-2.395	0.148	-2.362	0.158
Tetrahydrofuran	109-99-9	2.446	-0.134	2.506	-0.068	2.397	-0.189	2.417	-0.161	2.394	-0.197	2.414	-0.170
Tetrahydrothiophene	110-01-0	3.144	1.404	3.187	1.468	3.022	1.290	3.071	1.335	3.015	1.284	3.061	1.332
Thiophene	110-02-1	2.716	1.595	2.768	1.656	2.612	1.501	2.658	1.543	2.603	1.495	2.647	1.542
Toluene	108-88-3	2.845	2.193	2.888	2.254	2.746	2.097	2.787	2.131	2.738	2.090	2.778	2.129
trans 1,2-Dichloroethene	156-60-5	2.211	1.761	2.257	1.804	2.112	1.664	2.164	1.697	2.106	1.651	2.157	1.692
trans-1,2-Dimethylcyclohexane	6876-23-9	1.973	3.201	2.012	3.247	1.922	3.132	1.949	3.142	1.919	3.114	1.945	3.135
trans-1,2-Dimethylcyclopentane	822-50-4	1.282	2.688	1.340	2.733	1.268	2.653	1.286	2.657	1.265	2.636	1.283	2.650
trans-1,3-Dimethylcyclopentane	1759-58-6	1.256	2.678	1.312	2.722	1.238	2.639	1.259	2.644	1.236	2.622	1.256	2.636
trans-1,3-pentadiene	2004-70-8	1.235	1.652	1.310	1.704	1.216	1.621	1.240	1.636	1.212	1.610	1.234	1.631
trans-1,4-Dimethylcyclohexane	2207-04-7'	1.553	3.097	1.603	3.145	1.536	3.059	1.552	3.060	1.534	3.042	1.549	3.053
trans-2-butene	624-64-6	0.337	1.386	0.423	1.427	0.343	1.371	0.366	1.379	0.342	1.354	0.364	1.371
trans-2-hexene	4050-45-7	0.949	2.156	1.017	2.202	0.951	2.135	0.966	2.136	0.950	2.117	0.965	2.128
trans-2-octene	13389-42-9	1.550	2.920	1.601	2.971	1.553	2.897	1.558	2.891	1.552	2.880	1.556	2.883
trans-2-pentene	646-04-8	0.669	1.705	0.746	1.749	0.676	1.691	0.693	1.695	0.675	1.674	0.691	1.687
trans-3-octene	14919-01-8	1.564	2.929	1.615	2.980	1.564	2.903	1.571	2.898	1.562	2.886	1.569	2.890
trans-4-octene	14850-23-8	1.528	2.926	1.579	2.976	1.527	2.898	1.535	2.893	1.526	2.881	1.533	2.885
trans-Stilbene	103-30-0	7.341	4.084	7.315	4.198	7.160	3.946	7.181	3.990	7.141	3.959	7.159	4.001
Trichloroethene	79-01-6	2.518	2.190	2.559	2.241	2.436	2.114	2.475	2.139	2.429	2.104	2.467	2.137
Trichlorofluoromethane	75-69-4	1.013	1.482	1.083	1.523	0.970	1.424	1.007	1.445	0.967	1.407	1.004	1.437
Tricosane	638-67-5	5.952	9.397	5.863	9.474	5.915	9.314	5.871	9.259	5.915	9.290	5.871	9.249
Tridecane	629-50-5	2.835	5.306	2.837	5.360	2.823	5.257	2.815	5.233	2.823	5.235	2.815	5.223
Triethylamine	121-44-8	1.688	-0.686	1.788	-0.587	1.832	-0.570	1.767	-0.603	1.833	-0.573	1.768	-0.612
Triethylphosphate	78-40-0	5.267	-0.186	5.263	-0.096	5.127	-0.344	5.149	-0.308	5.132	-0.355	5.152	-0.330
Trifluoromethane	75-46-7	-0.264	0.540	-0.201	0.540	-0.362	0.408	-0.280	0.441	-0.356	0.374	-0.273	0.419
Trimethylamine	75-50-3	0.921	-1.311	1.035	-1.227	1.028	-1.224	0.993	-1.237	1.029	-1.229	0.993	-1.246
Undecan-2-one	112-44-7	4.700	3.120	4.680	3.187	4.559	2.959	4.589	2.983	4.560	2.943	4.589	2.968

	CAS	IL Specific		Lit (cation + anion)		Method 1		Method 2		Method 3		Method 4	
		log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*	log *K*	log *P*
Undecane	1120-21-4	2.213	4.487	2.232	4.537	2.206	4.446	2.205	4.428	2.206	4.424	2.205	4.418
Vinyl acetate	108-05-4	2.186	0.334	2.245	0.393	2.108	0.244	2.146	0.277	2.107	0.232	2.144	0.266
Vinyl chloride	75-01-4	1.090	1.238	1.158	1.273	0.996	1.135	1.058	1.175	0.993	1.118	1.054	1.166
Vinyl propionate	105-38-4	2.562	0.589	2.613	0.653	2.495	0.510	2.522	0.536	2.494	0.498	2.520	0.525
Vinylacetonitrile	109-75-1	3.195	0.414	3.224	0.466	3.021	0.238	3.092	0.298	3.019	0.224	3.089	0.285
Water	7732-18-5	4.541	-0.258	4.514	-0.230	4.396	-0.371	4.456	-0.368	4.398	-0.389	4.457	-0.384
Xenon	7440-63-3	-0.757	0.626	-0.651	0.655	-0.740	0.618	-0.707	0.630	-0.740	0.598	-0.707	0.620
α-Methylstyrene	98-83-9	3.904	2.850	3.934	2.928	3.792	2.751	3.825	2.785	3.781	2.750	3.812	2.786

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