Critical Properties, Normal Boiling Temperature, and Acentric Factor of Another 200 Ionic Liquids

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The critical properties, the normal boiling temperature, and the acentric factor of 200 ionic liquids have been determined using an extended group contribution method, which is based on the well-known concepts of Lydersen and Joback and Reid, that was developed by the authors. The method does not require any additional data besides knowledge of the structure of the molecule and its molecular mass. Because experimental critical properties of ionic liquids are not available, the accuracy of the method is checked by calculating the liquid density of the ionic liquids considered in the study for which experimental data are available in the literature. The results show that the values determined for the critical properties, the normal boiling temperature, and the acentric factor are sufficiently accurate for engineering calculations, generalized correlations, and equation of state methods, among other applications.

Introduction

The authors have recently presented a procedure to estimate the critical properties (temperature (T_C), pressure (P_C), and volume (V_C)), the normal boiling temperature (T_b), and the acentric factor (ω) of ionic liquids using a group contribution method that unifies the best characteristics of two of the most used simplest techniques: Lydersen[1] and Joback and Reid.[2] The accuracy of the estimated values were tested by determining the density of the ionic liquids using an independent equation that was not applied in determining the critical properties. The tests proved that the predicted values seem to be reasonable, considering the relatively low deviations between experimental and calculated densities.[3]

Ionic liquids recently have attracted special attention from the scientific community, and hundreds of studies that involve different aspects of ionic liquids have been presented in the literature. However, the critical properties that are required to estimate other properties for the modeling, simulation, and design of processes involving ionic liquids are not available. One reason for this is because the critical properties of ionic liquids cannot be experimentally determined, since most of these compounds start to decompose at low temperature and, in many cases, at temperatures approaching T_b. The estimated properties are useful approximations that must be interpreted as "these would be the values of T_C, P_C, T_b and ω, if the properties were possible to be measured". Because of the fact that experimental data do not exist and there is no reasonable and generally accepted theory yet available to estimate these properties for ionic liquids, the group contribution method recently presented by Valderrama and Robles[3] is considered to give reasonable estimates.

In addition to the aforementioned arguments, the critical properties (T_C, P_C, and V_C), normal boiling temperature (T_b), and acentric factor (ω) are widely used in correlations and predictive methods to estimate a series of thermophysical and transport properties (such as vapor pressure, liquid density, viscosity, and thermal conductivity, among others).[4] The corresponding state principle, which is based on equations of state or other methods of molecular nature, also makes use of the critical properties.[5] In the case of ionic liquids, our previous studies indicate that extending estimation procedures originally derived for organic substances to ionic liquids, instead of developing complete new procedures for treating these new fluids, is a reasonable way to obtain these hypothetical properties, which are needed for other calculations.[3]

Among the several proposals presented in the literature, the approach developed by Lydersen[1] is perhaps the most widely used group contribution method to estimate critical properties. Later, Joback and Reid[2] developed a method that is frequently mentioned in the literature and used in several applications. In all these methods, the property of a compound is calculated by summing the contributions of certain defined groups of atoms, while simultaneously considering the number frequency of each group that is present in the molecule. Although all these methods have been questioned in the literature,[4] they have the advantage of providing quick estimates without requiring sophisticated computational calculations.

Alvarez and Valderrama[6] combined the best results of Lydersen's method with the best results of the Joback−Reid method to proposed a "modified Lydersen−Joback−Reid" method that proved to give good results for molecules with high molecular mass. The method considers the equations of the Lydersen method for the critical pressure and critical volume, and the equations of the Joback−Reid method for the normal boiling temperature and the critical temperature. The authors modified the parameters involved in the different equations for the critical properties. The equation for the normal boiling point was the same as that given in the original method.

This modified Lydersen−Joback−Reid method was used by Valderrama and Robles[3] to estimate the critical properties of 50 ionic liquids. Because there are no experimental critical

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Table 1. Modified Group Contribution Method[a]

Model Equations	Constants
$T_b = 198.2 + \sum n\Delta T_{bM}$	$A_M = 0.5703$
$T_c = \dfrac{T_b}{\left[A_M + B_M \sum n\Delta T_M - \left(\sum n\Delta T_M\right)^2\right]}$	$B_M = 1.0121$
$P_c = \dfrac{M}{\left(C_M + \sum n\Delta P_M\right)^2}$	$C_M = 0.2573$
$V_c = E_M + \sum n\Delta V_M$	$E_M = 6.75$

[a] Data taken from ref 5. In the equations, M is given in units of g/mol, T_b and T_c are given in Kelvin, P_c is given in bars, and V_c is given in units of (cm^3/mol).

properties available to evaluate the accuracy of the estimates, these values were tested for accuracy and consistency by determining the density of the ionic liquids, for which experimental data are available. For this, an independent equation that was not applied in determining the critical properties was used. The deviations found between the experimental and calculated densities are within the experimental errors shown by the authors. However, the method has been questioned by Jones et al. in a recent communication.[7] These authors compared 8 of the 50 estimated boiling temperatures with values derived from experimentally determined heats of vaporization. According to Jones et al.,[7] the boiling temperatures of ionic liquids are not predicted well by the method used by Valderrama and Robles and, by inference, the critical properties and acentric factors also are likely to be erroneous. To reach this conclusion, Jones et al.[7] extrapolated their heat of vaporization data using a constant value for the heat capacity difference $[CP_L - CP_G] = 94$ J K^{-1} mol^{-1} for the 8 ionic liquids and then used Trouton's Law: $[\Delta H^{vap}(\text{at } 298 \text{ K}) - 94(T_b - 298 \text{ K})]/(T_b) = 85$.

In another communication, Valderrama and Robles[8] discussed their own calculated values and extensively explained why those values seem to be reasonable and can be accepted for correlation and other calculations in which critical properties are required. These authors demonstrated that the heat capacity difference $[CP_L - CP_G]$ that Jones et al.[7] assumed to be constant (94 J K^{-1} mol^{-1}) may vary from 15 J K^{-1} mol^{-1} to 287 J K^{-1} mol^{-1} for many fluids, and certainly this variation for ionic liquids is unknown. Also, Trouton's constant, which was assumed by Jones et al.[7] to be 85 J K^{-1} mol^{-1} ranges from 20 J K^{-1} mol^{-1} to 181 J K^{-1} mol^{-1} for many fluids. Also, in this case, the value of this constant, if it is constant, is unknown for ionic liquids. Therefore, assuming values of $[CP_L - CP_G] = 94$ J K^{-1} mol^{-1} and $[\Delta H^{vap}(\text{at } 298 \text{ K}) - 94(T_b - 298 \text{ K})]/T_b = 85$ are simply rough approximations that cannot be used for all ionic liquids without further analysis.

Because experimental data do not exist and there is no reasonable and generally accepted theory yet available to estimate these properties for ionic liquids, the extension of standard methods such as group contribution seems to be reasonable. Also, the independent test of using the estimated critical properties to calculate the density of ionic liquids gives an indication of the consistency of the estimated values.

The Group Contribution Method

Details of the group contribution method has been given by Valderrama and Robles;[3] therefore, it is only summarized in Tables 1 and 2. Table 1 shows the main equations for the normal boiling temperature and the critical properties, whereas Table 2 lists the groups used to estimate the properties of the selected 200 ionic liquids.

Table 2. Groups Considered in the Modified Lydersen−Joback−Reid Method[a]

group	ΔT_{bM}	ΔT_M	ΔP_M	ΔV_M
Without Rings				
$-CH_3$	23.58	0.0275	0.3031	66.81
$-CH_2-$	22.88	0.0159	0.2165	57.11
>CH−	21.74	0.0002	0.1140	45.70
>C< [>C−]$^-$	18.18	−0.0206	0.0539	21.78
$=CH_2$	24.96	0.0170	0.2493	60.37
=CH−	18.25	0.0182	0.1866	49.92
=C<	24.14	−0.0003	0.0832	34.90
−O− [−O]$^-$	22.42	0.0051	0.1300	15.61
>C=O	94.97	0.0247	0.2341	69.76
−COO−	81.10	0.0377	0.4139	84.76
>N− [>N<]$^+$	11.74	−0.0028	0.0304	26.70
−N=	74.60	0.0172	0.1541	45.54
−CN	125.66	0.0506	0.3697	89.32
−F [F^-]	−0.03	0.0228	0.2912	31.47
−Cl [Cl^-]	38.13	0.0188	0.3738	62.08
−I [I^-]	93.84	0.0148	0.9174	100.79
With Rings				
$-CH_2-$	27.15	0.0116	0.1982	51.64
=CH−	26.73	0.0114	0.1693	42.55
>C<	21.32	−0.0180	0.0139	17.62
=C<	31.01	0.0051	0.0955	31.28
>N− [>N<]$^+$	68.16	0.0063	0.0538	25.17
-N= [>N=]$^+$	57.55	−0.0011	0.0559	42.15
New Groups				
−B	−24.56	−0.0264	0.0348	22.45
−P	34.86	0.0067	0.1776	67.01
−S− [>S−]$^+$	117.52	−0.0004	0.6901	184.67
$-SO_2-$ *	147.24	−0.0563	−0.0606	112.19

[a] Data taken from ref 3. * Value determined in this work.

As a test of the "consistency" of the predicted properties, the liquid density of the ionic liquids has been estimated using a generalized correlation. In this work, a more flexible correlation that was proposed by one of the current authors have been used.[9] This correlation has been shown to give accurate predictions for many fluids and is based on the equation of Shah and Yaws.[10] It requires only the normal boiling temperature, the molecular mass, and the critical properties:

$$\rho_L = \left(0.01256 + \frac{0.9533M}{V_C}\right)\left[\left(\frac{0.0039}{M} + \frac{0.2987}{V_C}\right)V_C^{1.033}\right]^{\Psi} \quad (1)$$

where

$$\Psi = -\left[\frac{1 - T_R}{1 - T_{bR}}\right]^{2/7}$$

In these equations, ρ_L is the liquid density (given in units of g/cm^3), T_R is the reduced temperature ($T_R = T/T_C$), and T_{bR} is the reduced temperature at the normal boiling point ($T_{bR} = T_b/T_C$).

The acentric factors (ω) of the ionic liquids were estimated as described by Valderrama and Robles,[3] using the calculated critical properties and the calculated normal boiling temperature:

$$\omega = \frac{(T_b - 43)(T_c - 43)}{(T_c - T_b)(0.7T_c - 43)}\log\left(\frac{P_c}{P_b}\right) - \left(\frac{T_c - 43}{T_c - T_b}\right)\log\left(\frac{P_c}{P_b}\right) + \log\left(\frac{P_c}{P_b}\right) - 1 \quad (2)$$

Table 3. Critical Properties of Ionic Liquids Calculated by Group Contribution, Densities Calculated with the Generalized Correlation (eq 1), and Comparison with Literature Values[a]

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
1	[P11] [tsac]	$C_9H_{14}F_6N_2O_3S$	1,1-dimethylpyrrolidinium (2,2,2-trifluoro-*n*-(trifluoromethyl sulfonyl)acetamide	344	712.4	999.5	24.2	813.1	0.4673	298.15	1.4300[11]	1.4297	0.0
2	[emim] [tsac]	$C_9H_{11}F_6N_3O_3S$	1-ethyl-3-methylidimazolium (2,2,2-trifluoro-*n*-(trifluoromethyl sulfonyl)acetamide	355	764.4	1069.9	25.2	833.5	0.4977	298.15	1.4600[11]	1.4553	−0.3
3	[TEA] [tsac]	$C_{11}H_{20}F_6N_2O_3S$	tetraethylammonium (2,2,2-trifluoro-*n*-(trifluoromethyl sulfonyl)acetamide	374	686.1	913.2	19.1	970.2	0.6591	298.15	1.3700[11]	1.3401	−2.2
4	[TMAIA] [tsac]	$C_9H_{14}F_6N_2O_3S$	trimethylalylammonium (2,2,2-trifluoro-*n*-(trifluoromethyl sulfonyl)acetamide	344	637.0	875.2	22.5	842.3	0.5475	298.15	1.3800[11]	1.3736	−0.5
5	[TMEA] [tsac]	$C_8H_{14}F_6N_2O_3S$	trimethylethylammonium (2,2,2-trifluoro-*n*-(trifluoromethyl sulfonyl)acetamide	332	617.4	854.1	23.3	798.8	0.5257	298.15	1.4000[11]	1.3862	−1.0
6	[TMiPA] [tsac]	$C_9H_{16}F_6N_2O_3S$	trimethylisopropylammonium (2,2,2-trifluoro-*n*-(trifluoromethyl sulfonyl)acetamide	346	639.9	876.1	21.9	854.2	0.5536	298.15	1.4100[11]	1.3662	−3.1
7	[TMPA] [tsac]	$C_9H_{16}F_6N_2O_3S$	trimethylpropylammonium (2,2,2-trifluoro-*n*-(trifluoromethyl sulfonyl)acetamide	346	640.3	873.7	21.7	855.9	0.5700	298.15	1.3800[11]	1.3672	−0.9
8	[bmim] [TFES]	$C_{10}H_{16}N_2O_3SF_4$	1-butyl-3-methylidimazolium 1,1,2,2-tetrafluoroethane sulfonate	320	729.4	1030.5	25.7	827.8	0.4583	301.45	1.3240[12]	1.3016	−1.7
9	[dmim] [TFES]	$C_{18}H_{32}N_2O_3SF_4$	1-dodecyl-3-methylidimazolium 1,1,2,2-tetrafluoroethane sulfonate	433	912.5	1171.0	15.6	1284.7	0.8065	301.35	1.1360[12]	1.2497	10.0
10	[emim] [TFES]	$C_8H_{12}N_2O_3SF_4$	1-ethyl-3-methylidimazolium 1,1,2,2-tetrafluoroethane sulfonate	292	683.7	998.2	30.4	713.6	0.3743	301.45	1.5020[12]	1.3447	−10.5
11	[hpmim] [TFES]	$C_{13}H_{22}N_2SF_4$	1-heptyl-3-methylidimazolium 1,1,2,2-tetrafluoroethane sulfonate	362	798.1	1080.8	20.7	999.2	0.5903	301.15	1.2740[12]	1.2666	−0.6
12	[bmim] [HFPS]	$C_{11}H_{16}N_2F_6SO_3$	1-butyl-3-methylidimazolium 1,1,2,3,3,3-hexafluoropropane sulfonate	370	747.6	1032.1	21.3	912.6	0.4933	298.15	1.4090[12]	1.3909	−1.3
13	[4,4,4,14-P] [HFPS]	$C_{29}H_{57}O_3SF_6$	tributyl(tetradecyl) phosphonium 1,1,2,3,3,3-hexafluoropropane sulfonate	631	1058.5	1281.0	8.8	2003.3	0.9322	298.15	1.0700[13]	1.2701	18.7
14	[bmim] [TPES]	$C_{12}H_{16}N_2F_8SO_4$	1-butyl-3-methylidimazolium 1,1,2-trifluoro-2-(perfluoroethoxy)ethane sulfonate	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4230[12]	1.5136	6.4
15	[6,6,6,14-P] [TPES]	$C_{36}H_{69}O_4SF_8$	tetradecyl(trihexyl) phosphonium 1,1,2-trifluoro-2-(perfluoroethoxy)ethane sulfonate	750	1201.5	1481.4	7.0	2379.3	0.5555	298.15	1.0630[13]	1.2388	16.5
16	[bmim] [TTES]	$C_{11}H_{16}N_2O_4SF_8$	1-butyl-3-methylidimazolium 1,1,2-trifluoro-2-(trifluoromethoxy)ethane sulfonate	386	770.0	1058.3	20.9	928.2	0.5085	298.15	1.3930[12]	1.4371	3.2
17	[bmim] [FS]	$C_{12}H_{16}N_2F_8SO_4$	1-butyl-3-methylidimazolium 2-(1,2,2,2-tetrafluoroethoxy)- 1,1,2,2-tetrafluoroethane sulfonate	436	788.2	1061.3	17.9	1012.9	0.5488	298.15	1.4490[12]	1.5136	4.5
18	[TMG] [Ac]	$C_8H_{17}N_3O_2$	1,1,3,3-tetramethyl guanidine acetate	175	518.1	703.7	28.0	563.0	0.7326	298.15	1.2650[14]	1.0248	−19.0
19	[bmim] [Ac]	$C_{10}H_{18}N_2O_2$	1-butyl-3-methylidimazolium acetate	198	624.6	847.3	24.5	658.2	0.6681	298.15	1.0550[15]	1.0270	−2.6
20	[emim] [Ac]	$C_8H_{14}N_2O_2$	1-ethyl-3-methylidimazolium acetate	170	578.8	807.1	29.2	544.0	0.5889	298.15	1.0270[15]	1.0388	1.1
21	[emim] [BEI]	$C_{10}H_{11}N_3F_{10}S_2O_4$	1-ethyl-3-methylidimazolium *bis*(pentafluoroethylsulfonyl)imide	491	853.1	1231.4	21.9	1045.4	0.2895	298.15	1.5900[12]	1.5783	−0.7
22	[bmim] [BEI]	$C_{12}H_{15}F_{10}N_3O_4S_2$	1-butyl-3-methylidimazolium *bis*(pentafluoroethylsulfonyl)imide	505	841.3	1175.4	19.3	1117.4	0.3837	298.10	1.5140[16]	1.5478	2.2
23	[4MOPY] [BEI]	$C_{18}H_{24}N_2O_4S_2F$	4-methyl-*n*-octylpyridinium *bis*(pentafluoroethylsulfonyl)imide	587	979.9	1291.4	15.0	1436.7	0.5858	298.15	1.3900[17]	1.4815	6.6
24	[NH221] [BEI]	$C_9H_{14}N_2O_4S_2F$	diethyl methyl (quaternary)ammonium *bis* (pentafluoroethylsulfonyl)imide	468	743.8	1056.3	21.5	1053.3	0.3534	298.15	1.5100[18]	1.4833	−1.8
25	[NH11(i-3)] [BEI]	$C_9H_{14}N_2O_4S_2F$	dimethyl isopropyl (quaternary)ammonium *bis*(pentafluoroethylsulfonyl)imide	468	743.8	1056.3	21.5	1053.3	0.3534	298.15	1.5300[18]	1.4833	−3.1
26	[C27guan] [bti]	$C_{29}H_{58}N_4F_6S_2O_4$	[*bis*(bishexylamino)methylene]dimethylammonium *bis*[(trifluoromethyl)sulfonyl]imide	705	1262.0	1529.0	9.8	2167.1	1.0120	298.15	1.2000[19]	1.3305	10.9

Table 3. (Continued)

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
27	[C15guan][bti]	$C_{17}H_{34}N_4F_6S_2O_4$	[*bis*(butylethylamino)methylene]dimethylammonium *bis*[(trifluoromethyl)sulfonyl]imide	537	987.5	1271.0	15.6	1481.8	0.7803	298.15	1.3600[19]	1.3468	−1.0
28	[dmprim][bti]	$C_{10}H_{15}F_6N_3O_4S_2$	1,2-dimethyl-3-propylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide	419	867.4	1269.7	27.5	988.6	0.3226	295.15	1.4567[16]	1.4177	−2.7
29	[dbim][bti]	$C_{13}H_{21}N_3F_6S_2O_4$	1,3-dibutylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide	461	931.1	1305.0	22.3	1161.5	0.4349	298.15	1.4910[20]	1.3679	−8.3
30	[E1,3M4I][bti]	$C_{10}H_{15}N_3F_6S_2O_4$	1,3-diethyl-4-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	419	867.4	1269.7	27.5	988.6	0.3226	295.15	1.4320[20]	1.4177	−1.0
31	[dmim][bti]	$C_7H_9N_3F_6S_2O_4$	1,3-dimethylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	377	783.2	1235.7	35.8	835.8	0.1418	295.15	1.5590[16]	1.4417	−7.5
32	[MP4][bti]	$C_{11}H_{18}N_2F_6S_2O_4$	1-butyl-2-methylpyrrolidinium *bis*[(trifluoromethyl)sulfonyl]imide	421	832.9	1208.8	25.1	1017.8	0.3220	293.15	1.4300[20]	1.3810	−3.4
33	[bmpy][bti]	$C_{12}H_{16}N_2F_6S_2O_4$	1-butyl-3-methylpyridinium *bis*[(trifluoromethyl)sulfonyl]imide	430	852.0	1240.5	25.5	1038.8	0.3160	298.15	1.4120[12]	1.3821	−2.1
34	[decmim][bti]	$C_{16}H_{27}N_3F_6S_2O_4$	1-decyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	504	999.7	1345.1	18.7	1332.8	0.5741	298.15	1.2710[20]	1.3489	6.1
35	[N-epy][bti]	$C_9H_{10}F_6N_2O_4S_2$	1-ethylpyridinium *bis*[(trifluoromethyl)sulfonyl]imide	388	778.4	1207.9	32.7	869.0	0.1671	298.15	1.5360[16]	1.4341	−6.6
36	[hpmim][bti]	$C_{13}H_{21}N_3F_6S_2O_4$	1-heptyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	461	931.1	1305.0	22.3	1161.5	0.4349	298.15	1.3440[20]	1.3679	1.8
37	[nmim][bti]	$C_{15}H_{25}N_3F_6S_2O_4$	1-nonyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	490	976.8	1331.2	19.8	1275.7	0.5276	298.15	1.2990[20]	1.3535	4.2
38	[pmim][bti]	$C_{11}H_{17}N_3F_6S_2O_4$	1-pentyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	433	885.3	1281.1	25.6	1047.2	0.3442	298.15	1.4030[20]	1.3907	−0.9
39	[MP3][bti]	$C_{10}H_{16}N_2F_6S_2O_4$	1-propyl-2-methylpyrrolidinuim *bis*[(trifluoromethyl)sulfonyl]imide	407	810.0	1196.5	27.0	960.7	0.2783	293.15	1.4600[20]	1.3978	−4.3
40	[prmim][bti]	$C_9H_{13}N_3F_6S_2O_4$	1-propyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	405	839.6	1259.3	29.9	933.0	0.2573	298.15	1.4750[20]	1.4270	−3.3
41	[pmpy][bti]	$C_{11}H_{14}N_2F_6S_2O_4$	3-methyl-1-propylpyridinium *bis*[(trifluoromethyl)sulfonyl]imide	416	829.1	1228.9	27.5	981.7	0.2723	298.15	1.4440[12]	1.3986	−3.1
42	[N723′3′][bti]	$C_{17}H_{34}N_2F_6S_2O_4$	di(iso)propylethylheptylammonium *bis*[(trifluoromethyl)sulfonyl]imide	509	897.6	1176.6	16.1	1408.9	0.6653	293.15	1.2700[20]	1.3057	2.8
43	[dmeim][bti]	$C_9H_{16}N_3F_6S_2O_4$	dimethyl-3-ethylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide	405	833.9	1254.1	29.7	948.4	0.2447	298.15	1.4802[16]	1.3996	−5.4
44	[BNM2E][bti]	$C_{10}H_{20}N_2F_6S_2O_4$	dimethylethylbutylammonium *bis*[(trifluoromethyl)sulfonyl]imide	410	738.3	1054.3	24.1	1012.6	0.3777	293.15	1.3700[20]	1.3500	−1.5
45	[N1123][bti]	$C_9H_{18}N_2F_6S_2O_4$	dimethylethylpropylammonium *bis*[(trifluoromethyl)sulfonyl]imide	396	715.4	1038.7	25.9	955.5	0.3334	293.15	1.4100[20]	1.3647	−3.2
46	[N1134][bti]	$C_{11}H_{22}N_2F_6S_2O_4$	dimethylpropylbutylammonium *bis*[(trifluoromethyl)sulfonyl]imide	424	761.2	1070.1	22.5	1069.7	0.4228	293.15	1.3400[20]	1.3383	−0.1
47	[eomim][bti]	$C_9H_{13}N_3F_6S_2O_5$	ethoxymethyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	421	862.0	1285.2	29.0	948.6	0.2694	298.15	1.4960[20]	1.4675	−1.9
48	[N-bupy][bti]	$C_{11}H_{14}N_2F_6S_2O_4$	*n*-butylpyridinium *bis*[(trifluoromethyl)sulfonyl]imide	416	824.2	1229.1	27.7	983.3	0.2505	298.15	1.4490[20]	1.3900	−4.1
49	[prmpyr][bti]	$C_{10}H_{18}N_2F_6S_2O_4$	*n*-methyl-*n*-propylpyrrolidinium *bis*[(trifluoromethyl)sulfonyl]imide	408	810.4	1196.9	26.7	969.8	0.2754	293.15	1.4590[20]	1.3912	−4.6
50	[tda][bti]	$C_{42}H_{84}N_2F_6S_2O_4$	tetradecylammonium *bis*[(trifluoromethyl)sulfonyl]imide	859	1470.5	1831.8	7.0	2840.1	0.4734	298.15	1.0400[20]	1.1795	13.4
51	[thpa][bti]	$C_{30}H_{60}N_2F_6S_2O_4$	tetraheptylammonium *bis*[(trifluoromethyl)sulfonyl]imide	691	1195.9	1449.6	9.7	2154.8	0.9913	298.15	1.1000[20]	1.3034	18.5
52	[tha][bti]	$C_{26}H_{52}N_2F_6S_2O_4$	tetrahexylammonium *bis*[(trifluoromethyl)sulfonyl]imide	635	1104.4	1353.0	11.0	1926.4	0.9857	298.15	1.1100[20]	1.3119	18.2

Table 3. (Continued)

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
53	[tpa][bti]	$C_{22}H_{44}N_2F_6S_2O_4$	tetramylammonium *bis*[(trifluoromethyl)sulfonyl]imide	579	1012.9	1267.0	12.8	1697.9	0.8923	298.15	1.1600[20]	1.3100	12.9
54	[toa][bti]	$C_{34}H_{68}N_2F_6S_2O_4$	tetraoctylammonium *bis*[(trifluoromethyl)sulfonyl]imide	747	1287.4	1559.2	8.6	2383.2	0.8960	298.15	1.0600[20]	1.2782	20.6
55	[S444][bti]	$C_{14}H_{27}NF_6S_3O_4$	tributylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	484	934.9	1269.2	15.6	1389.3	0.4263	298.15	1.2900[20]	1.2200	−5.4
56	[N7444][bti]	$C_{21}H_{42}F_6N_2O_4S_2$	tributylheptylammonium *bis*[(trifluoromethyl)sulfonyl]imide	565	990.0	1247.0	13.3	1640.8	0.8585	293.15	1.1700[20]	1.3115	12.1
57	[N6444][bti]	$C_{20}H_{40}F_6N_2O_4S_2$	tributylhexylammonium *bis*[(trifluoromethyl)sulfonyl]imide	551	967.1	1227.4	13.9	1583.7	0.8216	293.15	1.1500[20]	1.3106	14.0
58	[N1444][bti]	$C_{15}H_{30}F_6N_2O_4S_2$	tributylmethylammonium *bis*[(trifluoromethyl)sulfonyl]imide	481	852.7	1136.3	17.7	1298.1	0.6068	296.9	1.2660[16]	1.3114	3.6
59	[N8444][bti]	$C_{22}H_{44}F_6N_2O_4S_2$	tributyloctylammonium *bis*[(trifluoromethyl)sulfonyl]imide	579	1012.9	1267.0	12.8	1697.9	0.8923	293.15	1.1200[20]	1.3126	17.2
60	[N7222][bti]	$C_{15}H_{30}N_2F_6S_2O_4$	triethylheptylammonium *bis*[(trifluoromethyl)sulfonyl]imide	481	852.7	1136.3	17.7	1298.1	0.6068	293.15	1.2600[20]	1.3136	4.3
61	[N6222][bti]	$C_{14}H_{28}N_2F_6S_2O_4$	triethylhexylammonium *bis*[(trifluoromethyl)sulfonyl]imide	467	829.8	1119.2	18.7	1241.0	0.5608	293.15	1.2700[20]	1.3171	3.7
62	[N8222][bti]	$C_{16}H_{32}N_2F_6S_2O_4$	triethyloctylammonium *bis*[(trifluoromethyl)sulfonyl]imide	495	875.6	1153.7	16.8	1355.3	0.6522	293.15	1.2500[20]	1.3113	4.9
63	[S222][bti]	$C_8H_{15}NF_6S_3O_4$	triethylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	399	797.6	1189.9	21.9	1046.6	0.1603	298.15	1.4600[20]	1.2435	−14.8
64	[N1114][bti]	$C_9H_{18}N_2F_6S_2O_4$	trimethylbutylammonium *bis*[(trifluoromethyl)sulfonyl]imide	396	715.4	1038.7	25.9	955.5	0.3334	293.15	1.4100[20]	1.3647	−3.2
65	[N7111][bti]	$C_{12}H_{24}N_2F_6S_2O_4$	trimethylheptylammonium *bis*[(trifluoromethyl)sulfonyl]imide	438	784.1	1086.1	21.1	1126.8	0.4685	293.15	1.2800[20]	1.3292	3.8
66	[N6111][bti]	$C_{11}H_{22}N_2F_6S_2O_4$	trimethylhexylammonium *bis*[(trifluoromethyl)sulfonyl]imide	424	761.2	1070.1	22.5	1069.7	0.4228	293.15	1.3300[20]	1.3383	0.6
67	[N111C2O][bti]	$C_7H_{14}N_2F_6S_2O_5$	trimethylmethoxymethylammonium *bis*[(trifluoromethyl)sulfonyl]imide	384	692.1	1035.7	29.5	856.9	0.2599	298.15	1.5100[20]	1.4469	−4.2
68	[N8111][bti]	$C_{13}H_{26}N_2F_6S_2O_4$	trimethyloctylammonium bis[(trifluoromethyl)sulfonyl]imide	452	807.0	1102.5	19.8	1183.9	0.5146	293.15	1.2700[20]	1.3222	4.1
69	[tmpa][bti]	$C_8H_{16}N_2F_6S_2O_4$	trimethylpropylammonium bis[(trifluoromethyl)sulfonyl]imide	382	692.6	1023.4	28.0	898.4	0.2900	298.15	1.4400[20]	1.3797	−4.2
70	[S111][bti]	$C_5H_9NF_6S_3O_4$	trimethylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	357	729.0	1156.5	27.3	875.3	0.0384	318.15	1.5800[20]	1.2758	−19.3
71	[Ph(CH2)mim][bti]	$C_{13}H_{13}N_3O_4S_2F_6$	1-(1-phenylalkyl)-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	453	948.1	1429.7	28.1	1039.5	0.2139	298.15	1.4910[21]	1.4395	−3.5
72	[Ph(CH2)2mim][bti]	$C_{14}H_{15}N_3O_4S_2F_6$	1-(2-phenylalkyl)-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	467	971.0	1436.9	26.1	1096.6	0.2573	298.15	1.4700[21]	1.4227	−3.2
73	[Ph(CH2)3mim][bti]	$C_{15}H_{17}N_3O_4S_2F_6$	1-(3-phenylalkyl)-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	481	993.8	1444.9	24.3	1153.7	0.3018	298.15	1.4550[21]	1.4089	−3.2
74	[dmeim][bti]	$C_8H_{12}N_3O_4S_2F_6$	1,2-dimethyl-3-ethylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide	392	817.8	1235.8	31.6	888.9	0.2492	293.15	1.5100[22]	1.4457	−4.3
75	[dmpim][bti]	$C_{10}H_{15}N_3F_6S_2O_4$	1,2-dimethyl-3-propylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide	419	867.4	1269.7	27.5	988.6	0.3226	299.15	1.4810[12]	1.4157	−4.4
76	[bdmim][bti]	$C_{11}H_{17}N_3F_6S_2O_4$	1-butyl-2,3-dimethylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	433	890.3	1281.1	25.5	1045.7	0.3669	298.15	1.4200[23]	1.3999	−1.4
77	[mbpyr][bti]	$C_{12}H_{16}N_2O_4S_2F_6$	1-butyl-4-methylpyridinium *bis*[(trifluoromethyl)sulfonyl]imide	430	852.0	1240.5	25.5	1038.8	0.3160	298.15	1.3500[24]	1.3821	2.4
78	[bmpyr][bti]	$C_{10}H_{17}N_2F_6S_2O_4$	1-butyl-1-methylpyrrolidinium *bis*[(trifluoromethyl)sulfonyl]imide	422	833.3	1209.2	24.8	1026.9	0.3191	298.15	1.3940[16]	1.3724	−1.6

Table 3. (Continued)

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
79	[bpyr][bti]	$C_{11}H_{14}F_6N_2O_4S_2$	1-butylpyridinium *bis*[(trifluoromethyl)sulfonyl]imide	416	824.2	1229.1	27.7	983.3	0.2505	298.10	1.4990[16]	1.3901	−7.3
80	[C12mim][bti]	$C_{18}H_{31}N_3O_4S_2F_6$	1-dodecyl-3-methylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide	532	1045.5	1374.6	16.8	1447.0	0.6662	293.15	1.2460[25]	1.3459	8.0
81	[memim][bti]	$C_8H_{12}N_3O_4S_2F_6$	1-methyl-3-ethyl-4-methylimidazolium *bis*[(trifluoromethyl)sulfonyl]imide	392	817.8	1235.8	31.6	888.9	0.2492	293.15	1.4700[22]	1.4457	−1.7
82	[mmim][bti]	$C_7H_9N_3F_6S_2O_4$	1-methyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	377	793.8	1239.9	35.8	818.8	0.1752	295.15	1.5590[26]	1.4827	−4.9
83	[pdmim][bti]	$C_{10}H_{15}N_3F_6S_2O_4$	1-propyl-2,3-dimethylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	419	867.4	1269.7	27.5	988.6	0.3226	295.15	1.4567[27]	1.4177	−2.7
84	[C2F3mim][bti]	$C_7H_6N_3O_4S_2F_9$	1-trifluoroethyl-3-methylidimazolium *bis*[(trifluoromethyl)sulfonyl]imide	431	788.8	1202.7	29.2	871.5	0.1879	293.15	1.6600[22]	1.6092	−3.1
85	[4MOPY][bti]	$C_{16}H_{24}N_2O_4S_2F_6$	4-methyl-*n*-octylpyridinium *bis*[(trifluoromethyl)sulfonyl]imide	487	943.5	1292.0	19.7	1267.2	0.4983	298.15	1.2900[17]	1.3439	4.2
86	[C23guan][bti]	$C_{25}H_{50}N_4O_4S_2F_6$	*bis*-hexyl-aminomethylene dimethylammonium *bis*[(trifluoromethyl)sulfonyl]imide	649	1170.5	1432.1	11.2	1938.7	1.0159	298.15	1.2000[20]	1.3437	12.0
87	[S224][bti]	$C_{10}H_{19}NO_4S_3F_6$	diethylbutylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	427	843.4	1214.5	19.3	1160.9	0.2465	298.15	1.3100[28]	1.2288	−6.2
88	[NH221][bti]	$C_7H_{14}N_2O_4S_2F_6$	diethylmethyl(quaternary)ammonium *bis*[(trifluoromethyl)sulfonyl]imide	368	707.4	1061.1	31.9	883.8	0.2805	298.15	1.4300[18]	1.3442	−6.0
89	[S221][bti]	C7H13NO4S3F$_6$	diethylmethylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	385	774.8	1178.3	23.4	989.5	0.1186	298.15	1.4300[28]	1.2544	−12.3
90	[S225][bti]	C11H$_{21}$NO$_4$S$_3$F$_6$	diethylpentylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	441	866.3	1227.5	18.2	1218.0	0.2908	298.15	1.3000[28]	1.2244	−5.8
91	[S223][bti]	$C_9H_{17}NO_4S_3F_6$	diethylpropylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	413	820.5	1202.0	20.5	1103.8	0.2030	298.15	1.3400[28]	1.2351	−7.8
92	[NH114][bti]	$C_8H_{16}N_2O_4S_2F_6$	dimethylbutyl (quaternary)ammonium *bis*[(trifluoromethyl)sulfonyl]imide	382	730.3	1075.3	29.3	940.9	0.3229	298.15	1.3900[18]	1.3265	−4.6
93	[S114][bti]	$C_8H_{15}NO_4S_3F_6$	dimethylbutylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	399	797.6	1189.9	21.9	1046.6	0.1603	298.15	1.5500[28]	1.2435	−19.8
94	[S112][bti]	$C_6H_{11}NO_4S_3F_6$	dimethylethylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	371	751.9	1167.2	25.2	932.4	0.0779	298.15	1.5600[28]	1.2683	−18.7
95	[NH11(i-3)][bti]	$C_7H_{14}N_2O_4S_2F_6$	dimethylisopropyl(quaternary)ammonium *bis*[(trifluoromethyl)sulfonyl]imide	368	707.4	1061.1	31.9	883.8	0.2805	298.15	1.4200[18]	1.3442	−5.3
96	[S115][bti]	$C_9H_{17}NO_4S_3F_6$	dimethylpentylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	413	820.5	1202.0	20.5	1103.8	0.2030	298.15	1.3500[28]	1.2351	−8.5
97	[S113][bti]	$C_7H_{13}NO_4S_3F_6$	dimethylpropylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	385	774.8	1178.3	23.4	989.5	0.1186	298.15	1.3900[28]	1.2544	−9.8
98	[S124][bti]	$C_9H_{17}NO_4S_3F_6$	methylethylbutylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	413	820.5	1202.0	20.5	1103.8	0.2030	298.15	1.2600[28]	1.2351	−2.0
99	[S125][bti]	$C_{10}H_{19}NO_4S_3F_6$	methylethylpentylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	427	843.4	1214.5	19.3	1160.9	0.2465	298.15	1.2600[28]	1.2288	−2.5
100	[S123][bti]	$C_8H_{15}NO_4S_3F_6$	methylethylpropylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	399	797.6	1189.9	21.9	1046.6	0.1603	298.15	1.3400[28]	1.2435	−7.2
101	[DEME][bti]	$C_{10}H_{20}N_2O_5S_2F_6$	*N*,*N*-diethyl-*N*-methyl-*N*-(2-methoxyethyl)ammonium *bis*[(trifluoromethyl)sulfonyl]imide	426	760.7	1080.7	23.5	1028.2	0.3915	293.15	1.4200[29]	1.3911	−2.0
102	[BMP][bti]	$C_{12}H_{22}N_2O_4S_2F_6$	*N*-butyl-*N*-methylpiperidinium *bis*[(trifluoromethyl)sulfonyl]imide	436	860.5	1233.4	23.4	1078.5	0.3472	298.15	1.3800[23]	1.3632	−1.2
103	[S444][bti]	$C_{14}H_{27}NO_4S_3F_6$	tributylsulfonium *bis*[(trifluoromethyl)sulfonyl]imide	484	934.9	1269.2	15.6	1389.3	0.4263	298.00	1.2900[30]	1.2200	−5.4
104	[N222(2O1)][bti]	$C_{11}H_{22}N_2O_5S_2F_6$	triethyl(2-methoxyethyl)ammonium *bis*[(trifluoromethyl)sulfonyl]imide	440	783.6	1096.3	22.0	1085.3	0.4370	298.15	1.4000[31]	1.3753	−1.8

Table 3. (Continued)

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
105	[*P*222(2O1)][bti]	$C_{11}H_{22}NO_5S_2F_6$	triethyl(2-methoxyethyl)phosphonium *bis*[(trifluoromethyl)sulfonyl]imide	457	806.7	1134.6	21.4	1125.6	0.3980	298.15	1.3900[31]	1.3747	−1.1
106	[N222(1O1)][bti]	$C_{10}H_{20}N_2O_5S_2F_6$	triethyl(methoxymethyl)ammonium *bis*[(trifluoromethyl)sulfonyl]imide	426	760.7	1080.7	23.5	1028.2	0.3915	298.15	1.4400[31]	1.3880	−3.6
107	[*P*222(1O1)][bti]	$C_{10}H_{20}NO_5S_2F_6$	triethyl(methoxymethyl)phosphonium *bis*[(trifluoromethyl)sulfonyl]imide	443	783.9	1119.8	22.8	1068.5	0.3525	298.15	1.4200[31]	1.3865	−2.4
108	[NH222][bti]	$C_8H_{16}N_2O_4S_2F_6$	triethyl(quaternary)ammonium *bis*[(trifluoromethyl)sulfonyl]imide	382	730.3	1075.3	29.3	940.9	0.3229	298.15	1.3600[18]	1.3265	−2.5
109	[N222(12)][bti]	$C_{20}H_{40}N_2O_4S_2F_6$	triethyldodecylammonium *bis*[(trifluoromethyl)sulfonyl]imide	551	967.1	1227.4	13.9	1583.7	0.8216	298.15	1.2200[31]	1.3079	7.2
110	[P222(12)][bti]	$C_{20}H_{40}NO_4S_2F_6$	triethyldodecyl phosphonium *bis*[(trifluoromethyl)sulfonyl]imide	568	990.2	1260.3	13.7	1624.0	0.7861	298.15	1.2100[31]	1.3122	8.4
111	[N2228][bti]	$C_{16}H_{32}N_2O_4S_2F_6$	triethyloctyl ammonium *bis*[(trifluoromethyl)sulfonyl]imide	495	875.6	1153.7	16.8	1355.3	0.6523	298.15	1.2800[31]	1.3085	2.2
112	[P2228][bti]	$C_{16}H_{32}NO_4S_2F_6$	triethyloctylphosphonium *bis*[(trifluoromethyl)sulfonyl]imide	512	898.7	1188.7	16.4	1395.6	0.6140	298.15	1.2600[31]	1.3117	4.1
113	[N2225][bti]	$C_{13}H_{26}N_2O_4S_2F_6$	triethylpentylammonium *bis*[(trifluoromethyl)sulfonyl]imide	452	807.0	1102.5	19.8	1183.9	0.5146	298.15	1.3300[31]	1.3193	−0.8
114	[P2225][bti]	$C_{13}H_{26}NO_4S_2F_6$	triethylpentylphosphonium *bis*[(trifluoromethyl)sulfonyl]imide	469	830.1	1139.5	19.3	1224.2	0.4757	298.15	1.3200[31]	1.3214	0.1
115	[bmim][Br]	$C_8H_{15}BrN_2$	1-butyl-3-methylidimazolium bromide	219	586.8	834.9	29.8	583.3	0.4891	298.40	1.2990[32]	1.2327	−5.1
116	[C27guan][Cl]	$C_{27}H_{58}N_3Cl$	[*bis*(*bis*-hexyl-amino)methylene]dimethylammonium chloride	460	957.6	1158.9	9.2	1745.7	0.9692	298.15	0.9000[19]	1.0530	17.0
117	[C35guan][Cl]	$C_{35}H_{74}N_3Cl$	[*bis*(*bis*-octyl-amino)methylene]dimethylammonium chloride	572	1140.7	1411.1	7.4	2202.6	0.5680	298.15	0.9600[19]	1.0105	5.3
118	[moeemim][Cl]	$C_9H_{17}N_2O_2Cl$	1-[2-(2-methoxyethoxy)ethyl]-3-methylidimazolium chloride	221	625.8	863.6	24.8	657.1	0.5707	298.15	1.1400[20]	1.1322	−0.7
119	[bmim][Cl]	$C_8H_{15}N_2Cl$	1-butyl-3-methylidimazolium chloride	175	558.0	789.0	27.8	568.8	0.4908	298.15	1.0800[20]	0.9998	−7.4
120	[hmim][Cl]	$C_{10}H_{19}N_2Cl$	1-hexyl-3-methylidimazolium chloride	203	603.8	829.2	23.5	683.0	0.5725	298.15	1.0300[20]	0.9944	−3.5
121	[omim][Cl]	$C_{12}H_{23}ClN_2$	1-octyl-3-methylidimazolium chloride	231	649.6	869.4	20.3	797.2	0.6566	298.1	1.0000[16]	0.9968	−0.3
122	[Bemim][Cl]	$C_{11}H_{13}ClN_2$	1-benzyl-3-methylidimazolium chloride	209	653.4	921.3	28.4	631.8	0.5145	298.15	1.1930[14]	1.1066	−7.2
123	[C12mim][Cl]	$C_{16}H_{31}N_2Cl$	1-dodecyl-3-methylidimazolium chloride	287	741.1	951.5	16.0	1025.6	0.8212	298.15	0.8806[32]	1.0153	15.3
124	[emim][Cl]	$C_6H_{11}ClN_2$	1-ethyl-3-methylidimazolium chloride	147	512.3	748.6	34.2	454.5	0.4165	294.65	1.1860[16]	1.0260	−13.5
125	[mmim][Cl]	$C_5H_9N_2Cl$	1-methyl-3-methylidimazolium chloride	133	489.4	728.2	38.5	397.4	0.3825	298.15	1.1399[20]	1.0446	−8.4
126	[mim][Cl]	$C_4H_7N_2Cl$	1-methylidimazolium chloride	119	461.1	687.7	48.2	316.1	0.4564	353.15	1.1832[15]	1.1121	−6.0
127	[ClBenmim][Cl]	$C_{11}H_{12}N_2Cl_2$	1-*p*-chlorobenzyl-3-methylidimazolium chloride	243	695.8	969.6	26.8	682.6	0.5521	298.15	1.2670[14]	1.2126	−4.3
128	[FBenMim][Cl]	$C_{11}H_{12}N_2ClF$	1-*p*-fluorobenzyl-3-methylidimazolium chloride	227	657.6	913.1	26.4	652.0	0.5660	298.15	1.2830[14]	1.1779	−8.2
129	[C23guan][Cl]	$C_{23}H_{50}N_3Cl$	*bis*-hexyl-amino-methylenedimethylammonium chloride	404	866.1	1052.1	10.5	1517.3	1.0428	298.15	0.9000[20]	1.0491	16.6
130	[dbim][Cl]	$C_{11}H_{21}N_2Cl$	1,3-dibutylimidazolium chloride	217	626.7	849.2	21.8	740.1	0.6144	298.15	1.0082[20]	0.9948	−1.3

Table 3. (Continued)

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
131	[bmim] [dca]	$C_{10}H_{15}N_5$	1-butyl-3-methylidimazolium dicyanamide	205	783.0	1035.8	24.4	712.0	0.8419	297.15	1.0580[16]	1.0406	−1.6
132	[emim] [dca]	$C_8H_{11}N_5$	1-ethyl-3-methylidimazolium dicyanamide	177	737.2	999.0	29.1	597.8	0.7661	298.15	1.0600[26]	1.0451	−1.4
133	[omim] [dca]	$C_{14}H_{23}N_5$	1-octyl-3-methylidimazolium dicyanamide	261	863.9	1103.9	18.4	957.4	0.9543	298.15	1.0000[24]	1.0229	2.3
134	[4MOPY] [dca]	$C_{16}H_{24}N_4$	4-methyl-*n*-octylpyridinium dicyanamide	272	864.1	1094.3	17.2	989.1	0.9923	298.15	0.9800[17]	1.0422	6.3
135	[emim] [dca]	$C_8H_{11}N_5$	1-ethyl-3-methylidimazolium dicyanoamides	177	737.2	999.0	29.1	597.8	0.7661	298.15	1.0600[20]	1.0451	−1.4
136	[mbpyr] [dca]	$C_{11}H_{20}N_4$	*n*-methyl-*n*-butylpyrrolidinium dicyanoamides	208	753.8	988.3	21.3	748.8	0.8316	298.15	0.9500[20]	1.0042	5.7
137	[mhpyr] [dca]	$C_{13}H_{24}N_4$	*n*-methyl-*n*-hexylpyrrolidinium dicyanoamides	236	799.6	1028.0	18.6	863.0	0.9087	298.15	0.9200[20]	1.0123	10.0
138	[mppyr] [dca]	$C_{10}H_{18}N_4$	*n*-methyl-*n*-propylpyrrolidinium dicyanoamides	194	730.9	968.8	22.9	691.7	0.7920	298.15	0.9200[20]	1.0018	8.9
139	[emim] [DEGlyMSO4]	$C_{11}H_{22}N_2O_6S$	1-ethyl-3-methylidimazolium diethyleneglycol monomethylethersulfate	310	826.2	1162.9	28.1	862.3	0.5176	298.15	1.2365[34]	1.2331	−0.3
140	[dmim] [DMPO4]	$C_7H_{15}N_2O_4P$	1,3-dimethylidimazolium dimethyl phosphate	222	623.0	880.4	28.6	598.4	0.5065	303.15	1.2530[16]	1.2322	−1.7
141	[py] [EOESO4]	$C_9H_{15}NO_5S$	pyridinium ethoxyethyl sulfate	248	696.1	1065.4	41.8	658.8	0.2994	298.15	1.2810[16]	1.2188	−4.9
142	[edmim] [ESO4]	$C_9H_{18}N_2O_4S$	1-ethyl-2,3-dimethylidimazolium ethyl sulfate	250	740.5	1082.6	35.8	715.3	0.4341	353.15	1.1970[15]	1.1327	−5.4
143	[emim] [ESO4]	$C_8H_{16}N_2O_4S$	1-ethyl-3-methylidimazolium ethyl sulfate	236	712.7	1067.5	40.5	659.8	0.3744	298.15	1.2388[35]	1.1699	−5.6
144	[moim] [PF6]	$C_{12}H_{23}N_2PF_6$	1-octyl-3-methylidimazolium hexafluorophosphate	340	635.5	800.1	14.0	1007.9	0.9069	298.15	1.2360[16]	1.2216	−1.1
145	[moeemim] [PF6]	$C_9H_{17}N_2O_2PF_6$	1-[2-(2-methoxyethoxy)ethyl]-3-methylidimazolium hexafluorophosphate	330	622.3	795.3	16.1	850.8	0.8676	298.15	1.3200[20]	1.3869	5.1
146	[bdmim] [PF6]	$C_9H_{17}F_6N_2P$	1-butyl-2,3-dimethylidimazolium hexafluorophosphate	298	582.4	746.3	16.2	818.0	0.8526	295.65	1.2416[16]	1.2832	3.4
147	[hpmim] [PF6]	$C_{11}H_{21}N_2PF_6$	1-heptyl-3-methylidimazolium hexafluorophosphate	326	623.2	787.8	14.7	933.8	0.9055	298.15	1.2620[20]	1.2577	−0.3
148	[nmim] [PF6]	$C_{13}H_{25}N_2PF_6$	1-nonyl-3-methylidimazolium hexafluorophosphate	354	669.0	834.1	13.4	1048.1	0.9680	298.15	1.2120[20]	1.2499	3.1
149	[oprim] [PF6]	$C_{14}H_{27}N_2PF_6$	1-octyl-3-propylimidazolium hexafluorophosphate	368	691.9	857.6	12.8	1105.2	0.9937	298.15	1.1182[20]	1.2473	11.5
150	[pmim] [PF6]	$C_9H_{17}F_6N_2P$	1-pentyl-3-methylidimazolium hexafluorophosphate	298	577.5	742.1	16.3	819.6	0.8316	294.1	1.3330[16]	1.2757	−4.3
151	[eommim] [PF6]	$C_7H_{13}N_2OPF_6$	ethoxymethyl-3-methylidimazolium hexafluorophosphate	286	554.1	723.7	18.2	721.0	0.7692	298.15	1.4000[20]	1.3595	−2.9
152	[mommim] [PF6]	$C_6H_{11}N_2OPF_6$	methyloxymethyl-3-methylidimazolium hexafluorophosphate	272	531.2	701.2	19.3	663.9	0.7274	298.15	1.4800[20]	1.3815	−6.7
153	[N-bupy] [PF6]	$C_9H_{14}NPF_6$	*n*-butylpyridinium hexafluorophosphate	281	516.3	674.4	17.3	755.6	0.7381	298.15	1.2144[20]	1.2487	2.8
154	[Ph(CH2)3mim] [PF6]	$C_{13}H_{17}N_2F_6P$	1-(3-phenylalkyl)-3-methylidimazolium hexafluorophosphate	346	686.0	883.8	16.3	926.1	0.8053	298.15	1.4070[21]	1.3452	−4.4
155	[prmim] [PF6]	$C_7H_{13}F_6N_2P$	1-propyl-3-methylidimazolium hexafluorophosphate	270	531.7	696.7	18.3	705.4	0.7504	293.00	1.3330[30]	1.3018	−2.3
156	[C2C6I] [PF6]	$C_{11}H_{21}N_2F_6P$	1-hexyl-3-ethylimidazolium hexafluorophosphate	326	623.2	787.8	14.7	933.8	0.9055	298.15	1.2622[20]	1.2577	−0.4

Table 3. (Continued)

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
157	[C2C8I][PF6]	$C_{13}H_{25}N_2F_6P$	1-octyl-3-ethylimidazolium hexafluorophosphate	354	669.0	834.1	13.4	1048.1	0.9680	298.15	1.2118[20]	1.2499	3.1
158	[bmim][HSO4]	$C_8H_{16}N_2O_4S$	1-butyl-3-methylidimazolium hydrogen sulfate	235	782.4	1103.8	43.2	664.9	0.7017	298.15	1.2770[15]	1.2161	−4.8
159	[emim][HSO4]	$C_6H_{12}N_2O_4S$	1-ethyl-3-methylidimazolium hydrogen sulfate	207	736.7	1073.8	57.4	550.7	0.6394	298.15	1.3673[15]	1.2656	−7.4
160	[mim][HSO4]	$C_4H_8N_2SO_4$	1-methylidimazolium hydrogen sulfate	179	685.5	1019.6	91.7	412.2	0.7158	298.15	1.4835[15]	1.4488	−2.3
161	[bmim][I]	$C_8H_{15}N_2I$	1-butyl-3-methylidimazolium iodide	266	613.7	871.2	28.6	607.5	0.4831	298.15	1.4400[20]	1.4500	0.7
162	[TMG][Lac]	$C_8H_{19}N_3O_3$	1,1,3,3-tetramethyl guanidine lactate	204	632.7	816.9	27.1	639.1	1.1160	298.15	1.2220[14]	1.1461	−6.2
163	[bmim][mesy]	$C_9H_{18}N_2O_3S$	1-butyl-3-methylidimazolium methane sulfonate	234	713.1	1054.8	37.4	701.3	0.3990	373.15	1.1284[15]	1.0581	−6.2
164	[emim][mesy]	$C_7H_{14}N_2O_3S$	1-ethyl-3-methylidimazolium methane sulfonate	206	667.4	1026.0	48.1	587.1	0.3307	298.15	1.2437[36]	1.1275	−9.3
165	[dmim][MOESO4]	$C_8H_{16}N_2O_5S$	1,3-dimethylidimazolium methoxyethyl sulfate	252	735.1	1094.4	38.9	675.4	0.3854	298.15	1.3140[16]	1.2286	−6.5
166	[dmim][MSO4]	$C_6H_{12}N_2O_4S$	1,3-dimethylidimazolium methyl sulfate	208	666.9	1040.0	52.9	545.6	0.3086	298.15	1.3280[16]	1.2208	−8.1
167	[bmim][MSO4]	$C_9H_{18}N_2O_4S$	1-butyl-3-methylidimazolium methyl sulfate	250	735.6	1081.6	36.1	716.9	0.4111	298.15	1.2124[16]	1.1534	−4.9
168	[MMMPZ][MSO4]	$C_7H_{14}N_2O_4S$	1,2,4-trimethylpyrazolium methylsulfate	222	694.8	1054.2	45.4	601.1	0.3627	353.15	1.2500[37]	1.1702	−6.4
169	[MTEOA][MSO4]	$C_8H_{21}NO_7S$	*tris*(2-hydroxyethyl)methylammonium methyl sulfate	273	865.1	1093.4	34.9	744.3	1.5130	353.15	1.3100[37]	1.3770	5.1
170	[bmim][NfO]	$C_{12}H_{15}N_2F_9SO_3$	1-butyl-3-methylidimazolium nonafluorobutane sulfonate	438	762.3	1028.8	17.3	1004.8	0.5150	295.15	1.4730[20]	1.5249	3.5
171	[omim][NfO]	$C_{16}H_{23}N_2O_3SF_9$	1-octyl-3-methylidimazolium nonafluorobutane sulfonate	494	843.2	1094.2	14.2	1250.2	0.6591	298.15	1.3300[24]	1.4408	8.3
172	[bmim][C8S]	$C_{16}H_{32}N_2O_4S$	1-butyl-3-methylidimazolium octyl sulfate	349	895.7	1189.8	20.2	1116.7	0.7042	298.15	0.9971[38]	1.1204	12.4
173	[tibmp][pTSO3]	$C_{20}H_{37}O_3PS$	triisobutylmethyl phosphonium *p*-toluene sulfonate	389	874.8	1176.4	18.2	1249.9	0.5628	298.15	1.0690[16]	1.0941	2.3
174	[Ch][Sa]	$C_{12}H_{19}NO_4$	choline salicylate	240	762.2	950.5	23.7	726.4	1.3953	353.15	1.1467[37]	1.2288	7.2
175	[C27guan][BF4]	$C_{27}H_{58}N_3BF_4$	[*bis*(*bis*-hexylamino)methylene]dimethylammonium tetrafluoroborate	512	894.8	1100.3	8.2	1832.0	0.7076	298.15	0.9700[19]	1.0751	10.8
176	[C15guan][BF4]	$C_{15}H_{34}N_3BF_4$	[*bis*(butyl-ethylamino)methylene]dimethylammonium tetrafluoroborate	343	620.3	755.9	12.2	1146.7	1.1454	298.15	1.0500[19]	1.1164	6.3
177	[moeoemim][BF4]	$C_9H_{17}N_2O_2BF_4$	1-[2-(2-methoxyethoxy)ethyl]-3-methylidimazolium tetrafluoroborate	272	562.9	720.2	18.8	743.3	0.9644	298.15	1.2200[20]	1.2824	5.1
178	[bdmim][BF4]	$C_9H_{17}N_2BF_4$	1-butyl-2,3-dimethylidimazolium tetrafluoroborate	240	523.1	671.0	18.9	710.5	0.9476	300.15	1.0935[16]	1.1565	5.8
179	[dmim][BF4]	$C_{14}H_{27}N_2BF_4$	1-decyl-3-methylidimazolium tetrafluoroborate	310	632.5	784.6	14.5	997.7	1.0817	298.15	1.0400[20]	1.1444	10.0
180	[N-epy][BF4]	$C_7H_{10}BF_4N$	1-ethylpyridinium tetrafluoroborate	195	411.2	549.9	23.5	533.9	0.7495	293.1	1.3020[16]	1.1412	−12.4
181	[prmim][BF4]	$C_7H_{13}N_2BF_4$	1-propyl-3-methylidimazolium tetrafluoroborate	212	472.3	619.7	21.8	597.9	0.8479	298.15	1.2400[20]	1.1642	−6.1
182	[moemim][BF4]	$C_7H_{13}N_2OBF_4$	ethyloxymethyl-3-methylidimazolium tetrafluoroborate	228	494.8	647.0	21.7	613.5	0.8686	298.15	1.2600[20]	1.2404	−1.6

Table 3. (Continued)

No.	ionic liquid	global formula	IUPAC name	M	T_b (K)	T_C (K)	P_C (bar)	V_C (cm^3/mol)	ω	T (K)	ρ^{lit} (g/cm^3)[a]	ρ^{calc} (g/cm^3)	%$\Delta\rho$
183	[mommim] [BF4]	$C_6H_{11}N_2OBF_4$	methyloxymethyl-3-methylidimazolium tetrafluoroborate	214	471.9	623.7	23.3	556.4	0.8291	298.15	1.3300[20]	1.2599	−5.3
184	[bpyr] [BF4]	$C_9H_{14}BF_4N$	1-butylpyridinium tetrafluoroborate	223	456.9	597.6	20.3	648.1	0.8307	298.20	1.2144[39]	1.1174	−8.0
185	[4MOPY] [BF4]	$C_{14}H_{24}BF_4N$	4-methyl-*n*-octylpyridinium tetrafluoroborate	293	576.3	720.8	15.1	932.1	1.0289	298.15	1.0800[17]	1.1237	4.0
186	[C23guan] [BF4]	$C_{23}H_{50}N_3F_4B$	*bis*-hexyl-amino-methylene dimethylammonium tetrafluoroborate	455	803.3	975.1	9.2	1603.5	0.9385	298.15	0.9700[20]	1.1050	13.9
187	[DEME] [BF4]	$C_8H_{20}NOF_4B$	*N*,*N*-diethyl-*N*-methyl-*N*-(2-methoxyethyl)ammonium tetrafluoroborate	233	393.5	501.4	17.1	693.1	0.9465	293.15	1.1800[29]	1.0539	−10.7
188	[bmim] [tca]	$C_9H_{15}N_3S$	1-butyl-3-methylidimazolium thiocyanate	197	763.1	1047.4	19.4	780.7	0.4781	298.15	1.0696[15]	0.8738	−18.3
189	[emim] [SCN]	$C_7H_{11}N_3S$	1-ethyl-3-methylidimazolium thiocyanate	169	717.3	1013.6	22.3	666.4	0.3931	298.15	1.1140[15]	0.8573	−19.0
190	[N-epy] [ta]	$C_9H_{10}F_3NO_2$	1-ethylpyridinium trifluoroacetate	221	535.1	739.9	24.2	586.5	0.5483	293.1	1.2730[16]	1.2409	−2.5
191	[emim] [ta]	$C_8H_{11}N_2F_3O_2$	1-ethyl-3-methylidimazolium trifluoroacetate	224	562.8	775.7	24.2	610.4	0.5664	298.15	1.3900[16]	1.2180	−12.4
192	[mpmi] [TfO]	$C_{12}H_{13}N_2F_3SO_4$	1-(4-methoxyphenyl)-3-methylidimazolium trifluoromethane sulfonate	338	830.4	1184.7	28.0	827.7	0.4481	323.15	1.3200[20]	1.3778	4.4
193	[dbim] [TfO]	$C_{12}H_{21}N_2F_3SO_3$	1,3-dibutylimidazolium trifluoromethane sulfonate	330	776.4	1072.0	23.2	922.0	0.5325	303.15	1.3000[20]	1.2295	−5.4
194	[N8444] [TfO]	$C_{21}H_{44}NF_3SO_3$	tributyloctylammonium trifluoromethane sulfonate	448	858.2	1066.7	12.6	1458.4	0.9461	293.15	1.0200[20]	1.1737	15.1
195	[Bemim] [TfO]	$C_{12}H_{13}N_2O_3SF_3$	1-benzyl-3-methylidimazolium trifluoromethane sulfonate	322	803.0	1158.0	29.0	813.7	0.4118	303.15	1.3000[40]	1.3313	2.4
196	[mbpyr] [TfO]	$C_{11}H_{16}NO_3F3$	1-butyl-4-methylpyridinium trifluoromethane sulfonate	299	697.3	997.8	26.9	799.3	0.4153	298.15	1.1700[24]	1.2441	6.3
197	[omim] [TfO]	$C_{13}H_{23}F_3N_2O_3S$	1-octyl-3-methylidimazolium trifluoromethane sulfonate	344	799.2	1088.7	21.6	979.1	0.5766	298.15	1.1200[24]	1.2248	9.4
198	[4MOPY] [TfO]	$C_{15}H_{24}NO_3SF_3$	4-methyl-*n*-octylpyridinium trifluoromethane sulfonate	355	788.8	1065.7	20.1	1027.8	0.5898	298.15	1.1700[17]	1.2079	3.2
199	[dmpim] [TMEM]	$C_{12}H_{15}F_9N_2O_6S_3$	1,2-dimethyl-3-propylimidazolium *tris*(trifluoromethylsulfonyl)methide	550	1039.3	1568.6	23.9	1212.0	0.1526	298.15	1.5970[12]	1.5007	−6.0
200	[bmim] [TMEM]	$C_{12}H_{15}F_9N_2O_6S_3$	1-butyl-3-methylimidazolium *tris*(trifluoromethylsulfonyl)methide	550	1034.4	1571.4	24.0	1213.6	0.1320	297.65	1.5630[27]	1.4913	−4.6

[a] The reference (noted as a superscript) corresponds to the source from which the literature density value was obtained.

Table 4. Average, Absolute and Maximum Deviations Found between Predicted and Experimental Densities for the 200 Ionic Liquids

parameter	value
number of ionic liquids with $\%\Delta\rho > 10\%$	36
number of ionic liquids with $\%\Delta\rho < 10\%$	164
number of ionic liquids with $\%\Delta\rho < 5\%$	109
maximum absolute deviation, $\%\Delta\rho_{max}$	20.6%
average deviation, $\overline{\%\Delta\rho}$	−0.4%
average absolute deviation, $\overline{\lvert\%\Delta\rho\rvert}$	5.9%

[a] The symbol $\%\Delta\rho$ represents deviation.

In this equation, T_b is the boiling temperature at the normal boiling pressure ($P_b = 1.01325$ bar).

Results and Discussion

The calculated critical properties, the normal boiling temperature (T_b for $P_b = 1.01325$ bar), and the acentric factors are presented in Table 3. The molecular mass is also included in Table 3; this value is needed in the density calculations (see eq 1).

As explained previously, the calculation of the density is done as a global test of the consistency of the estimated critical properties. In fact, the 200 ionic liquids considered in this study are those for which density values are available in the literature, so that the test could be performed. As observed in Table 3, the predicted densities, using exclusively the calculated critical properties and the calculated normal boiling temperature, are within acceptable margins of errors for the purpose of the test.

Although other additional tests could be done, there is not much information available in the literature to perform such tests. One approach that could be done if data were available is to determine the vapor pressure using one of the several correlations to estimate this property. However, few data are available, in regard to the vapor pressure of ionic liquids, and some of the data are calculated values with unknown uncertainty.[41,42]

Table 4 summarizes some statistical values, such as the average, absolute, and maximum deviations found between predicted and experimental densities. As observed, the overall average deviations are less than −0.40% and the overall absolute deviations are less than 5.9%, whereas deviations greater than 10% are observed for only 36 of the 200 ionic liquids. The deviations between calculated and experimental densities are randomly distributed, and no relationship between the errors and some of the characteristics or properties of the ionic liquids has been observed. For instance, there is a group of tetra alkyl ammonium [bti] compounds (Nos. 50−54 in Table 3) for which deviations are close to 20%, but other compounds of the same group show lower deviations (Nos. 64−69 in Table 3).

Note that these deviations are relatively small if we consider the deviations between some experimental data published in the open literature. Table 5 shows the experimental densities that have been published by different authors for two ionic liquids. Deviations up to 17% are observed between some values. Finally, it should be mentioned that the generalized correlation used to estimate the density of ionic liquids (eq 1) was derived totally independent from the group contribution method used to estimate the critical properties (Table 3). Therefore, the density calculation is a reliable independent test to show that the values of the critical properties of ionic liquids are acceptable and can be used in other applications where these properties are needed.

Table 5. Deviations between Experimental Density Data Published by Different Authors for Some Ionic Liquids at 298 K

r	$\%\Delta\rho$	reference
	[bmin][BF4]	
1.12	*[a]	Huddleson et al.[43]
1.12	0	Visser et al.[44]
1.19	6.3	Wu et al.[45]
1.21	8.0	Nishida et al.[46]
1.26	12.5	Branco et al.[47]
	[omim][PF6]	
1.19	*[a]	Branco et al.[47]
1.22	2.5	Huddleson et al.[43]
1.23	2.9	Gu and Brennecke[39]
1.24	3.9	Chun et al.[48]
1.40	17.6	Wu et al.[45]

[a] The value with an asterisk (*) was used as a reference to determine the deviations for the other values.

Conclusions

A consistent group contribution method has been extended to evaluate the critical properties of 200 ionic liquids. In addition, estimated values for the normal boiling temperatures and the acentric factors of these substances were determined. The consistency of the method has been checked using literature values of ionic liquid densities and comparing them with calculated values, using a generalized correlation that makes use of those estimated critical properties. The values provided for the critical properties, the normal boiling temperature, and the acentric factors are believed to be sufficiently accurate for use in engineering calculations, generalized correlations, and equation of state methods, among other applications. The values provided, plus the results previously presented by the authors,[3] represent the most complete database on the critical properties of ionic liquids available in the open literature.

Nomenclature

A_M, B_M, C_M, D_M, E_M = coefficients in the modified Lydersen−Joback−Reid method

M = molecular mass

No. = number of ionic liquids

N = number of times that a group appears in a molecule (number frequency)

P_b = normal boiling pressure = 1.01325 bar

P_c = critical pressure

T = temperature

T_b = normal boiling temperature

T_{bR} = reduced temperature at the normal boiling point

T_c = critical temperature

T_R = reduced temperature

V_c = critical volume

Abbreviations

eq = equation

log = base 10 logarithm

Greek Letters

ρ_L = liquid density

ρ^{calc} = liquid density calculated using the proposed method

ρ^{lit} = liquid density from the literature

$\%\Delta\rho$ = percent relative deviation between calculated and literature values for the liquid density

ω = acentric factor

ΔT_M, ΔP_M, ΔV_M = contribution to the critical properties in the modified Lydersen−Joback−Reid method

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