Supporting information for:

Investigation of 1,2,3-trialkylimidazolium ionic liquids: experiment and density functional theory calculations

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Table S1. Provenance and purity of the samples.

Ionic liquid	Provenance	Product Number	Purification method	Mass fraction	Water content (ppm)	Halide content (ppm)
[emmim][NTf_2][a]	IoLiTec	174899-90-2	Vacuum drying	$\omega \geq 0.99$	70	75
[pmmim][NTf_2][b]	IoLiTec	169051-76-7	Vacuum drying	$\omega \geq 0.99$	80	68
[bmmim][NTf_2][c]	Merck	350493-08-2	Vacuum drying	$\omega \geq 0.99$	83	72

[a]1-ethyl-2,3-dimethylimidazolium *bis*(trifluoromethylsulfonyl)imide
[b]1,2-dimethyl-3-propylimidazolium *bis*(trifluoromethylsulfonyl)imide
[c]1-butyl-2,3-dimethylimidazolium *bis*(trifluoromethylsulfonyl)imide

Table S2. Linear fitting coefficients, b_i, of the density of the [emmim][NTf_2], [pmmim][NTf_2] and [bmmim][NTf_2] ionic liquids as a function of the temperature calculated from the experimental data provided in Table 1 using the eq. (S1) along with their standard deviations, (σ), (eq. (S2)).

Ionic liquid	b_o/ (g·cm^{-3})	$b_1 \cdot 10^4$/ (g·cm^{-3}·K^{-1})	$\sigma \cdot 10^4$/ (g·cm^{-3})
[emmim][NTf_2]	1.77720	-9.58	0.72
[pmmim][NTf_2]	1.73552	-9.43	1.00
[bmmim][NTf_2]	1.69350	-9.20	1.16

$$d = \sum_{i=0}^{1} b_i \cdot T^i \qquad \text{(S1)}$$

$$\sigma = \left(\frac{\sum (d_i^{\text{exp}} - d_i^{\text{cal}})^2}{n - v} \right)^{0.5} \qquad \text{(S2)}$$

Table S3. Thermal expansion coefficients, (α_p), as a function of temperature for the investigated ionic liquids (calculated from values given in Table 1 and references[1,2,3] by eq. (S3)).

T/(K)	$\alpha_p \cdot 10^4$ / (K^{-1})					
	[emmim][NTf_2]	[emim][NTf_2][3]	[pmmim][NTf_2]	[pmim][NTf_2][2]	[bmmim][NTf_2]	[bmim][NTf_2][1]
293.15	6.40	6.83	6.46	6.66	6.46	6.84
298.15	6.42	6.85	6.48	6.68	6.48	6.87
303.15	6.44	6.88	6.50	6.71	6.50	6.89
308.15	6.47	6.90	6.52	6.73	6.53	6.91
313.15	6.49	6.92	6.55	6.75	6.55	6.94
318.15	6.51	6.95	6.57	6.77	6.57	6.96
323.15	6.53	6.97	6.59	6.80	6.59	6.99

$$\alpha_p = -\frac{1}{d}\left(\frac{\partial d}{\partial T}\right)_P, \tag{S3}$$

Table S4. VFT fitting parameters for the viscosity, (η), (eq. S4), along with Angell strength parameter, ($D=b/T_o$), as a function of temperature for [emmim][NTf_2], [pmmim][NTf_2] and [bmmim][NTf_2] ionic liquids with the deviations of their fit, (σ), (eq. (S5)), calculated from the experimental data given in Table 1.

Ionic liquid	ln$a$	b	T_o	D	σ
[emmim][NTf_2]	-0.8265	564.80	187.02	3.02	0.025
[pmmim][NTf_2]	-0.9345	583.50	191.31	3.05	0.022
[bmmim][NTf_2]	-1.0338	592.97	193.15	3.07	0.028

$$\eta = a\exp\left(b/\left(T - T_0\right)\right) \tag{S4}$$

$$\sigma_\eta = \left(\frac{\sum\left(\eta_i^{\exp} - \eta_i^{\mathrm{cal}}\right)^2}{\eta - \nu}\right)^{0.5}, \tag{S5}$$

where n is the number of experimental points and ν is the number of adjustable parameters.

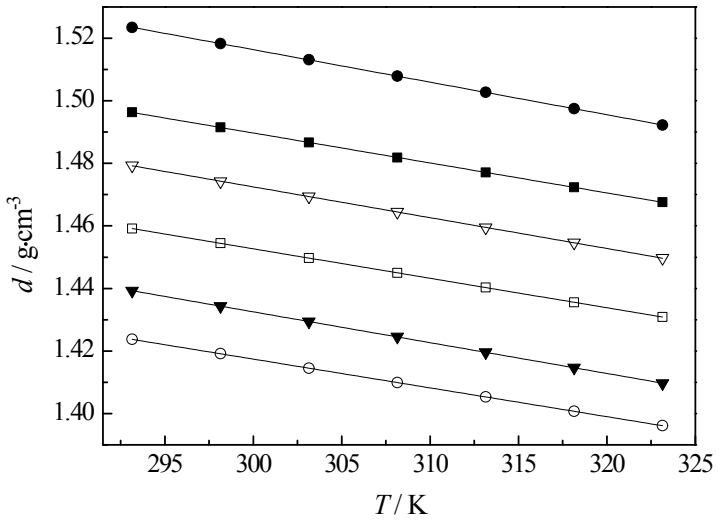

Figure S1. Experimental density, (*d*), of the ionic liquids: (❍) [emmim][NTf_2] (this paper), (❍) [pmmim][NTf_2] (this paper), (ᘓ) [bmmim][NTf_2] (this paper) (ᔓ) [emim][NTf_2][3], (⧫) [pmim][NTf_2][2] and (❑) [bmim][NTf_2][1] on temperature T = 298.15 K and atmospheric pressure (p = 0.1 MPa). The lines represent linear type fitting of the experimental data with parameters reported in Table S2 in the supporting information of this manuscript and in references[1-3].

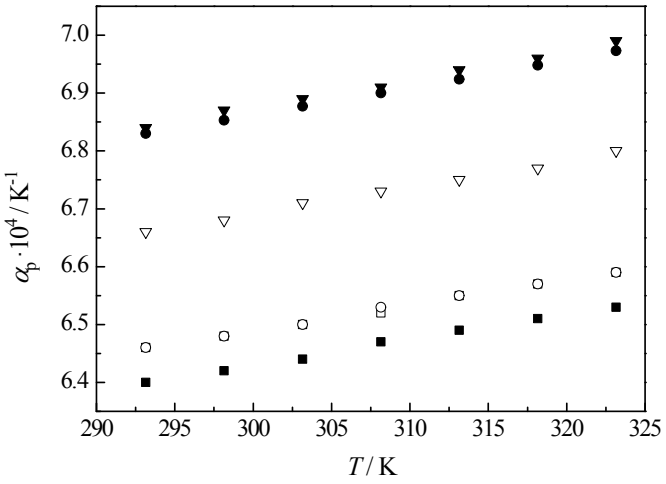

Figure S2. Variation of thermal expansion coefficients, (α_p), with temperature (293.15 – 323.15) K obtained by eq. (S3), for different ILs: (❍) [emmim][NTf_2] (this paper), (❍) [pmmim][NTf_2] (this paper), (ᘓ) [bmmim][NTf_2] (this paper) (ᔓ) [emim][NTf_2][3], (⧫) [pmim][NTf_2][2] and (❑) [bmim][NTf_2][1].

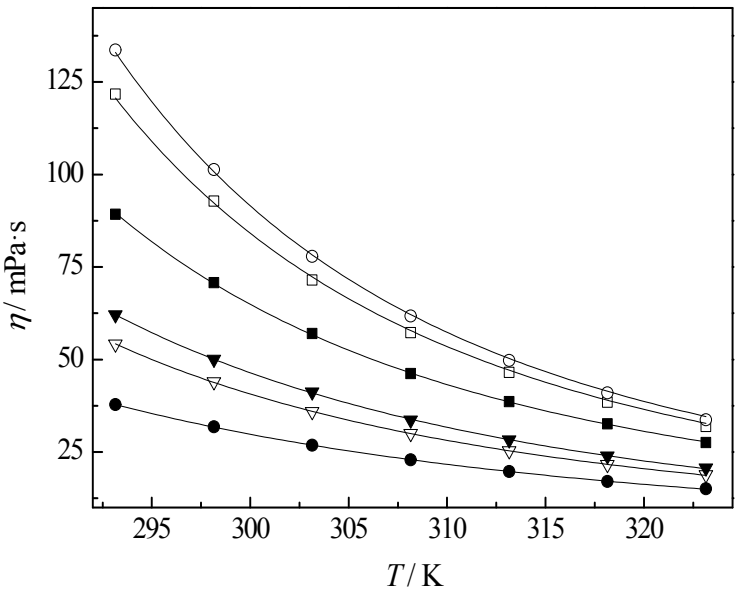

Figure S3. Viscosity, (η), of (O) [emmim][NTf_2] (this paper), (O) [pmmim][NTf_2] (this paper), (ᘓ) [bmmim][NTf_2] (this paper), (ᘐ) [emim][NTf_2][3], (♦) [pmim][NTf_2][2] and (❑) [bmim][NTf_2][1] in the temperature range from (293.15 to 323.15) K. The lines represent the Vogel–Fulcher–Tammann fitting of the experimental data with parameters reported in Table S4 in the supporting information of this manuscript and references[1-3].

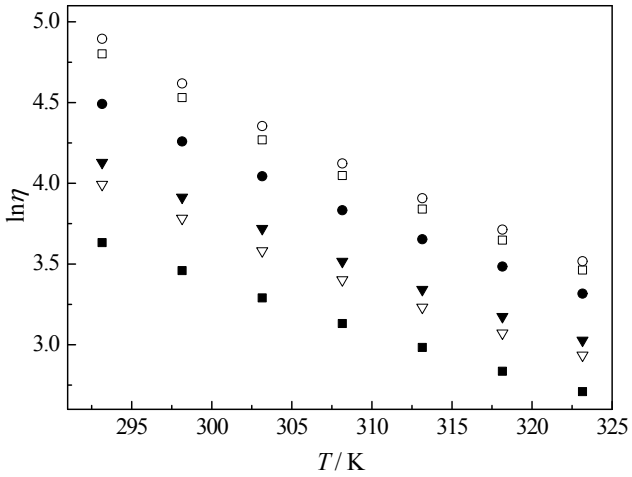

Figure S4. Logarithm of viscosity, (lnη), of (O) [emmim][NTf_2] (this paper), (O) [pmmim][NTf_2] (this paper), (ᘓ) [bmmim][NTf_2] (this paper), (ᘐ) [emim][NTf_2][3], (♦) [pmim][NTf_2][2] and (❑) [bmim][NTf_2][1] in the temperature range from (293.15 to 323.15) K.

References

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