

Supplementary Information

Critical behaviour and vapour-liquid coexistence of 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide ionic liquids via Monte Carlo simulations

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Supplementary Table 1. Calculated coexistence properties and standard deviations (SD) for [C₁mim][NTf₂].

<i>T</i> (K)	$\rho_{\text{liq.}}$ (g/cm ³)	SD	$\rho_{\text{vap.}}$ (g/cm ³)	SD	<i>P</i> ^{sat} (kPa)	SD	ΔH^{vap} (kJ/mol)	SD
900.00	1.019	0.00080	0.003696	0.000075	49.64	0.84	75.80	0.3429
950.00	0.963	0.00110	0.005354	0.000106	74.36	0.87	72.65	0.2893
1000.00	0.909	0.00120	0.008284	0.000146	113.98	1.12	68.31	0.2416
1025.00	0.879	0.00150	0.009245	0.000200	130.57	1.84	67.16	0.2861
1050.00	0.848	0.00140	0.010469	0.000280	148.33	3.08	65.74	0.3379
1075.00	0.819	0.00140	0.013769	0.000468	185.59	3.04	62.41	0.4132
1100.00	0.788	0.00240	0.019406	0.000552	235.53	3.38	57.55	0.4149

Supplementary Table 2. Calculated coexistence properties and standard deviations (SD) for [C₂mim][NTf₂].

<i>T</i> (K)	$\rho_{\text{liq.}}$ (g/cm ³)	SD	$\rho_{\text{vap.}}$ (g/cm ³)	SD	<i>P</i> ^{sat} (kPa)	SD	ΔH^{vap} (kJ/mol)	SD
900.00	0.965	0.00080	0.004047	0.000112	54.16	1.09	74.64	0.3800
950.00	0.911	0.00100	0.005908	0.000108	80.60	1.18	71.26	0.2498
1000.00	0.852	0.00130	0.008636	0.000208	118.02	1.75	66.98	0.3123
1025.00	0.822	0.00180	0.010088	0.000296	139.47	2.21	65.06	0.3682
1050.00	0.792	0.00180	0.012028	0.000147	165.68	1.71	62.94	0.2014
1075.00	0.756	0.00170	0.015377	0.000420	198.82	2.60	59.55	0.3181
1100.00	0.728	0.00140	0.022054	0.000651	253.40	3.58	54.91	0.3886

Supplementary Table 3. Calculated coexistence properties and standard deviations (SD) for [C₄mim][NTf₂].

<i>T</i> (K)	$\rho_{\text{liq.}}$ (g/cm ³)	SD	$\rho_{\text{vap.}}$ (g/cm ³)	SD	<i>P</i> ^{sat} (kPa)	SD	ΔH^{vap} (kJ/mol)	SD
900.00	0.890	0.00120	0.004518	0.000111	56.00	0.94	72.45	0.3458
950.00	0.838	0.00170	0.006898	0.000179	87.62	1.86	68.38	0.3482
1000.00	0.780	0.00160	0.009862	0.000318	126.06	2.76	64.20	0.4101
1025.00	0.753	0.00180	0.012613	0.000621	157.60	3.97	61.52	0.5430
1050.00	0.717	0.00250	0.013096	0.000475	169.82	5.45	60.17	0.4948
1075.00	0.677	0.00510	0.015642	0.000477	199.83	4.06	57.28	0.4095
1100.00	0.638	0.00350	0.020252	0.000968	246.36	5.59	53.33	0.5732

Supplementary Table 4. Calculated coexistence properties and standard deviations (SD) for [C₆mim][NTf₂].

<i>T</i> (K)	$\rho_{\text{liq.}}$ (g/cm ³)	SD	$\rho_{\text{vap.}}$ (g/cm ³)	SD	<i>P</i> ^{sat} (kPa)	SD	ΔH^{vap} (kJ/mol)	SD
900.00	0.833	0.00180	0.005245	0.000140	60.34	1.43	71.15	0.4847
950.00	0.780	0.00140	0.006639	0.000182	82.60	1.65	68.86	0.4296
1000.00	0.723	0.00190	0.009759	0.000337	121.66	2.41	64.07	0.4390
1025.00	0.691	0.00140	0.012305	0.000311	148.59	2.39	60.68	0.3293
1050.00	0.659	0.00160	0.014885	0.000312	177.90	2.35	57.90	0.2775
1075.00	0.624	0.00200	0.018565	0.000444	216.40	3.30	54.57	0.3181
1100.00	0.581	0.00380	0.024159	0.000913	261.38	5.48	49.94	0.4816