

Supporting Information for

Experimental and Computational Study of the Properties of Imidazole Compounds with Branched and Cycloalkyl Substituents

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Table S1: Compilation of densities (ρ) of linear alkyl imidazoles at different temperatures (T) and $P = 101$ kPa [1].

$\frac{T}{K}$	$\frac{\rho}{g \cdot cm^{-3}}$			
	1-propylimidazole	1-butylimidazole	1-pentylimidazole	1-octylimidazole
293.15	0.9729	0.9514	0.9389	0.9115
303.15	0.9646	0.9434	0.9311	0.9043
313.15	0.9562	0.9354	0.9233	0.8971
323.15	0.9479	0.9274	0.9156	0.8898
333.15	0.9395	0.9194	0.9078	0.8826
343.15	0.9311	0.9113	0.8999	0.8753
353.15	0.9227	0.9032	0.8921	0.8680

Table S2: Dynamic viscosities (η) of imidazole compounds from measurements and COSMOtherm calculations at different temperatures (T) and $P = 101$ kPa.^a

$\frac{T}{K}$	$\frac{\eta_m^b}{mPa \cdot s}$	$\frac{\eta_c^c}{mPa \cdot s}$	$\frac{Error^d}{\%}$	$\frac{T}{K}$	$\frac{\eta_m}{mPa \cdot s}$	$\frac{\eta_c}{mPa \cdot s}$	$\frac{Error}{\%}$
(1) <i>N</i> -isopropylimidazole				(2) <i>N</i> -isobutylimidazole			
293.15	3.11	2.38	23.42	293.15	4.76	2.85	40.21
298.15	2.74	2.14	21.76	298.15	4.08	2.55	37.57
303.15	2.46	1.94	21.28	303.15	3.54	2.29	35.36
308.15	2.20	1.75	20.23	308.15	3.10	2.06	33.46
313.15	1.99	1.60	19.83	313.15	2.75	1.87	32.16
318.15	1.80	1.45	19.18	318.15	2.45	1.69	30.91
323.15	1.64	1.33	18.88	323.15	2.18	1.54	29.33
333.15	1.35	1.12	16.93	333.15	1.78	1.29	27.71
343.15	1.10	0.95	13.20	343.15	1.50	1.09	27.59
353.15	0.93	0.82	11.79	353.15	1.21	0.93	23.50
(3) <i>N</i> -sec-butylimidazole				(4) <i>N</i> -cyclopropylmethylimidazole			
293.15	4.22	2.81	33.45	293.15	7.06	3.78	46.40
298.15	3.62	2.51	30.53	298.15	6.00	3.36	44.06
303.15	3.15	2.26	28.25	303.15	5.14	2.99	41.85
308.15	2.75	2.04	25.88	308.15	4.48	2.67	40.37
313.15	2.45	1.84	24.73	313.15	3.94	2.40	39.17
318.15	2.19	1.67	23.57	318.15	3.49	2.16	38.19

323.15	1.95	1.52	21.85	323.15	3.12	1.95	37.56
333.15	1.60	1.27	20.39	333.15	2.55	1.60	37.12
343.15	1.32	1.08	18.50	343.15	2.15	1.33	37.92
353.15	0.99	0.92	7.34	353.15	1.87	1.12	39.96
(5) N-cyclopentylimidazole				(6) N-cyclohexylmethylimidazole			
293.15	7.16	5.00	30.16	293.15	N/A (Solid)		
298.15	6.17	4.40	28.75	298.15	N/A (Solid)		
303.15	5.34	3.88	27.31	303.15	N/A (Solid)		
308.15	4.68	3.44	26.48	308.15	N/A (Solid)		
313.15	4.13	3.06	25.86	313.15	N/A (Solid)		
318.15	3.65	2.73	25.07	318.15	N/A (Solid)		
323.15	3.27	2.45	25.04	323.15	11.42	3.63	68.22
333.15	2.67	1.99	25.52	333.15	7.94	2.87	63.82
343.15	2.24	1.63	27.09	343.15	5.83	2.30	60.46
353.15	1.91	1.36	28.99	353.15	4.45	1.87	57.92

^aTemperature variance is +/-0.01 K. Viscosity measurements variance is +/- 0.1% of the reported value

^bMeasured viscosity

^cCOSMOtherm calculated viscosity

^dError = $\frac{\eta_m - \eta_c}{\eta_c} * 100$

Table S3: Compilation of viscosities (η) of linear alkyl imidazoles at different temperatures (T) and $P = 101$ kPa [1].

$\frac{T}{K}$	$\frac{\eta}{mPa \cdot s}$			
	1-propylimidazole	1-butylimidazole	1-pentylimidazole	1-octylimidazole
293.15	3.17	3.95	5.13	9.17
298.15	2.81	3.47	4.49	7.77
303.15	2.50	3.05	3.89	6.56
308.15	2.26	2.71	3.42	5.63
313.15	2.05	2.43	3.02	4.87
318.15	1.86	2.19	2.70	4.25
323.15	1.69	1.99	2.42	3.76
333.15	1.45	1.66	2.00	3.00
343.15	1.25	1.43	1.68	2.44
353.15	1.23	1.42	1.43	2.04

Table S4: Vapor pressure (P) and enthalpies of vaporization (ΔH) of imidazole compounds from measurements and COSMOtherm calculations at different temperatures (T).^a

Compound	$\frac{T}{K}$	$\frac{P_m^b}{Pa}$	$\frac{P_c^c}{Pa}$	$\frac{\text{Error}(P)^d}{\%}$	$\frac{\Delta H_{vap}^m^e}{kJ \cdot mol^{-1}}$	$\frac{\Delta H_{vap}^c^f}{kJ \cdot mol^{-1}}$	$\frac{\text{Error}(\Delta H_{vap})^g}{\%}$
1	283.4	5.04	5.23	-3.74	59.39	54.61	8.04
	286.5	6.62	6.72	-1.47	59.18	54.52	7.88
	289.4	8.51	8.45	0.74	58.98	54.43	7.72
	292.4	10.89	10.65	2.19	58.77	54.33	7.55
	295.3	13.80	13.26	3.89	58.58	54.24	7.41
	298.2	16.97	16.44	3.13	58.37	54.15	7.23
	303.1	24.51	23.39	4.58	58.04	53.99	6.97
	304.5	28.32	25.81	8.87	57.95	53.95	6.90
	306.0	31.02	28.65	7.65	57.84	53.90	6.81
	309.0	40.17	35.18	12.41	57.64	53.81	6.65
	312.0	49.53	43.02	13.14	57.43	53.71	6.48
	314.1	56.73	49.41	12.91	57.29	53.64	6.37
	316.0	64.34	55.90	13.12	57.15	53.58	6.25
	318.0	74.82	63.54	15.07	57.01	53.52	6.13
	320.0	84.70	72.11	14.87	56.88	53.45	6.03
	321.0	90.13	76.76	14.83	56.81	53.42	5.97
	323.0	103.60	86.88	16.14	56.67	53.35	5.85
2	289.6	4.42	4.37	1.07	62.81	56.97	9.30
	292.6	5.85	5.57	4.75	62.57	56.88	9.10
	295.6	7.50	7.06	5.83	62.34	56.78	8.91
	298.3	9.55	8.70	8.85	62.14	56.70	8.75
	301.2	12.07	10.85	10.14	61.91	56.61	8.56
	302.5	13.16	11.95	9.18	61.81	56.57	8.48
	303.2	13.91	12.59	9.50	61.76	56.55	8.44
	306.0	17.49	15.45	11.64	61.55	56.46	8.28
	307.1	19.30	16.73	13.31	61.46	56.42	8.20
	308.1	20.50	17.98	12.31	61.39	56.39	8.15
	309.2	22.80	19.44	14.74	61.30	56.35	8.07
	310.0	24.06	20.57	14.50	61.24	56.33	8.02
	311.3	26.08	22.54	13.59	61.14	56.29	7.94
	311.4	27.01	22.69	15.98	61.13	56.28	7.93
	313.3	30.71	25.89	15.70	60.99	56.22	7.82
	314.2	33.17	27.54	16.97	60.92	56.19	7.76
	316.6	38.96	32.41	16.80	60.73	56.12	7.60

	317.1	40.21	33.52	16.63	60.69	56.10	7.56
	319.1	47.08	38.30	18.65	60.54	56.03	7.44
	319.2	47.83	38.56	19.39	60.53	56.03	7.43
	320.4	51.47	41.73	18.93	60.44	55.99	7.36
	322.1	58.12	46.62	19.79	60.31	55.94	7.25
	323.2	63.21	50.05	20.81	60.22	55.90	7.17
	324.0	67.39	52.69	21.81	60.16	55.87	7.13
	324.4	68.34	54.06	20.90	60.13	55.86	7.10
	326.1	78.34	60.21	23.14	60.00	55.80	6.99
3	295.7	7.11	6.84	3.78	64.78	56.81	12.31
	298.4	8.99	8.43	6.22	64.57	56.72	12.16
	301.7	11.98	10.82	9.66	64.32	56.61	11.98
	304.4	14.84	13.22	10.92	64.11	56.52	11.83
	307.6	19.39	16.67	14.01	63.86	56.42	11.65
	310.3	23.75	20.20	14.95	63.65	56.33	11.50
	314.3	32.90	26.66	18.96	63.35	56.20	11.28
	316.8	39.32	31.59	19.66	63.16	56.12	11.15
	317.0	40.65	32.02	21.24	63.14	56.11	11.13
	320.1	51.73	39.34	23.95	62.90	56.01	10.96
	324.3	69.99	51.65	26.21	62.58	55.87	10.72
	324.5	70.09	52.31	25.37	62.56	55.86	10.71
	326.3	80.12	58.64	26.81	62.42	55.80	10.60
	328.4	93.00	66.87	28.09	62.26	55.73	10.49
	330.2	105.33	74.74	29.04	62.13	55.67	10.40
4	303.0	3.70	7.25	-95.88	59.49	57.46	3.42
	305.4	4.54	8.67	-90.95	59.32	57.38	3.27
	308.2	5.48	10.64	-94.21	59.12	57.29	3.09
	309.3	5.99	11.52	-92.38	59.04	57.26	3.02
	311.3	6.98	13.29	-90.46	58.90	57.19	2.90
	312.2	7.39	14.17	-91.73	58.83	57.16	2.83
	314.2	8.43	16.30	-93.35	58.69	57.10	2.71
	316.8	9.98	19.50	-95.38	58.50	57.01	2.54
	317.2	10.4	20.04	-92.68	58.47	57.00	2.51
	320.2	12.76	24.53	-92.26	58.26	56.90	2.33
	320.3	12.75	24.70	-93.70	58.25	56.90	2.32
	323.1	15.55	29.71	-91.09	58.05	56.81	2.14
	325.5	18.34	34.72	-89.34	57.88	56.73	1.99
	329.1	23.29	43.66	-87.47	57.62	56.61	1.76
	331.5	27.09	50.71	-87.20	57.45	56.53	1.61

	334.3	31.87	60.21	-88.91	57.24	56.43	1.41
	337.5	39.17	72.97	-86.30	57.01	56.32	1.21
	340.4	47.33	86.57	-82.91	56.81	56.22	1.03
	343.3	56.46	102.37	-81.32	56.60	56.12	0.84
	305.0	2.42	2.16	10.79	70.10	61.53	12.23
	308.0	3.19	2.73	14.29	69.87	61.43	12.08
	310.8	3.90	3.39	13.00	69.65	61.34	11.93
	312.7	4.64	3.92	15.54	69.51	61.27	11.85
	313.6	5.06	4.19	17.13	69.44	61.24	11.80
	316.9	6.37	5.35	15.95	69.19	61.13	11.64
	317.8	6.92	5.72	17.37	69.12	61.10	11.60
	318.8	7.44	6.15	17.37	69.04	61.07	11.54
5	321.2	9.10	7.30	19.76	68.86	60.99	11.43
	321.5	9.41	7.46	20.73	68.83	60.98	11.40
	324.2	11.73	9.02	23.12	68.62	60.89	11.27
	324.8	12.44	9.40	24.42	68.58	60.87	11.24
	327.9	15.79	11.63	26.32	68.34	60.76	11.09
	328.3	16.52	11.95	27.64	68.31	60.75	11.07
	330.9	20.43	14.24	30.32	68.11	60.66	10.94
	334.0	24.61	17.47	29.03	67.87	60.55	10.78
	336.9	30.09	21.07	29.98	67.65	60.45	10.64
	340.1	39.46	25.81	34.60	67.40	60.34	10.48
	343.2	48.81	31.29	35.90	67.16	60.23	10.32
	346.1	58.67	37.34	36.36	66.94	60.13	10.18
	314.0	1.12	0.86	23.66	76.17	67.47	11.42
	316.6	1.43	1.06	26.08	75.95	67.38	11.29
	323.0	2.52	1.75	30.40	75.41	67.15	10.95
	323.1	2.55	1.77	30.69	75.41	67.15	10.96
	326.0	3.24	2.21	31.88	75.16	67.04	10.80
	319.9	1.95	1.38	29.43	75.67	67.26	11.11
6	329.0	4.07	2.77	32.06	74.91	66.94	10.64
	325.8	3.23	2.17	32.69	75.18	67.05	10.81
	330.8	4.80	3.16	34.19	74.76	66.87	10.55
	334.9	6.65	4.25	36.05	74.42	66.72	10.35
	340.9	10.67	6.48	39.28	73.92	66.50	10.04
	343.8	13.46	7.90	41.34	73.67	66.39	9.89
	343.9	13.78	7.95	42.32	73.66	66.38	9.88
	346.8	16.86	9.65	42.76	73.42	66.27	9.73
	349.9	21.23	11.83	44.29	73.17	66.15	9.59

	352.8	26.47	14.26	46.14	72.92	66.04	9.43
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^aUncertainties are $u(T) = 0.1$ K and $u(P) = 0.01$ Pa

^bMeasured vapor pressure [2]

^cCOSMOtherm calculated vapor pressure

^d $\text{Error}(P) = \frac{P_m - P_c}{P_m} * 100$

^eEnthalpy of vaporization from measurement

^fEnthalpy of vaporization from COSMOtherm calculation

^g $\text{Error}(\Delta H_{vap}) = \frac{\Delta H_{vap}^m - \Delta H_{vap}^n}{\Delta H_{vap}^m} * 100$

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