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Supplementary material

SUPPLEMENTARY MATERIAL TO

Prediction of high pressure liquid heat capacities of organic compounds by a group contribution method

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TABLE I-S. The literature experimental data used for correlation and prediction results

Compound	Ref.	n	T_{min} K	T_{max} K	T_c K	p_{min} MPa	p_{max} MPa	Kolská %	New %
1,1,1,2,3,3,3-Heptafluoropropane	40	62	223.150	283.150	375.900	1.100	20.000	10.20	2.27
1,1,1,2,3,3,3-Heptafluoropropane	41	46/30	273.150	333.150	375.900	0.600	15.000	8.08	2.15
1,1,1,2-Tetrafluoroethane	42	59/32	273.000	333.000	374.100	0.500	30.000	5.20	5.73
1,1,1,2-Tetrafluoroethane	41	52	223.150	283.150	374.100	0.750	18.200	4.18	4.85
1,1,2-Trichlorotrifluoroethane	43	77/49	288.150	423.150	487.300	0.600	30.000	4.83	2.79
1,2-Dimethybenzene	44	36	318.150	373.150	630.300	0.100	10.000	0.91	0.78
1,3-Dimethybenzene	44	36	318.150	373.150	617.000	0.100	10.000	2.96	1.51
1,4-Dimethybenzene	44	36	318.150	373.150	616.200	0.100	10.000	2.61	1.46
1-Bromobutane	45	21	298.000	348.000	569.400	0.098	147.000	9.18	6.61
1-Bromoheptane	45	21	298.000	348.000	647.400[a]	0.098	147.000	13.10	3.42
1-Bromohexane	45	21	298.000	348.000	623.900[a]	0.098	147.000	11.60	1.49
1-Butanol	46	58/52	321.050	472.950	562.000	0.100	50.000	5.32	5.96
1-Decanol	47	94	325.700	570.700	687.300	2.000	30.000	15.12	4.52
1-Decanol	48	79	304.050	522.950	687.300	0.100	50.000	6.46	2.84
1-Heptanol	47	94/91	325.700	560.700	632.600	2.000	30.000	15.04	4.17
1-Heptanol	48	77	303.350	522.150	632.600	0.100	50.000	8.08	2.51
1-Hexanol	47	110/103	325.700	540.700	610.300	1.500	30.000	12.31	3.66
1-Nonanol	49	78	303.100	522.450	670.700	0.100	50.000	7.09	2.47
1-Octanol	47	92	325.700	570.700	652.500	2.000	30.000	14.79	4.13
1-Octanol	49	77	303.200	523.150	652.500	0.100	50.000	7.66	2.46
2,2,4-Trimethylpentane	50	18/14	360.000	480.000	543.800	2.000	10.000	7.56	4.61
2-Methyl-1-propanol	51	65/53	300.650	471.150	547.700	0.100	50.000	10.07	6.08
2-Methylaniline	52	57	303.150	523.150	717.000	0.100	25.000	29.08	1.45
2-Methylbutane	53	35/18	288.800	299.100	460.400	0.100	280.300	15.41	5.62
2-Methylpentane	54	20/10	298.300	299.500	497.700	0.100	257.000	8.43	0.42
2-Propanol	55	27/14	323.150	423.150	508.300	4.760	30.000	8.87	6.56
3-Methyl-1-butanol	51	64/58	302.050	496.850	577.200	0.100	50.000	10.26	4.64
3-Methylaniline	52	57	303.150	523.150	709.100	0.100	25.000	29.21	1.75

TABLE I-S. Continued

Compound	Ref.	n	T_{min} K	T_{max} K	T_c K	p_{min} MPa	p_{max} MPa	Kolská %	New %
3-Methylpentane	56	8/3	298.950	299.250	504.600	0.101	227.778	15.00	5.08
3-Methylpentane	57	137	110.310	291.060	504.600	0.100	108.000	5.40	2.34
Benzene	58	86/48	302.550	505.150	562.100	5.000	25.000	4.09	2.18
Benzene	59	8	298.300	298.600	562.100	0.100	68.100	2.84	4.01
Benzene	46	50	322.050	489.350	562.100	0.100	50.000	2.85	1.65
Chlorobenzene	60	240/175	301.260	568.240	632.300	0.500	15.000	1.45	1.49
Cyclohexane	61	128/82	295.420	493.700	553.800	0.500	50.000	3.58	3.71
Decane	62	72	318.150	373.150	617.600	0.100	10.000	2.10	0.51
Decane	63	12	298.800	299.200	617.600	0.100	254.500	4.58	4.25
Decane	64	69/62	292.650	548.420	617.600	0.101	60.000	4.93	0.53
Ethyl cyanide	65	64/59	303.150	503.150	564.400	0.100	25.000	25.69	1.00
Ethylbenzene	66	72/57	301.560	554.060	617.200	8.000	25.000	3.99	1.53
Ethylbenzene	44	36	318.150	373.150	617.200	0.100	10.000	0.75	2.93
Ethylbenzene	50	33	350.000	550.000	617.200	2.000	20.000	2.55	1.16
Ethylcyclohexane	50	21/18	380.000	540.000	609.100	2.000	10.000	11.10	1.54
Fluorobenzene	67	146/86	301.760	501.290	560.100	0.500	15.000	2.37	1.71
Fluorotrichloromethane	43	52/44	288.150	423.150	471.200	0.600	30.000	8.24	3.92
Heptane	68	52/44	303.150	483.150	540.100	0.100	25.000	5.03	1.35
Heptane	64	47/37	292.490	485.080	540.100	5.000	60.000	6.65	1.27
Hexadecane	62	60	318.150	373.150	720.600	0.100	10.000	1.52	0.41
Hexane	69	73	313.150	373.150	507.900	0.100	100.000	5.32	0.73
Hexane	70	65/52	293.390	453.240	507.900	0.500	60.000	5.46	1.04
Hexane	68	42/32	303.150	443.150	507.900	5.000	25.000	4.01	1.67
Hexane	65	44/32	313.150	443.150	507.900	5.000	25.000	4.40	1.70
Hexane	49	57/44	308.350	447.150	507.900	0.100	50.000	1.78	3.27
Hexane	71	18	298.120	348.170	507.900	0.098	147.000	10.73	5.30
Methyl cyanide	68	63/53	303.150	483.150	548.000	0.100	25.000	6.57	3.54
Nonane	62	72	318.150	373.150	594.600	0.100	10.000	2.30	0.89

TABLE I-S. Continued

Compound	Ref.	n	T_{min} K	T_{max} K	T_c K	p_{min} MPa	p_{max} MPa	Kolská %	New %
Nonane	64	41/32	323.820	524.370	594.600	5.000	60.000	7.51	0.85
Octane	62	60	318.150	373.150	568.800	0.100	10.000	2.39	0.63
Octane	72	18/13	298.100	299.100	568.800	0.100	294.300	10.38	6.34
Octane	64	34/25	323.920	494.380	568.800	5.000	60.000	8.16	1.16
Pentane	73	24/18	293.450	412.760	469.800	10.000	60.000	5.65	0.92
Propyl cyanide	65	65	303.150	523.150	582.300	0.100	25.000	25.33	2.56
Toluene	74	193/128	302.870	531.860	591.700	0.500	25.000	2.54	2.50
Toluene	75	60/48	300.000	520.000	591.700	5.000	30.000	4.00	2.49
Toluene	76	80/40	255.500	401.500	591.700	3.500	291.100	2.43	7.00
Toluene	77	24	297.460	423.920	591.700	0.100	100.000	4.64	4.77
Tridecane	78	77	313.150	373.150	676.200	0.100	100.000	2.41	0.58
Overall	–	4072/3449	–	–	–	–	–	7.52	2.55

[a]Predicted values