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HEAT OF VAPORIZATION FROM THE CORRESPONDING STATES PRINCIPLE

The heat of vaporization was estimated from the corresponding states principle. The reported values of the functions $\Delta S^{(0)}$ and $\Delta S^{(1)}$, or their analytical expressions, are presented. Tabulated values of $\Delta S^{(0)}$ and $\Delta S^{(1)}$ were correlated. Estimation procedures were tested on 80 non–polar substances with 397 experimental data points. The model proposed by Sivaraman, Magee and Kobayashi had the best predictive characteristics.

Key words: Heat of vaporization, Acentric factor, Corresponding states principle.

Using the three–parameter corresponding states principle, the heat of vaporization ΔH_v of a pure non–polar substance is given by the following relation [1]

$$\Delta H_v / T = \Delta S^{(0)} (T_r) + \omega \Delta S^{(1)} (T_r) + \omega^2 \Delta S^{(2)} (T_r) \quad (1)$$

where $T_r = T/T_c$ is the reduced temperature, T the temperature [K], T_c the critical temperature [K], ΔS the entropy of vaporization [J/molK] and ω the acentric factor. The quadratic term in ω is almost always negligible [2].

Pitzer et al. [1] (PLCHP) and Carruth and Kobayashi [2] (CK) have reported the values of $\Delta S^{(0)}$ and $\Delta S^{(1)}$ (Table 1). Reid et al. [3] (P) reported the following relation from the tabulated $\Delta S^{(0)}$ and $\Delta S^{(1)}$ values given by Pitzer et al. [1]

$$\Delta H_v / RT_c = 7.08 (1–T_r)^{0.354} + 10.95 \omega (1–T_r)^{0.456}, \quad 0.6 < T_r \leq 1.0 \quad (2)$$

where R=8.31451 J/molK is the universal gas constant.

Sivaraman et al. [4] (SMK) have reported dimensionless relations as follows

$$\Delta H_v / RT_c = (\Delta H_v)^{(0)} + (\omega / 0.490) (\Delta H_v)^{(1)}, \quad 0.31 < T_r < 0.98 \quad (3)$$

$$(\Delta H_v)^{(0)} = –0.932980 (1 – T_r)^{1/3} + 275.553255 (1 – T_r)^{5/6} + 416.646872 (1 – T_r)^{29/24} – 617.767986 (1 – T_r) – 94.438858 (1 – T_r)^2 + 29.557315 (1 – T_r)^3 \quad (4)$$

$$(\Delta H_v)^{(1)} = 10.494541 (1 – T_r)^{1/3} – 351.097613 (1 – T_r)^{5/6} – 617.139173 (1 – T_r)^{29/24} + 854.731448 (1 – T_r) + 155.934841 (1 – T_r)^2 – 50.592504 (1 – T_r)^3 \quad (5)$$

In order to avoid interpolation, in this study the values of $\Delta S^{(0)}$ and $\Delta S^{(1)}$ from Table 1 were united and correlated as follows (PLCHPCK)

$$\Delta S^{(0)} (T_r) = 2.8656 – 0.0077686 / (1 – T_r) + 52.926 (1 – T_r) – 38.353 (1 – T_r)^{1.5} + 93.993 (1 – T_r)^4 \quad (6)$$

$$\Delta S^{(1)} (T_r) = 3.8100 – 0.014418 / (1 – T_r) + 46.531 (1 – T_r) + 0.92683 (1 – T_r)^{1.5} + 190.74 (1 – T_r)^5 \quad (7)$$

The same procedure was performed with the functions $f^{(0)}$ and $f^{(1)}$ in the three–parameter expression for reduced vapor pressures

$$f^{(0)} (T_r) = [–5.6297 (1 – T_r) + 0.76024 (1 – T_r)^2 + 4.7372 (1 – T_r)^5 – 43.988 (1 – T_r)^7 + 54.514 (1 – T_r)^{8.5}]/T_r \quad (8)$$

$$f^{(1)} (T_r) = [–4.6784 (1 – T_r) – 0.63774 (1 – T_r)^2 – 79.885 (1 – T_r)^5 + 327.50 (1 – T_r)^7 – 347.27 (1 – T_r)^{8.5}]/T_r \quad (9)$$

Thus, in this procedure, the acentric factor ω can be determined using the three–parameter corresponding states principle

$$\omega = \{ – \ln (p_c [\text{atm}]) – f^{(0)} (T_{br}) \} / f^{(1)} (T_{br}) \quad (10)$$

rather than the literature values from Table 2, where $T_{br} = T_b/T_c$ is the reduced normal boiling point, T_b the normal boiling point and p_c the critical pressure.

RESULTS AND DISCUSSION

All the expressions were tested on selected experimental data from Table 2, where ΔT was the temperature interval of the experimental data and n the number of experimental data points per set. The experimental values for T_b, T_c, p_c and ω were taken from reference [40]. The results are also presented in Table 2.

The overall percent errors, were calculated as follows

$$P_{av} = \sum_{i=1}^{N} n_i p_{av,i} / \sum_{i=1}^{N} n_i \quad ,$$

$$p_{av} = (100/n) \sum_{i=1}^{n} \left| (\Delta H_{v,exp,i} – \Delta H_{v,cal,i}) / \Delta H_{v,exp,i} \right| \quad (11)$$

where N is the number of experimental data sets.

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Table 1. Values of $f^{(0)}$, $f^{(1)}$, $\Delta S^{(0)}$ and $\Delta S^{(1)}$

T_r	$f^{(0)}$		$f^{(1)}$		$\Delta S^{(0)}$ [cal/molK]		$\Delta S^{(1)}$ [cal/molK]	
	PLCHP	CK	PLCHP	CK	PLCHP	CK	PLCHP	CK
0.250		–15.312		–36.611				
0.260		–14.690		–32.812				
0.270		–14.138		–30.164				
0.280		–13.608		–27.539				
0.290		–13.079		–25.144				
0.300		–12.549		–22.888		40.20		71.50
0.310		–12.019		–20.677				
0.320		–11.524		–19.111		37.55		63.60
0.330		–11.052		–17.615				
0.340		–10.592		–16.302		35.10		57.40
0.350		–10.154		–15.289				
0.360		–9.717		–14.368		32.80		53.00
0.370		–9.302		–13.539				
0.380		–8.911		–12.802		30.70		49.20
0.390		–8.520		–12.158				
0.400		–8.151		–11.536		28.83		46.00
0.410		–7.794		–10.983				
0.420		–7.460		–10.454		27.05		43.50
0.430		–7.138		–9.947				
0.440		–6.839		–9.441		25.50		41.14
0.450		–6.562		–8.980				
0.460		–6.286		–8.508		24.05		38.80
0.470		–6.033		–8.174				
0.480		–5.791		–7.622		22.70		36.48
0.490		–5.556		–7.207				
0.500		–5.330		–6.820		21.60		34.22
0.510		–5.107		–6.475				
0.520		–4.905		–6.125		20.55		32.00
0.530		–4.697		–5.761				
0.540		–4.525		–5.457		19.56		29.84
0.550		–4.352		–5.162				
0.560	–4.223	–4.186	–4.789	–4.881	18.64		27.80	
0.570		–4.023		–4.651				
0.580	–3.887	–3.868	–4.329	–4.393	17.74		26.20	
0.590		–3.707		–4.168				
0.600	–3.574	–3.555	–3.914	–3.937	16.92		24.60	
0.610		–3.419		–3.749				
0.620	–3.283	–3.279	–3.546	–3.557	16.12		23.20	
0.630		–3.150		–3.369				
0.640	–3.012	–3.012	–3.201	–3.201	15.36		21.80	
0.650		–2.878		–3.039				
0.660	–2.758	–2.758	–2.878	–2.878	14.62		20.50	
0.670		–2.636		–2.729				
0.680	–2.524	–2.524	–2.579	–2.579	13.89		19.30	
0.690		–2.411		–2.441				
0.700	–2.303	–2.303	–2.303	–2.303	13.19		18.10	
0.720	–2.093		–2.061		12.49		17.00	
0.740	–1.895		–1.842		11.84		16.00	
0.760	–1.709		–1.623		11.20		14.90	
0.780	–1.531		–1.428		10.57		13.90	
0.800	–1.363		–1.255		9.97		13.00	
0.820	–1.202		–1.094		9.37		12.10	
0.840	–1.048		–0.933		8.79		11.20	
0.860	–0.900		–0.794		8.19		10.30	
0.880	–0.760		–0.656		7.58		9.39	
0.900	–0.622		–0.530		6.95		8.53	
0.920	–0.488		–0.414		6.23		7.54	
0.940	–0.359		–0.306		5.44		6.51	
0.950	–0.297		–0.251		5.00		5.96	
0.960	–0.235		–0.198		4.52		5.39	
0.970	–0.175		–0.147		4.00		4.72	
0.980	–0.115		–0.097		3.38		3.91	
0.990	–0.058		–0.048		2.57		2.83	
1.000	0.000		0.000		0.00		0.00	
1 J = 4.1868 cal								

Table 2. Experimental data reported in the literature and the results of prediction

Substance	Ref.	n	T_b [K]	T_c [K]	p_c [bar]	ω [1]	ΔT [K]	PLCHPCK		P	SMK
								ω_{cal} [1]	p_{av} [%]	p_{av} [%]	p_{av} [%]
1,2,3–trimethylbenzene	[5]	1	449.3	665.3	35.2	0.366	298.15	0.368	0.83	0.79	0.35
1,2,4–trimethylbenzene	[5]	1	442.5	649.1	32.3	0.376	298.15	0.376	0.49	0.79	0.47
1,2–dimethylbenzene	[5]	1	417.6	630.3	37.3	0.310	298.15	0.310	0.55	1.26	0.40
1,2–dimethylcyclohexane,cis	[6]	2	402.9	606.0	29.6	0.236	369.85–386.85	0.241	3.75	4.15	2.77
1,2–dimethylcyclohexane,cis	[5]	1					298.15		4.60	5.18	4.79
1,2–dimethylcyclohexane,trans	[6]	2	396.6	596.0	29.0	0.242	373.25–387.25	0.237	3.96	3.46	1.93
1,2–dimethylcyclohexane,trans	[5]	1					298.15		3.99	3.43	2.92
1,3,5–trimethylbenzene	[7]	1	437.9	638.6	31.6	0.399	298.15	0.394	0.71	0.07	1.40
1,3,5–trimethylbenzene	[5]	1					298.15		0.91	0.13	1.60
1,3–dimethylbenzene	[5]	1	412.3	617.1	35.4	0.325	298.15	0.325	0.22	0.84	0.20
1,3–dimethylcyclohexane,cis	[6]	2	393.3	591.0	29.6	0.224	361.15–384.95	0.244	3.96	5.99	4.65
1,3–dimethylcyclohexane,cis	[5]	1					298.15		4.01	6.06	5.68
1,3–dimethylcyclohexane,trans	[6]	3	397.6	598.0	29.7	0.189	340.65–376.45	0.242	1.48	6.77	5.87
1,3–dimethylcyclohexane,trans	[5]	1					298.15		5.02	10.44	10.40
1,3–dimethylcyclopentane,cis	[8]	3	363.9	551.0	34.0	0.272	322.62–363.93	0.265	0.51	0.19	1.81
1,4–dimethylbenzene	[9]	7	411.5	616.2	35.1	0.321	347.77–439.48	0.320	0.42	0.55	1.38
1,4–dimethylbenzene	[5]	1					298.15		0.29	0.77	0.24
1,4–dimethylcyclohexane,cis	[5]	1	397.5	598.0	29.7	0.234	298.15	0.241	4.71	5.47	5.05
1,4–dimethylcyclohexane,trans	[5]	1	392.5	587.7	29.7	0.242	298.15	0.259	2.32	4.08	3.53
1–butene	[10]	6	266.9	419.6	40.2	0.187	202.31–266.72	0.190	1.13	1.23	1.07
1–butyne	[11]	6	281.2	440.0	46.0	0.245	262.53–282.52	0.247	1.36	1.52	0.48
1–cyclohexyldecane	[12]	1	570.8	750.0	15.4	0.583	298.15	0.641	5.68	13.05	11.14

Substance	Ref.	n	T_b [K]	T_c [K]	p_c [bar]	ω [1]	ΔT [K]	PLCHPCK		P	SMK
								ω_{cal} [1]	p_{av} [%]	p_{av} [%]	p_{av} [%]
1–methyl–1–ethylcyclopentane	[9]	8	394.7	592.0	30.0	0.250	332.00–422.44	0.256	3.50	4.29	2.77
1–pentene	[13]	3	303.1	464.7	35.3	0.245	283.96–303.13	0.233	1.12	0.18	1.75
2,2,3–trimethylbutane	[5]	1	354.0	531.1	29.5	0.250	298.15	0.249	1.56	1.13	0.10
2,2,3–trimethylbutane	[14]	2					313.83–353.95		1.41	1.37	0.17
2,2,3–trimethylpentane	[5]	1	383.0	563.5	27.3	0.297	298.15	0.297	1.81	1.82	0.72
2,2,4–trimethylpentane	[15]	4	372.4	543.8	25.7	0.303	298.15–353.15	0.305	1.38	1.58	0.16
2,2,4–trimethylpentane	[5]	1					298.15		1.33	1.43	0.16
2,2,5–trimethylhexane	[5]	1	397.2	569.8	23.3	0.357	298.15	0.343	3.89	2.81	1.39
2,2–dimethylbutane	[16]	3	322.8	489.0	31.0	0.232	296.05–322.85	0.231	1.41	1.22	0.19
2,2–dimethylbutane	[5]	1					298.15		1.48	1.13	0.17
2,2–dimethylhexane	[5]	1	380.0	549.8	25.3	0.338	298.15	0.339	2.20	2.35	0.93
2,2–dimethylpentane	[5]	1	352.4	520.5	27.7	0.287	298.15	0.287	1.76	1.55	0.22
2,3,3–trimethylpentane	[5]	1	387.9	573.5	28.2	0.290	298.15	0.290	0.84	0.85	0.16
2,3,4–trimethylpentane	[17]	2	386.6	566.4	27.3	0.315	361.45–386.25	0.315	2.36	2.80	0.78
2,3,4–trimethylpentane	[5]	1					298.15		1.34	1.43	0.22
2,3,5–trimethylhexane	[5]	1	404.5	579.2	24.0	0.364	298.15	0.364	2.46	2.88	1.46
2,3–dimethyl–2–butene	[18]	4	346.4	524.0	33.6	0.239	292.13–346.37	0.264	3.17	5.64	4.39
2,3–dimethylbutane	[19]	4	331.1	499.9	31.5	0.247	295.95–331.14	0.249	1.17	1.31	0.16
2,3–dimethylbutane	[5]	1					298.15		1.20	1.12	0.15
2,3–dimethylbutene	[20]	4					293.15–353.15		0.69	1.12	0.60
2,3–dimethylhexane	[17]	1	388.8	563.5	26.3	0.346	388.35	0.347	1.64	2.56	0.22
2,3–dimethylhexane	[5]	1					298.15		1.66	1.97	0.57
2,3–dimethylpentane	[15]	4	362.9	537.5	29.1	0.296	298.15–353.15	0.294	1.55	1.41	0.21
2,3–dimethylpentane	[5]	1					298.15		1.58	1.28	0.01
2,4–dimethylhexane	[5]	1	382.6	553.5	25.6	0.343	298.15	0.344	1.93	2.16	0.73
2,4–dimethylpentane	[5]	1	353.6	519.8	27.4	0.302	298.15	0.302	1.80	1.66	0.25
2,5–dimethylhexane	[5]	1	382.3	550.0	24.9	0.356	298.15	0.358	1.77	2.10	0.57
2,6–dimethylnaphthalene	[21]	5	535.2	777.2	32.2	0.443	383.32–420.00	0.421	1.06	2.34	4.30
2,7–dimethylnaphthalene	[21]	5	536.2	775.0	32.3	0.440	368.81–400.00	0.446	1.61	0.12	1.88
2–butene,cis	[22]	7	276.9	435.6	42.0	0.202	246.18–292.25	0.201	1.77	1.45	0.37
2–cyclohexyl–2–methylpropane	[23]	4	444.7	659.0	26.6	0.252	328.15–368.15	0.258	6.84	7.32	6.55
2–cyclopentylpropan	[5]	1	399.6	601.0	30.0	0.240	298.15	0.246	4.56	5.23	4.78
2–methyl–1–butene	[13]	3	304.3	465.0	34.5	0.236	277.96–304.32	0.237	2.14	2.18	0.72
2–methyl–2–butene	[13]	3	311.7	470.0	34.5	0.244	289.00–311.73	0.286	0.29	4.07	2.55
2–methyl–3–ethylpentane	[17]	1	388.8	567.1	27.0	0.330	388.15	0.330	1.47	2.18	0.08
2–methyl–3–ethylpentane	[5]	1					298.15		1.78	1.91	0.62
2–methylbutane	[13]	3	301.0	460.4	33.8	0.227	279.48–301.01	0.226	0.85	0.77	0.70
2–methylbutane	[24]	2					293.92–293.98		0.14	0.23	1.74
2–methylheptane	[15]	4	390.8	559.7	25.0	0.378	298.15–353.15	0.381	1.40	1.87	0.38
2–methylheptane	[5]	1					298.15		1.62	2.18	0.59
2–methylhexane	[15]	4	363.2	530.4	27.4	0.329	298.15–353.15	0.330	1.36	1.64	0.32
2–methylpentane	[19]	3	333.4	497.7	30.4	0.278	298.15–333.45	0.279	1.09	1.38	0.34
2–methylpentane	[20]	4					293.15–353.15		0.87	1.33	0.97
2–methylpentane	[5]	1					298.15		1.18	1.15	0.31
2–phenylpropane	[5]	1	425.6	631.0	32.1	0.335	298.15	0.327	2.39	2.47	1.44
3,3–dimethylhexane	[5]	1	385.1	562.0	26.5	0.320	298.15	0.320	1.53	1.59	0.33
3,3–dimethylpentane	[5]	1	359.2	536.4	29.5	0.267	298.15	0.267	1.18	0.91	0.19
3,4–dimethylhexane	[17]	1	390.9	568.8	26.9	0.338	390.45	0.339	1.42	2.26	0.04
3,4–dimethylhexane	[5]	1					298.15		1.61	1.88	0.55
3–ethylhexane	[17]	1	391.7	565.5	26.1	0.361	391.35	0.362	1.47	2.40	0.02
3–ethylhexane	[5]	1					298.15		1.87	2.21	0.73
3–ethylpentane	[5]	1	366.6	540.6	28.9	0.310	298.15	0.310	1.96	1.87	0.55
3–methyl–3–ethylpentane	[17]	1	391.4	576.5	28.1	0.303	391.15	0.304	1.14	1.84	0.27
3–methyl–3–ethylpentane	[5]	1					298.15		0.65	0.86	0.22
3–methylheptane	[5]	1	392.1	563.6	25.5	0.370	298.15	0.372	1.82	2.32	0.78
3–methylhexane	[15]	4	365.2	535.3	28.1	0.323	298.15–353.15	0.324	1.32	1.55	0.25
3–methylpentane	[15]	4	336.4	504.6	31.2	0.272	298.15–353.15	0.270	1.12	1.16	0.58
3–methylpentane	[19]	3					303.25–336.45		1.27	1.22	0.48
3–methylpentane	[25]	1					298.15		1.19	0.77	0.60
3–methylpentane	[5]	1					298.15		1.37	0.96	0.42
4–methylheptane	[15]	4	390.9	561.7	25.4	0.371	298.15–353.15	0.372	1.82	2.10	0.41

Substance	Ref.	n	T_b [K]	T_c [K]	p_c [bar]	ω [1]	ΔT [K]	PLCHPCK		P	SMK
								ω_{cal} [1]	p_{av} [%]	p_{av} [%]	p_{av} [%]
4–methylheptane	[5]	1					298.15		1.94	2.31	0.76
benzene	[26]	3	353.2	562.1	48.9	0.209	314.75–353.25	0.210	2.50	2.25	1.23
benzene	[27]	4					298.15–353.25		2.65	2.40	1.49
benzene	[28]	6					298.15–353.25		2.63	2.36	1.42
benzene	[16]	4					314.75–353.25		2.56	2.27	1.29
benzene	[29]	1					298.15		3.20	2.90	2.42
benzene	[30]	7					298.10–377.58		2.43	2.25	1.30
benzene	[5]	1					298.15		3.04	2.74	2.26
butylcyclohexane	[12]	1	454.1	667.0	31.5	0.362	298.15	0.360	1.60	2.83	1.75
butylcyclopentane	[23]	4	429.8	621.2	27.6	0.372	328.15–368.15	0.380	0.36	1.15	0.68
cyclohexane	[15]	6	353.8	553.8	40.8	0.212	298.15–353.15	0.209	2.65	2.00	0.93
cyclohexane	[28]	5					313.15–353.85		2.75	2.08	0.98
cyclohexane	[25]	1					298.15		2.88	2.09	1.51
cyclohexane	[31]	3					291.73–292.94		4.16	3.43	2.95
cyclohexane	[6]	2					327.25–346.45		2.34	1.68	0.52
cyclohexane	[5]	1					298.15		2.92	2.13	1.55
cyclohexane	[32]	5					293.15–353.85		2.55	1.90	0.94
cyclopentane	[8]	3	322.4	511.7	45.1	0.196	298.16–322.42	0.195	1.61	1.10	0.11
cyclopentane	[33]	3					295.01–295.70		3.97	3.30	2.51
decane	[25]	1	447.3	617.6	21.1	0.489	298.15	0.494	2.57	4.30	2.32
decane	[5]	1					298.15		2.53	4.26	2.28
decane	[34]	10					344.26–444.26		1.33	2.30	0.78
ethylbenzene	[9]	9	409.3	617.2	36.1	0.302	345.96–437.22	0.302	1.25	1.47	0.37
ethylbenzene	[5]	1					298.15		1.60	2.12	1.26
ethylcyclohexane	[23]	5	404.9	609.0	30.0	0.243	313.15–368.15	0.246	5.12	5.14	4.19
ethylcyclohexane	[5]	1					298.15		5.21	5.62	5.20
ethylcyclopentane	[23]	5	376.6	569.5	34.0	0.271	313.15–368.15	0.270	1.68	1.47	0.20
heptane	[14]	3	371.6	540.1	27.4	0.350	331.21–363.63	0.351	1.27	1.76	0.32
heptane	[15]	4					298.15–353.15		1.52	1.80	0.24
heptane	[5]	1					298.15		1.63	1.81	0.27
heptane	[35]	8					288.16–371.51		1.46	1.95	0.30
heptane	[36]	1					310.93		1.87	2.00	0.33
hexane	[15]	4	341.9	507.6	30.2	0.298	298.15–353.15	0.299	1.36	1.70	0.17
hexane	[16]	4					298.15–341.85		1.43	1.66	0.18
hexane	[20]	4					298.15–353.15		0.62	0.87	1.08
hexane	[5]	1					298.15		1.61	1.55	0.06
hexane	[37]	13					310.93–444.26		0.39	1.23	1.23
methylbenzene	[5]	1	383.8	591.8	42.3	0.263	298.15	0.272	0.23	1.28	0.58
methylcyclohexane	[15]	4	374.1	572.2	34.8	0.236	298.15–353.15	0.236	1.88	1.61	0.63
methylcyclohexane	[25]	1					298.15		1.96	1.76	1.14
methylcyclohexane	[5]	1					298.15		1.87	1.67	1.05
methylcyclopentane	[8]	3	345.0	532.7	37.9	0.231	304.09–344.97	0.231	1.64	1.49	0.26
methylcyclopentane	[5]	1					298.15		1.79	1.41	0.52
nonane	[5]	1	424.0	594.6	22.9	0.445	298.15	0.448	2.15	3.25	1.43
octane	[15]	4	398.8	568.8	24.9	0.400	298.15–353.15	0.399	1.81	2.01	0.32
octane	[25]	1					298.15		2.04	2.41	0.73
octane	[17]	2					373.65–398.45		1.40	2.11	0.38
octane	[5]	1					298.15		1.92	2.29	0.61
octane	[36]	11					310.93–444.26		0.85	1.33	1.14
pentane	[38]	16	309.2	469.8	33.7	0.251	301.09–366.48	0.249	0.93	1.60	0.47
pentane	[5]	1					298.15		1.16	0.99	0.60
pentane	[39]	11					310.93–427.59		0.51	1.00	1.40
propane	[38]	16	231.1	369.8	42.5	0.154	312.82–348.15	0.153	2.85	2.60	1.31
propylbenzene	[5]	1	432.4	638.4	32.0	0.344	298.15	0.344	1.43	2.42	1.35
propylcyclohexane	[12]	1	429.9	639.0	28.0	0.258	298.15	0.266	7.07	8.35	7.97
propylcyclohexane	[5]	1					298.15		6.88	8.15	7.77
propylcyclopentane	[5]	1	404.1	596.2	30.0	0.335	298.15	0.322	1.69	0.85	0.35
undecane	[25]	1	469.1	638.7	19.5	0.530	298.15	0.537	3.43	5.69	3.58
P_{av} [%]		397							1.81	2.11	1.28

From the results presented in Table 2 it may be concluded that the expressions derived by Sivaraman et al. [4] (Eqs. 3–5) have the best predictive characteristics.

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IZVOD

ODREĐIVANJE TOPLOTE ISPARAVANJA NA BAZI PRINCIPA KORESPONDENTNIH STANJA

(Naučni rad)

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U ovom radu razmotrene su mogućnosti predskazivanja vrednosti toplote isparavanja na bazi principa korespondentnih stanja. Prikazane su predložene funkcije $\Delta S^{(0)}$ i $\Delta S^{(1)}$, kako u diskretnoj, tako i u analitičkoj formi. Diskretne vrednosti su korelisanjem prevedene u analitičke izraze. Predskazivanje vrednosti toplote isparavanja testirano je na podacima za 80 nepolarnih supstanci sa ukupno 397 eksperimentalnih vrednosti. Najbolje prediktivne osobine pokazao je model, koji su predložili Sivaraman, Magee i Kobayashi.

Ključne reči: Toplota isparavanja, Faktor acentričnosti, Princip korespondentnih stanja, Nepolarne supstance.