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A correlation for heat of vaporization of pure compounds

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Abstract−Twenty-seven selected equations were tested on 162 compounds with 1958 calorimetric data for their abilities to reflect the temperature influence on the heat of vaporization of pure compounds. A new equation is recommended (overall percent deviation 0.27% and percent deviation 0.59% above $0.9T_r$).

Key words: Heat of Vaporization, Correlation, Pure Compound, Equation, Calorimetric Data

INTRODUCTION

In many calculations associated with process design and simulations it is necessary to know the physical properties of pure compounds, including their heat of vaporization [1-3]. Although many equations have been developed, the problem of the correlation of heat of vaporization for pure compounds has not been fully addressed yet. Most of the recommended equations very well correlate heat of vaporization data in a limited temperature range near the normal boilinig point. On the other hand, due to thermal degradation it is difficult to measure heat of vaporization at elevated temperatures. As a result, experimental data in the temperature range $0.9 \le T_r \le 1$ are scarce [4,5] and testing and development of correlation equations over the full temperature range $T_t \le T \le T_c$ has been limited. The objective of this work is to investigate the performance of the recommended equations with respect to the correlation of calorimetrically measured heats of vaporization and to develop a new equation.

EXISTING EQUATIONS

Correlation equations listed in chronological order are presented in Table 1. The number of parameters varies from one to six. All equations are linear in the parameters or can be linearized except the Lin-Silberberg-McKetta and Vetere equations. Preliminary investigation indicates that these nonlinear equations do not result in a significantly better correlation than linear equations with the same number of parameters. As the problem of convergence and global optima arises in correlation with nonlinear equations, this work investigates only linear equations.

DATA SELECTION

In all, 1958 experimental calorimetric data for 162 compounds, presented in Table 2, are selected from the database with 819 compounds and 3415 data points. Table 2 lists only compounds with at least five experimental data, as that number of data enables realistic correlation by equations with one, two or three parameters (minimum number of data is n=m+2). Used experimental normal freezing points and critical temperatures are also included in Table 2. Columns 6 and 7 in Table 2 contain temperature and reduced temperature intervals of the selected data points. The last column of Table 2 lists references for selected experimental calorimetric heats of vaporization.

It is obvious from Table 2 that most reduced temperatures fall between 0.45-0.65, which is away from both triple and critical temperature. Heat of vaporization has a maximum value at triple point and a zero value at critical point. Heat of vaporization rapidly decreases to zero in the vicinity of the critical point and correlation in this region is very difficult.

RESULTS AND DISCUSSION

Results of correlation are presented in Table 3. The number of parameters is shown in the third column, number of compounds in the fourth column, number of data in the fifth column and absolute mean percent deviation in the sixth column. The absolute mean percent deviation is defined as

$$p_{abs}[\%] = 100\left|(\Delta H_{v,exp} - \Delta H_{v,cal})/\Delta H_{v,exp}\right| \quad (1)$$

$$p_{av}[\%] = \left(\sum_{i=1}^{N} p_{abs,i}\right)/N \quad (2)$$

Torquato-Stell and Armstrong equations are used with only first four parameters as preliminary investigation indicated that these equations yield the best results with the first four parameters. In the Somayajulu II equation, normal freezing point, T_f, is used instead a triple point, T_t, as this value is more common.

All 1958 data for 162 selected compounds were correlated with all equations with one, two and three parameters. Equations with four parameters were used for 131 compounds and 1801 data points with n≥6. In absence of experimental values of normal freezing point for some compounds, the Somayajulu II equation was used for only 125 compounds and 1733 data points. For the Guermouche-Vergnaud, Todd-Hossenlopp-Scott, Svoboda and Xiang equations, data correlation of certain compounds was not successfull (ordinal number of compounds is given in parentheses).

Results presented in Table 3 indicate that all equations, except Mollier, Thiesen, Pilling, Tyrer and Eggert equations, are excellent in correlation of selected heats of vaporization (average mean percent deviation is less or equal to 1%). The best are Guermouche-

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Table 1. Recommended heat of vaporization correlation equations

i	Author	Equation
1	Mollier [6]	$\Delta H_v = A[T(1-T_r)]^B$
2	Thiesen [7]	$\Delta H_v = A(1-T_r)^{1/3}$
3	Pilling [8]	$\Delta H_v = A/T^{1/2}$
4	Tyrer [9]	$\Delta H_v = A(1-T_r)^{0.5}$
5	Kendall [10]	$\Delta H_v = A(1-T_r)^{0.386}$
6	Osborne-van Dusen [11]	$\Delta H_v = A(1-T_r)^{1/2} + B(1-T_r)$
7	Keyes-Taylor-Smith [12]	$\ln(\Delta H_v) = A + B(1-T_r) + C\ln(1-T_r)$
8	Winter [13]	$\Delta H_v = A(1-T_r)^{0.4}$
9	Nutting [14]	$\Delta H_v = A(1-T_r)^B$
10	Eggert [15]	$\Delta H_v = A(1-T_r)$
11	Jones-Bowden [16]	$\Delta H_v = A(1-T_r)^{7/18}$
12	Silverberg-Wenzel [17]	$\Delta H_v = A(1-T_r)^{0.378}$
13	Graue-Berry-Sage I [18]	$\Delta H_v = A(1-T_r)^{1/3} + B(1-T_r)^{2/3}$
14	Graue-Berry-Sage II [18]	$\Delta H_v = A(1-T_r)^{1/3} + B(1-T_r)^{2/3} + C(1-T_r)$
15	Lin-Silberberg-McKetta [19]	$\Delta H_v = A(T_c-T) + B(T_c-T)^2 + C(T_c-T)^D$
16	Chueh-Swanson [20,21]	$\Delta H_v = A(1-T_r)^{B+C(1-T_r)}$
17	Guermouche-Vergnaud [22]	$\Delta H_v = A(1-T_r)^{B+CT_r+DT_r^2}$
18	Todd-Hossenlopp-Scott [23]	$\ln(\Delta H_v) = A + B\ln[1/(1-T_r)] + C\ln[1/(1-T_r)]^{1/3} + D\ln[1/(1-T_r)]^{2/3}$
19	Radosz-Lydersen [24]	$\Delta H_v = A(1-T_r)^{1/3} + B(1-T_r)^{2/3} + C(1-T_r)^{5/3} + D(1-T_r)^2$
20	Tekač-Majer-Svoboda-Hynek [25]	$\Delta H_v = A(1-T_r)^B \exp(-BT_r)$
21	Torquato-Stell [26]	$\Delta H_v = A(1-T_r)^{1/3} + B(1-T_r)^{5/6} + C(1-T_r)^{29/24} + \sum_{j=1}^{m} D_j(1-T_r)^j,\ m \le 3$
22	Armstrong [27]	$\Delta H_v = A(1/T_r-1)^{1/3} + B(1/T_r-1) + C(1/T_r-1)^{4/3} + D(1/T_r-1)^{5/3} + E(1/T_r-1)^2 + F(1/T_r-1)^{19/3}$
23	Vetere [28]	$\Delta H_v/RT_c = A + BT_r + CT_r^D$
24	Somayajulu I [29]	$\Delta H_v = A(1/T_r-1) + B(1-T_r)^{3/8} + C(1-T_r)^{18/8}$
25	Somayajulu II [29]	$\Delta H_v = AX_t^{3/8} + BX_t^{11/8} + CX_t^{19/8} + DX_t^{27/8},\ X_t = (T_c-T)/(T_c-T_t)$
26	Svoboda [30]	$\Delta H_v = A + B\ln[1/(1-T_r)] + C\ln[1/(1-T_r)]^{1/3} + D\ln[1/(1-T_r)]^{2/3}$
27	Xiang [31]	$\Delta H_v/RT_c = [A(1/T_r-1) + B(1-T_r)]/[1 + C(1-T_r)]$

Table 2. Survey of experimental calorimetric heats of vaporization

i	Compound	n	T_f [K]	T_c [K]	ΔT [K]	ΔT_r [1]	Reference
1	1,1,1-Trichloroethane	12	240.0	545.0	284.34-358.15	0.52-0.66	[32], [33], [34], [35], [36]
2	1,1,1-Trichlorotrifluoroethane	5	287.5	482.9	298.15-328.15	0.61-0.68	[37]
3	1,1,2,2-Tetrachloroethane	9	237.0	661.2	298.15-419.35	0.45-0.63	[33], [34], [38], [39], [40]
4	1,1,2-Trichloroethane	9	235.8	606.0	298.15-358.48	0.49-0.59	[33], [34], [41]
5	1,2-Dibromo-1-chlorotrifluoroethane	5	182.7	560.7	298.15-358.15	0.53-0.64	[42]
6	1,2-Dibromomethane	6	282.9	646.0	298.15-338.15	0.46-0.52	[43], [44]
7	1,2-Dichloroethane	11	237.5	566.0	293.15-358.15	0.52-0.63	[34], [44], [45], [46], [47]
8	1,2-Dichlorotetrafluoroethane	5	297.9	551.0	308.15-338.15	0.56-0.61	[43]
9	1,2-Dimethylbenzene	11	248.2	630.3	298.15-445.80	0.47-0.71	[38], [48], [49]
10	1,4-Dimethylbenzene	23	286.4	616.2	298.15-557.25	0.48-0.90	[38], [49], [50], [51]
11	1-Bromo-1-chloro-2,2,2-trifluoroethane	6	157.4	496.3	298.15-343.15	0.60-0.69	[37]
12	1-Bromobutane	8	160.4	569.4	298.15-372.55	0.52-0.65	[44], [52], [53], [54]
13	1-Bromopropane	7	163.0	535.5	298.15-352.35	0.56-0.66	[44], [52], [53], [54]
14	1-Butanol	20	188.0	562.0	298.15-500.80	0.53-0.89	[24], [54], [55], [56], [57], [58], [59]
15	1-Butene	14	87.7	419.6	202.31-377.61	0.48-0.90	[60], [61]
16	1-Butyne	6	147.3	440.0	262.53-282.52	0.60-0.64	[62]
17	1-Decanol	20	280.1	687.3	281.50-338.41	0.41-0.49	[59], [63], [64]

Table 2. Continued

i	Compound	n	T_f [K]	T_c [K]	ΔT [K]	ΔT_r [1]	Reference
18	1-Dodecanol	14	297.1	719.4	298.15-348.30	0.41-0.48	[63], [64], [65]
19	1-Hexadecanol	12	322.4	770.0	327.90-362.40	0.43-0.47	[63]
20	1-Hexanol	19	226.0	610.3	298.15-368.15	0.49-0.60	[54], [63], [65], [66]
21	1-Chloro-3-methylbutane	6	169.0	558.9	298.15-368.15	0.53-0.66	[25]
22	1-Chlorobutane	8	150.1	542.0	298.15-368.15	0.55-0.68	[25], [44], [52]
23	1-Chloropentane	7	174.0	552.0	298.15-378.15	0.54-0.68	[25], [44], [52]
24	1-Methyl-1-ethylcyclopentane	8	129.3	592.0	332.00-422.44	0.56-0.71	[50]
25	1-Octanol	15	257.6	652.5	282.30-469.15	0.43-0.72	[63], [67]
26	1-Octene	6	171.4	567.0	298.15-368.15	0.53-0.65	[65], [68]
27	1-Pentanol	14	195.0	586.1	298.15-499.65	0.51-0.85	[24], [54], [66], [69]
28	1-Propanol	32	146.9	536.7	298.15-499.05	0.56-0.93	[24], [41], [54], [57], [58], [59], [70], [71], [72]
29	1-Tetradecanol	14	312.6	743.0	298.15-346.60	0.40-0.47	[63], [65]
30	1-Tridecanol	23	305.6	732.0	307.00-348.30	0.42-0.48	[63]
31	1-Undecanol	14	292.0	703.6	313.20-354.30	0.45-0.50	[63]
32	2,2,3-Trimethylpentane	9	160.9	563.5	298.15-368.15	0.53-0.65	[73]
33	2,2,4-Trimethylpentane	12	165.8	543.8	298.15-372.33	0.55-0.68	[49], [68], [74], [75]
34	2,2-Dimethyl-1-propanol	22	327.0	549.0	274.20-312.30	0.50-0.57	[76]
35	2,2-Dimethyl-3-butanone	7	223.4	562.9	308.15-348.15	0.55-0.62	[77]
36	2,2-Dimethylpentane	10	149.4	520.5	298.15-368.15	0.57-0.71	[49], [73]
37	2,2-Dimethylpropane	9	256.6	433.8	264.81-303.50	0.61-0.70	[78], [79]
38	2,3,3-Trimethylpentane	10	172.5	573.5	298.15-368.15	0.52-0.64	[49], [73]
39	2,3,4-Trimethylpentane	10	163.9	566.4	298.15-413.76	0.53-0.73	[49], [79], [80]
40	2,3-Dimethylbutane	9	144.6	499.9	293.15-353.15	0.59-0.71	[49], [81], [82]
41	2,3-Dimethylpentane	5	149.0	537.5	298.15-353.15	0.55-0.66	[49], [74]
42	2,3-Dimethylpyridine	5	257.9	655.5	313.15-368.15	0.48-0.56	[83]
43	2,4-Dimethylpentane	8	154.0	519.8	298.15-348.15	0.57-0.67	[49], [73]
44	2,4-Dimethylpyridine	5	209.4	647.0	313.15-368.15	0.48-0.57	[83]
45	2,6-Dimethylnaphthalene	5	383.3	777.2	383.32-420.00	0.49-0.54	[84]
46	2,6-Dimethylpyridine	5	267.1	623.8	313.15-368.15	0.50-0.59	[83]
47	2,7-Dimethylnaphthalene	5	368.8	775.0	368.81-400.00	0.48-0.52	[84]
48	2-Bromopropane	7	184.2	532.0	298.15-337.65	0.56-0.63	[44], [52], [53], [54]
49	2-Butanol	15	158.5	536.1	298.15-503.05	0.56-0.94	[24], [38], [52], [57], [85]
50	2-Butanone	15	186.5	535.5	298.15-370.57	0.56-0.69	[86], [87], [88], [89], [90]
51	2-Butanethiol	5	133.0	551.0	298.16-358.14	0.54-0.65	[91], [92]
52	2-Butene,trans	18	167.6	428.6	272.44-394.26	0.64-0.92	[93], [94]
53	2-Hexanol	18	-	583.0	274.50-368.15	0.47-0.63	[66], [76]
54	2-Hexanone	12	216.2	586.6	298.15-368.15	0.51-0.63	[77], [90]
55	2-Chloro-1,1,2-trifluoroethyl ethyl ether	6	-	524.4	298.15-368.15	0.57-0.70	[95]
56	2-Chlorobutane	5	141.8	520.6	298.15-358.15	0.57-0.69	[25], [44]
57	2-Methyl-1-pentanol	14	-	604.4	275.10-313.20	0.46-0.52	[76]
58	2-Methyl-1-propanol	18	165.2	547.7	298.15-498.85	0.54-0.91	[24], [54], [57], [69], [96]
59	2-Methyl-2-butanol	25	264.4	545.1	274.30-444.25	0.50-0.81	[24], [66], [76]
60	2-Methyl-2-pentanol	6	170.2	559.5	298.15-368.15	0.53-0.66	[66]
61	2-Methyl-2-propanol	20	298.0	506.2	298.15-440.55	0.59-0.87	[24], [54], [57], [96], [97], [98]
62	2-Methyl-3-pentanol	13	-	576.0	274.90-307.50	0.48-0.53	[76]
63	2-Methylbutane	5	113.3	460.4	279.48-301.01	0.61-0.65	[99], [100]
64	2-Methylheptane	5	164.2	559.7	298.15-353.15	0.53-0.63	[49], [74]
65	2-Methylpentane	8	119.5	497.7	293.15-353.15	0.59-0.71	[49], [81], [82]
66	2-Methylpyridine	9	207.0	621.0	298.15-402.54	0.48-0.65	[101], [102]
67	2-Pentanol	6	-	560.0	298.15-368.15	0.53-0.66	[66]
68	2-Pentanone	11	196.3	561.1	298.15-394.57	0.53-0.70	[86], [88], [90]

Table 2. Continued

i	Compound	n	T_f [K]	T_c [K]	ΔT [K]	ΔT_r [1]	Reference
69	2-Propanol	32	184.7	508.3	298.15-477.03	0.59-0.94	[24], [38], [41], [54], [57], [72], [103], [104], [105]
70	3,3-Dimethyl-2-butanone	5	223.4	562.9	298.15-378.44	0.53-0.67	[86], [87], [106]
71	3,5-Dimethylpyridine	5	267.3	667.7	313.15-368.15	0.47-0.55	[83]
72	3-Ethylpentane	8	154.6	540.6	298.15-348.15	0.55-0.64	[49], [73]
73	3-Hexanone	8	217.5	583.2	298.15-396.65	0.51-0.68	[90], [107]
74	3-Methyl-1-butanol	10	156.0	577.2	303.15-496.80	0.53-0.86	[24], [38], [42]
75	3-Methyl-2-butanol	9	203.0	556.1	280.30-301.40	0.50-0.54	[76], [108]
76	3-Methyl-2-butanone	7	181.0	553.0	298.15-367.48	0.54-0.66	[86], [90], [107]
77	3-Methyl-3-pentanol	11	249.5	575.6	275.20-301.50	0.48-0.52	[76]
78	3-Methylpentane	10	110.3	504.6	298.15-353.15	0.59-0.70	[49], [74], [82], [109], [110]
79	3-Methylpyridine	9	255.0	645.0	298.15-417.29	0.46-0.65	[101], [111]
80	3-Pentanone	10	234.2	561.5	298.15-375.11	0.53-0.67	[86], [90], [107], [112]
81	4-Methyl-2-pentanol	11	-	603.5	273.70-301.30	0.45-0.50	[66], [76]
82	4-Methyl-2-pentanone	8	189.2	571.4	298.15-388.62	0.52-0.68	[87], [90]
83	4-Methylheptane	6	152.2	561.7	298.15-390.35	0.53-0.69	[38], [49], [74]
84	4-Methylpyridine	13	276.9	646.0	298.15-434.26	0.46-0.67	[101], [113]
85	Acenaphthene	6	366.6	803.2	366.56-410.00	0.46-0.51	[84]
86	Acetone (2-propanone)	15	178.5	508.2	293.15-505.20	0.58-0.99	[45], [114], [115], [116]
87	Ammonia	34	195.4	405.5	231.14-324.95	0.57-0.80	[11]
88	Benzene	59	278.7	562.1	293.15-560.93	0.52-1.00	[23], [38], [41], [45], [46], [49], [58], [70], [117], [118], [119], [120], [121], [122], [123], [124]
89	Benzenethiol	5	258.0	685.0	298.15-416.90	0.43-0.61	[125], [126]
90	Butylamine	5	222.7	531.9	298.15-358.15	0.56-0.67	[127], [128]
91	Butyl ethanoate	7	199.7	575.4	298.15-397.35	0.52-0.69	[54], [56], [67], [129]
92	Butyl isopropylamine	5	-	563.6	298.15-358.15	0.53-0.64	[130]
93	Butyl methanoate	7	183.2	565.2	298.15-378.27	0.53-0.67	[38], [129], [131]
94	Cyclohexane	47	279.6	553.8	291.73-427.62	0.53-0.77	[38], [49], [58], [72], [74], [109], [110], [127], [132], [133], [134], [135], [136], [137], [138], [139], [140], [141], [142]
95	Cyclohexanone	8	242.6	664.3	298.15-348.15	0.45-0.52	[77], [143]
96	Cyclohexene	6	169.7	553.5	313.15-354.75	0.57-0.64	[38], [58]
97	Cyclopentane	7	179.3	511.8	295.01-322.42	0.58-0.63	[140], [144], [145]
98	Decane	24	243.5	617.6	298.15-444.26	0.48-0.72	[49], [59], [109], [110], [125], [127], [135], [146], [147]
99	Dibenzothiophene	5	371.8	897.0	590.00-630.00	0.66-0.70	[148]
100	Diborane	18	108.0	289.8	179.79-284.01	0.62-0.98	[149], [150]
101	Dibutyl ether	6	175.3	580.0	298.15-414.45	0.51-0.71	[52], [151]
102	Diethylamine	5	223.2	496.6	298.15-343.15	0.60-0.69	[128], [152]
103	Diethyl ether	8	156.9	466.7	280.69-313.15	0.60-0.67	[38], [67], [151], [153]
104	Diphenyl	19	342.4	789.0	298.15-755.35	0.38-0.96	[154], [155], [156]
105	Diisopropylamine	6	212.2	523.1	298.15-358.15	0.57-0.68	[130], [152]
106	Diisopropyl ether	8	187.7	500.3	298.15-358.15	0.60-0.72	[151], [157]
107	Dipropyl ether	9	151.0	530.6	298.15-363.22	0.56-0.68	[134], [151], [158]
108	Ethanal	9	149.7	461.0	294.15-422.04	0.64-0.92	[117], [159]
109	Ethanol	33	159.1	514.0	298.15-508.71	0.58-0.99	[24], [54], [57], [69], [72], [97], [105], [108], [122], [160]
110	Ethylbenzene	14	178.2	617.2	298.15-437.22	0.48-0.71	[38], [49], [50], [68]
111	Ethyl butylamine	5	194.9	547.1	298.15-358.15	0.54-0.65	[130]
112	Ethyl butyl ether	5	170.2	531.0	298.15-358.15	0.56-0.67	[151]

Table 2. Continued

i	Compound	n	T_f [K]	T_c [K]	ΔT [K]	ΔT_r [1]	Reference
113	Ethylcyclohexane	6	161.4	609.1	298.15-368.15	0.49-0.60	[49], [161]
114	Ethylcyclopentane	5	134.7	569.5	313.15-368.15	0.55-0.65	[161]
115	Ethyl ethanoate	13	189.2	523.2	298.15-363.40	0.57-0.69	[38], [54], [129], [162], [163]
116	Ethyl methanoate	5	193.8	508.4	304.00-343.15	0.60-0.67	[38], [129], [131]
117	Ethyl propanoate	10	199.3	548.0	298.15-372.35	0.54-0.68	[38], [67], [129], [163], [164]
118	Ethyl propyl ether	6	194.2	500.2	298.15-358.15	0.60-0.72	[84], [151]
119	Phenanthrene	7	372.4	873.0	298.15-420.00	0.34-0.48	[84], [156]
120	Hexafluorobenzene	8	278.0	516.7	300.57-376.53	0.58-0.73	[113], [165]
121	Hexafluoroethane	8	172.4	293.0	179.96-195.21	0.61-0.67	[166]
122	Hexane	39	177.8	507.9	298.15-498.20	0.59-0.98	[49], [72], [74], [81], [167], [168]
123	Heptane	21	182.6	540.1	288.16-371.51	0.53-0.69	[38], [49], [57], [74], [75], [169], [170], [171]
124	Indane	8	221.5	684.9	381.70-450.96	0.56-0.66	[50]
125	Methane	10	90.7	190.6	111.85-184.71	0.59-0.97	[172]
126	Methanol	39	175.5	512.5	298.15-510.20	0.58-1.00	[24], [38], [54], [57], [58], [67], [72], [97], [105], [120], [173], [174], [175]
127	Methyl tert-butyl ether	5	165.0	497.1	298.15-343.15	0.60-0.69	[134], [151]
128	Methylamine	24	179.7	430.0	297.04-380.37	0.69-0.88	[176]
129	Methyl butyl ether	6	157.7	512.8	298.15-358.15	0.58-0.70	[134], [151]
130	Methylcyclohexane	16	146.6	572.2	298.15-493.15	0.52-0.86	[49], [74], [110], [141], [177], [178]
131	Methyl ethanoate	12	175.1	506.8	295.51-343.15	0.58-0.68	[38], [67], [89], [129], [162], [163]
132	Methyl phenyl ether	5	235.7	645.6	298.15-426.73	0.46-0.66	[97], [134]
133	Methyl methanoate	5	173.2	487.2	293.25-313.45	0.60-0.64	[38], [67], [129]
134	Methyl propanoate	10	185.7	530.6	298.15-363.40	0.56-0.68	[38], [86], [89], [129], [163]
135	N,N'-dimethylhydrazine	5	264.2	530.0	296.46-298.97	0.56	[179]
136	N,N-diethylethanolamine	31	203.1	616.0	278.20-318.30	0.45-0.52	[180]
137	N-methylethanolamine	16	268.6	630.0	274.90-320.20	0.44-0.51	[180]
138	Nitromethane	8	244.8	588.0	298.10-374.44	0.51-0.64	[38], [181], [182], [183], [184]
139	Nonane	6	219.7	594.6	298.15-368.15	0.50-0.62	[49], [56], [185]
140	Oxetane	10	176.1	507.9	271.50-342.24	0.53-0.67	[113]
141	Oxirane	11	161.0	469.0	283.66-422.04	0.60-0.90	[186], [187]
142	Octane	35	216.4	568.8	298.15-444.26	0.52-0.78	[49], [59], [74], [79], [80], [109], [110], [125], [134], [142], [170], [178]
143	Pentadecane	8	283.0	706.8	298.15-373.15	0.42-0.53	[188], [189], [190]
144	Pentane	44	143.4	469.8	259.55-465.37	0.55-0.99	[54], [79], [122], [191], [192], [193], [194]
145	Pyridine	15	231.6	620.0	298.00-389.90	0.48-0.63	[97], [101], [119], [195], [196], [197], [198]
146	Propane	31	85.5	369.8	231.04-348.15	0.62-0.94	[194], [199], [200]
147	Propyl ethanoate	16	178.1	549.4	298.15-374.91	0.54-0.68	[38], [54], [87], [129], [162], [163]
148	Propyl methanoate	8	180.3	538.0	298.15-363.40	0.55-0.68	[129], [131]
149	Propyl propanoate	6	197.3	578.0	313.15-395.75	0.54-0.68	[38], [67], [129]
150	Tetradecane	10	279.0	693.0	298.15-358.15	0.43-0.52	[189], [190], [201]
151	Tetrahydronaphthalene	5	237.4	720.1	498.33-604.52	0.69-0.84	[51]
152	Tetrachloroethene	6	251.0	620.2	298.15-393.84	0.48-0.64	[34], [38]
153	Tetrachloromethane	12	250.5	556.4	297.32-358.15	0.53-0.64	[34], [110], [120], [141], [193], [202]
154	Thiacyclohexane	5	292.0	657.1	351.44-414.91	0.53-0.63	[203]
155	Toluene	25	178.2	591.1	298.15-521.13	0.50-0.88	[38], [40], [47], [49], [51], [136], [204]

Table 2. Continued

i	Compound	n	T_f [K]	T_c [K]	ΔT [K]	ΔT_r [1]	Reference
156	Tridecane	7	267.8	676.2	298.15-348.15	0.44-0.51	[189], [190]
157	Triethylamine	6	158.4	535.0	298.15-358.15	0.56-0.67	[128], [152]
158	Trichloroethene	6	186.8	571.0	298.15-358.84	0.52-0.63	[34], [38]
159	Trichloromethane	6	209.6	536.4	293.15-343.15	0.55-0.64	[34], [38], [45]
160	Carbon dioxide	10	216.6	304.1	168.90-172.70	0.56-0.57	[205]
161	Water	42	273.2	647.3	273.15-373.20	0.42-0.58	[49], [57], [70], [105], [110], [120], [139], [196], [206], [207], [208], [209]
162	sec-Butylamine	5	168.6	514.3	298.15-343.15	0.58-0.67	[128], [152]
	Total	1958					

Table 3. Heat of vaporization data correlation results

i	Author	m	S	N	p_{av} [%]
1	Mollier	2	162	1958	1.51
2	Thiesen	1	162	1958	1.61
3	Pilling	1	162	1958	4.81
4	Tyrer	1	162	1958	1.99
5	Kendall	1	162	1958	1.01
6	Osborne-van Dusen	2	162	1958	0.59
7	Keyes-Taylor-Smith	3	162	1958	0.33
8	Winter	1	162	1958	1.03
9	Nutting	2	162	1958	0.45
10	Eggert	1	162	1958	9.29
11	Jones-Bowden	1	162	1958	1.01
12	Silverberg-Wenzel	1	162	1958	1.04
13	Graue-Berry-Sage I	2	162	1958	0.48
14	Graue-Berry-Sage II	3	162	1958	0.34
15	Lin-Silberberg-McKetta	4	-	-	-
16	Chueh-Swanson	3	162	1958	0.33
17	Guermouche-Vergnaud	4	130	1791 (160)	0.27
18	Todd-Hossenlopp-Scott	4	129	1785 (16,160)	0.29
19	Radosz-Lydersen	4	131	1801	0.31
20	Tekač-Majer-Svoboda-Hynek	2	162	1958	0.59
21	Torquato-Stell	4	131	1801	0.50
22	Armstrong	4	131	1801	0.29
23	Vetere	4	-	-	-
24	Somayajulu I	3	162	1958	0.37
25	Somayajulu II	4	125	1733	0.29
26	Svoboda	4	130	1791 (160)	0.28
27	Xiang	3	157	1927 (11, 70,133,135,160)	0.35
28	New	4	131	1801	0.27

Remarks: Number in parenthesis presents number of data sets for failed correlation

Vergnaud (p_{av}=0.27%), Svoboda (p_{av}=0.28%), Todd-Hossenlopp-Scott (p_{av}=0.29%), Armstrong (p_{av}=0.29%) and Somayajulu II (p_{av}= 0.29%) equations, all with four parameters. However, the absolute percent deviation value increases for all equations when the reduced temperature approaches one. Detailed results of correlation for compounds with $T_r \geq 0.9$ for the best equations, along with results for Torquato-Stell and Armstrong equations with all six parameters, are presented in Table 4. The best results are obtained with Torquato-Stell (p_{av}=0.40%) and Armstrong equations (p_{av}=0.48%), both with six parameters. Based on results presented in Table 3 and Table 4 it is be recommended to use the Somayajulu II equation for $T_r<0.9$ and Torquato-Stell equation for $T_r \geq 0.9$.

The best results for correlation of all selected heats of vaporization were obtained with the following empirical equation:

$$\ln(\Delta H_v)=A+B/T_r+C/(1/T_r-1)+D\ln(1/T_r-1) \quad (3)$$

Table 4. Absolute mean percent deviation for compounds with $T_r \geq 0.9$

i	Compound/Equation	Guermouche-Vergnaud	Todd-Hossenlopp-Scott	Torquato-Stell m=6	Armstrong m=4	Armstrong m=6	Somayajulu II	Svoboda	New
1	1-butene	0.39(0.81)	0.40(0.79)	0.28(0.96)	0.33(0.89)	0.26(1.01)	0.35(0.89)	0.43(0.78)	0.44(0.73)
2	1,4-dimethylbenzene	0.20(0.40)	0.20(0.41)	0.12(0.31)	0.22(0.53)	0.14(0.24)	0.20(0.44)	0.20(0.47)	0.21(0.51)
3	1-propanol	0.18(0.64)	0.18(0.65)	0.17(0.64)	0.18(0.67)	0.18(0.64)	0.18(0.63)	0.20(0.74)	0.17(0.66)
4	2-butanol	0.27(1.17)	0.26(1.18)	0.25(1.11)	0.42(1.39)	0.25(1.15)	0.44(1.33)	0.38(1.15)	0.30(1.22)
5	2-butene,trans	0.20(0.88)	0.20(0.88)	0.18(0.77)	0.25(0.90)	0.16(0.55)	0.26(0.90)	0.19(0.88)	0.20(0.88)
6	2-methyl-1-propanol	0.40(1.44)	0.41(1.43)	0.25(1.45)	0.36(1.54)	0.34(1.63)	0.38(1.47)	0.47(1.78)	0.41(1.46)
7	2-propanol	0.23(0.67)	0.23(0.67)	0.22(0.61)	0.22(0.70)	0.20(0.56)	0.23(0.67)	0.23(0.64)	0.22(0.67)
8	Acetone	0.34(0.96)	0.33(0.93)	0.22(0.49)	0.26(0.62)	0.25(0.89)	0.31(0.67)	0.28(0.72)	0.42(1.23)
9	Benzene	0.61(5.72)	0.62(5.42)	0.55(3.31)	0.69(6.40)	0.66(7.87)	0.62(6.56)	0.63(7.06)	0.69(5.81)
10	Diborane	0.20(0.52)	0.19(0.51)	0.16(0.36)	0.29(1.37)	0.19(0.53)	0.28(1.45)	0.21(0.52)	0.16(0.38)
11	Diphenyl	3.02(6.45)	2.64(5.75)	1.14(2.98)	2.38(5.03)	1.62(4.81)	3.20(7.70)	3.45(6.49)	2.49(5.58)
12	Ethanal	0.14(0.42)	0.14(0.44)	0.10(0.25)	0.11(0.26)	0.11(0.24)	0.14(0.35)	0.30(0.62)	0.21(0.54)
13	Ethanol	0.74(2.09)	0.69(2.29)	0.74(2.05)	0.91(5.80)	0.77(2.02)	1.09(9.33)	0.94(2.86)	0.76(2.90)
14	Hexane	0.47(1.73)	0.46(1.55)	0.41(1.43)	0.56(3.57)	0.46(1.52)	0.57(4.45)	0.44(1.41)	0.41(1.37)
15	Methane	0.29(0.69)	0.23(0.60)	0.19(0.53)	0.42(1.02)	0.23(0.56)	0.42(1.17)	0.22(0.50)	0.21(0.53)
16	Methanol	0.34(2.10)	0.34(1.96)	0.21(0.90)	0.35(2.62)	0.33(2.32)	0.41(4.85)	0.25(1.03)	0.34(1.55)
17	Oxirane	0.78(2.21)	0.82(2.31)	0.17(0.33)	0.62(1.34)	0.07(0.18)	0.58(1.31)	1.07(2.51)	0.92(2.58)
18	Pentane	0.99(5.94)	0.97(5.74)	0.47(3.96)	0.90(9.33)	0.85(6.64)	0.87(6.50)	0.87(5.70)	0.86(5.52)
19	Propane	1.22(2.73)	1.22(2.72)	0.83(2.25)	1.22(2.76)	0.75(2.41)	1.23(2.80)	1.22(2.65)	1.22(2.68)
	p_{av} [%]	0.61	0.59	0.40	0.61	0.48	0.65	0.64	0.59

Remarks: Data in parenthesis are maximum (single) absolute percent deviations

Correlation results obtained with use of the above equation are included in Table 3 and Table 4.

Overall percent error deviation obtained by using the proposed equation is among the lowest (0.27%), and percent error deviation (0.59%) around the T_c (T_r>0.9) calssifies it among the best four-parameter equations; however, it performs worse than six-parameter equations.

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NOMENCLATURE

ΔH_v : heat of vaporization
m : number of parameters
n : number of data per set
N : number of data
p_{abs} : absolute mean percent deviation
S : number of compounds
T : temperature
ΔT : temperature range
T_c : critical temperature
T_f : normal freezing point
$T_r = T/T_c$: reduced temperature
ΔT_r : reduced temperature range
T_t : triple point

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