Erratum: New Group-Contribution Approach to Thermochemical Properties of Organic Compounds: Hydrocarbons and Oxygen-Containing Compounds [J. Phys. Chem. Ref. Data 42, 033102 (2013)]

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Erratum: New Group-Contribution Approach to Thermochemical Properties of Organic Compounds: Hydrocarbons and Oxygen-Containing Compounds [J. Phys. Chem. Ref. Data 42, 033102 (2013)]

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Corrections are required for several of the symbols and values in Table 33 of the original article.[1] Corrected entries are underlined in the revised table below.

TABLE 33. Group-contribution parameters for calculation of enthalpies of formation (kJ mol^{-1}) and enthalpies of vaporization (kJ mol^{-1}) at the temperature 298.15 K

Structural group[a]	$\Delta_f H^0_m(l)$	Variance	$\Delta^g_l H_m$	Variance	$\Delta_f H^0_m(g)$	Variance
CH_3-C	−45.98	0.48	6.02	0.13	−41.31[b]	0.50
CH_2-2C	−28.85	0.32	4.57	0.12	−23.70	0.38
CH-3C	−16.45	0.92	1.51	0.37	−12.23	1.11
C-4C	−6.61[b]	3.00	−2.09[b]	0.50	−4.49[b]	3.00
$(C\text{-}C)_{1\text{-}4}$	2.96	0.09	0.35	0.03	3.12	0.11
$(C\text{-}C)_{1\text{-}5}$	7.41	4.20	−0.80	0.50	6.39[b]	4.00
CH_3-Cd	−45.98	0.00	6.02	0.00	−41.31	0.00
CdH_2-Cd	22.04	1.33	4.91	0.08	26.36	0.85
CdH-Cd,C	28.12	0.44	4.69	0.23	34.59	0.49
Cd-Cd, 2C	30.53	1.55	3.30	0.21	37.07	1.58
CH_2-C,Cd	−28.02	1.38	4.44	0.16	−23.84	1.25
CH-2C,Cd	−16.71	2.87	0.94	0.50	−13.47	2.30
C-3C,Cd	−5.06	4.33	−2.31	0.35	−3.71	3.76
cis-interaction	4.37	3.11	<u>−0.04</u>	0.54	4.43	2.65
CbH-2Cb	8.17	0.10	5.63	0.05	13.80	0.10
<u>CH_3-Cb</u>	−45.98	0.00	6.02	0.00	−41.31	0.00
Cb-C,2Cb	16.53	0.22	3.78	0.08	21.79	0.30
CH_2-C,Cb	−23.81	0.63	3.94	0.26	−19.93	1.09
CH-2C,Cb	−6.34	1.29	0.87	0.73	−4.58	1.33
C-3C,Cb	9.42	2.64	−2.92	0.44	9.08	2.52
ortho(alkyl-alkyl)	3.40	0.97	1.26	0.32	4.03	1.16
meta(alkyl-alkyl)	−0.10	0.87	0.32	0.22	0.25	0.84
para(alkyl-alkyl)	−0.32	0.73	0.72	0.30	0.70	0.99
CH_3-Ct	−45.98	0.00	6.02	0.00	−41.31	0.00
CtH-Ct	106.79	1.35	6.81	0.45	<u>112.25</u>	1.00
Ct-Ct,C	105.65	0.56	6.80	0.10	<u>113.98</u>	0.50
CH_2-C,Ct	−22.38[b]	1.55	3.44	0.26	<u>−19.47</u>[b]	1.50
CH-2C,Ct	15.92[b]	3.00	–	–	–	–
C-3C,Ct	3.40[b]	2.00	–	–	–	–
OH-C	−193.48	0.00	31.50	0.00	−159.82	0.00
<u>CH_2-C,OH</u>	−36.44	1.59	5.48	0.66	−33.86	2.79
<u>CH-2C,OH</u>	−33.30	1.62	0.16	0.78	−32.44	3.60
<u>C-3C,OH</u>	−28.06	1.22	−5.17	0.90	−30.52	3.03
CH_3-O	−45.98	0.00	6.02	0.00	−41.31	0.00

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TABLE 33. Group-contribution parameters for calculation of enthalpies of formation (kJ mol^{-1}) and enthalpies of vaporization (kJ mol^{-1}) at the temperature 298.15 K—Continued

Structural group[a]	$\Delta_f H^0_m$(l)	Variance	$\Delta^g_l H_m$	Variance	$\Delta_f H^0_m$(g)	Variance
O-2C	−108.84[b]	2.00	8.60	0.91	−97.26[b]	2.50
CH_2-C,O	−35.79	0.63	3.05	0.12	−33.38	0.60
CH-2C,O	−29.95	1.46	−0.14	0.22	−28.72	1.38
C-3C,O	−21.93	1.03	−3.58	0.29	−22.36	1.70
CH_3-CO	−45.98	0.00	6.02	0.00	−41.31	0.00
CHO-C	−145.30	1.15	19.97	0.37	−126.31[b]	1.50
CO-2C	−152.15[b]	2.00	17.93	1.19	−134.85[b]	1.50
CH_2-C,CO	−31.58	0.51	2.64	0.15	−26.80	0.44
CH-2C,CO	−20.28	1.10	−1.21	0.27	−16.77[b]	1.00
C-3C,CO	−10.40	1.78	−6.51	0.56	−9.14	1.71
CH_2-C,COOH	−28.85	0.00	4.57	0.00	−23.70	0.00
CH-2C,COOH	−16.45	0.00	1.51	0.00	−12.23	0.00
C-3C,COOH	−6.61	0.00	−2.09	0.00	−4.49	0.00
COOH,C	−438.41	0.79	41.68	0.54	−395.77	0.80
O-C,CO	−108.84	0.00	8.59	0.00	−97.27	0.00
CHO-O	−231.63	5.00	13.92[b]	0.72	−219.36	5.00
CO-C,O	−238.01	1.26	10.39	0.97	−230.57	1.00
CO-2O	−299.61	0.29	8.31	0.54	−294.10	0.33

[a]Cd is a double-bonded C-atom; Cb is a C-atom in the aromatic ring; Ct is a triple-bonded C-atom; *ortho*(alkyl-alkyl), *meta*(alkyl-alkyl), and *para*(alkyl-alkyl) are interactions of small alkyl substituents (methyl and ethyl) in di-substituted benzenes.

[b]The calculated variance for this parameter was overestimated due to the existence of few or only low quality experimental data involving the group of interest. The variance was subsequently reduced individually for practical use.

References

[1]S. P. Verevkin, V. N. Emel'yanenko, V. Diky, C. D. Muzny, R. D. Chirico, and M. Frenkel, J. Phys. Chem. Ref. Data **42**, 033102 (2013).