

**Group Contribution Values of the Infinite Dilution Thermodynamic  
Functions of Hydration for Aliphatic Non-Cyclic Hydrocarbons,  
Alcohols and Ketones at 298.15 K and 0.1 MPa**

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## **Abstract**

A compilation of experimental values of the infinite dilution partial molar Gibbs energy, enthalpy and heat capacity of hydration, together with molar volumes in water at 298.15 K and 0.1 MPa is presented for aliphatic non-cyclic ketones. These data, combined with the related results for aliphatic non-cyclic hydrocarbons and monohydric alcohols, were treated in the framework of a simple first order group additivity scheme. Numerical values of the contributions to the each of the thermodynamic properties are obtained by the least-square procedure for the following groups: CH<sub>3</sub>, CH<sub>2</sub>, CH, C, OH and CO.

## Introduction

Values of thermodynamic properties of organic compounds in aqueous solutions at infinite dilution are needed for many applications in chemistry, biology, medicine, geochemistry, chemical engineering etc. An experimental study of all the variety of organic compounds is out of the question: there are simply too many substances to make a comprehensive study possible. Instead, group additivity methods are used to estimate the properties of organic species in gas, liquid and solid phases (see: Benson et al.<sup>1</sup>, Domalski and Hearing<sup>2</sup>, Frenkel et al.<sup>3</sup>). In 1981, Cabani et al.<sup>4</sup> presented an extensive data base of thermodynamic functions of hydration of organic compounds at 298.15 K, and derived group contribution values for many functional groups. Recently, we attempted an update of the data base and group contribution values for aliphatic and monoaromatic hydrocarbons and monohydric alcohols (Plyasunov and Shock<sup>5</sup>). Here we present the results for aliphatic non-cyclic ketones.

## Data compilation

The infinite dilution partial molar functions of hydration under consideration are the Gibbs energy,  $\Delta_{\text{h}}G^{\circ}$ , the enthalpy,  $\Delta_{\text{h}}H^{\circ}$ , the heat capacity,  $\Delta_{\text{h}}C_p^{\circ}$ , and volume,  $V_2^{\circ}$ . The standard state adopted for gaseous species is unit fugacity of the ideal gas at any temperature and pressure  $P^{\circ} = 0.1$  MPa; that for aqueous species calls for unit activity of a hypothetical one molal solutions referenced to infinite dilution at any temperature and pressure. The hydration process refers to transfer of one mole of a solute from an ideal gas to a standard one molal solution. We note two main reasons to work with the functions of hydration rather than with the partial molar properties, like the Gibbs energy of formation of an aqueous compound. First, functions of hydration typically have lower uncertainties, because they do not include the uncertainties of the

enthalpy of combustion measurements. Second, as discussed by Cabani et al.<sup>4</sup>, there is a universal contribution to the properties of aqueous species, which is seen as the non-zero intercept of a plot of properties for a homologous series versus molecular mass or number of groups. The nature of this term is obvious for the thermodynamic functions of hydration, where it arises as the functions of hydration of a material point (Pierotti<sup>6</sup>). This term can be calculated independently using the thermophysical properties of pure water, thus reducing the dimension of the fitting task.

***The Gibbs energy of hydration at 298.15 K.*** Literature values of the various modifications of Henry's law constants and gas/water partition coefficients were recalculated to yield equilibrium constants,  $K^\circ$ , for a gas dissolution reaction  $A(g) \rightleftharpoons A(aq)$ , for which  $\Delta_h G^\circ = -RT \ln K^\circ = -RT \ln \frac{aP^\circ}{f}$ , where  $a$  and  $f$  stand for the activity and fugacity of a solute in water, respectively.

Results for the infinite dilution activity coefficient of a solute for the symmetrical normalization of activities, reported as  $\gamma^\infty$ , were converted to  $\Delta_h G^\circ$  values as follows (see Plyasunov and Shock<sup>5</sup>):  $\Delta_h G^\circ = -\Delta_{\text{vap}} G^\circ + RT \ln \gamma^\infty - RT \ln 1000/M_w$ , where  $M_w$  stands for the molecular mass of water in  $\text{g}\cdot\text{mol}^{-1}$ ;  $\Delta_{\text{vap}} G^\circ = -RT \ln \frac{\psi P_s}{P^\circ}$ , where  $P_s$  stands for the saturated vapor pressure over the pure liquid/solid compound, and  $\psi$  represents the fugacity coefficient of a pure compound, evaluated using the second virial coefficient.

The mutual solubility data were converted to  $\Delta_h G^\circ$  values as follows (see Plyasunov and Shock<sup>5</sup>):  $\Delta_h G^\circ = \Delta_{\text{sol}} G^\circ - \Delta_{\text{vap}} G^\circ$ , where  $\Delta_{\text{sol}} G^\circ = -RT \ln \frac{m_s \gamma_s}{X_s \Lambda_s}$ , where  $m_s$  and  $\gamma_s$  stand for the molality and the molal activity coefficient (for the unsymmetrical normalization) at saturation for an organic compound in the water-rich phase, respectively;  $X_s$  and  $\Lambda_s$  represent the mole fraction

and the mole fraction activity coefficient (for the symmetrical normalization) of the organic compound in the coexisting organic-rich phase. The UNIQUAC model (Reid et al.<sup>7</sup>) was employed to evaluate  $\Lambda_s$ . Values of  $\gamma_s$  were estimated using the Savage and Wood<sup>8</sup> group contribution scheme. In the Savage-Wood formalism,  $\ln \gamma_s = 2g_{xx}m_s / RT$ , where  $g_{xx}$  is the solute-solute self-interaction coefficient, given by  $g_{xx} = \sum_{i,j} n_i n_j G_{ij} - RTM_w / 2000$ , where  $n_i$  and  $n_j$  represent the number of groups  $i$  and  $j$  in two interacting molecules, and  $G_{ij}$  stand for the excess Gibbs energy of an  $i$ - $j$  interaction. To characterize the ketone-ketone interactions one needs  $G_{CH_2-CH_2} = -34 \text{ J}\cdot\text{mol}^{-1}$  (Suri et al.<sup>9</sup>),  $G_{CH_2-CO} = 41 \text{ J}\cdot\text{mol}^{-1}$  and  $G_{CO-CO} = -64 \text{ J}\cdot\text{mol}^{-1}$  (the two later values were evaluated from  $g_{xx}$  for acetone (Kozak et al.<sup>10</sup>) and 2-butanone (Wong et al.<sup>11</sup>)).

The values of  $\Delta_h G^\circ$  obtained for ketones are presented in Table 1. Where necessary, results measured within 10-20 K from 298.15 K were recalculated to this temperature using the approximation that  $\Delta_h H^\circ$  is constant. Results based on the mutual solubility studies are given in italics. Values considered unreliable are given in parentheses and were excluded from consideration.

***The enthalpy and heat capacity of hydration, and partial molar volume at 298.15 K, 0.1 MPa.***

Calorimetric values of the standard enthalpy of solution of a pure liquid ketone in water,  $\Delta_s H^\circ$ , were converted to  $\Delta_h H^\circ$  by means of  $\Delta_h H^\circ = \Delta_s H^\circ - \Delta_{\text{vap}} H^\circ$ , where  $\Delta_{\text{vap}} H^\circ$  stands for the standard enthalpy of vaporization of a pure compound. Results are presented in Table 2.

Published values of the infinite dilution partial molar heat capacity of aqueous solutes,  $Cp_2^\circ$ , were used to calculate  $\Delta_h Cp^\circ$  as follows:  $\Delta_h Cp^\circ = Cp_2^\circ - Cp(\text{ig})$ , where  $Cp(\text{ig})$  represents the heat capacity of a compound in the ideal gas state. Results are given in Table 3.

Literature values of the infinite dilution partial molar volumes of ketones in water are presented in Table 4.

### **Group contributions values**

The values of the thermodynamic functions of hydration of ketones at 298.15 K and 0.1 MPa were combined with those for aliphatic non-cyclic hydrocarbons and monohydric alcohols, which were presented elsewhere (Plyasunov and Shock<sup>5</sup>). The first order group additivity scheme, in which the properties of a group are assumed to be independent of the group's neighbors, was chosen to treat the data. The following groups are necessary to represent the selected compounds: CH<sub>3</sub>, CH<sub>2</sub>, CH, C, OH and CO. Assuming the properties of the groups are additive, any thermodynamic property of interest,  $Y$ , can be estimated from  $Y = Y_0 + \sum_i n_i Y_i$ , where  $n_i$  stands for the number of times the  $i$ -th group is present in the compound,  $Y_i$  designates the contribution to the  $Y$  property of the  $i$ -th group,  $Y_0$  represents the values of thermodynamic functions of hydration of a material point, i.e. an imaginable compound without any groups at all. Values of  $Y_0$  can be calculated independently using the thermophysical properties of water (Pierotti<sup>6</sup>, for details see Plyasunov and Shock<sup>5</sup>). The numerical values of the group contributions given in Table 5 were derived by a weighted least-square fit of the selected data set. In general, our results are very close to the values obtained by Cabani et al.<sup>4</sup> based on the data set available more than twenty years ago.

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Table 1. Values of the Gibbs energy of hydration of ketones at 298.15 K, 0.1 MPa (see text for details)

Compound	Formula	$\Delta_{\text{vap}}G^\circ /$ kJ·mol <sup>-1</sup>	$\Delta_{\text{h}}G^\circ /$ kJ·mol <sup>-1</sup>	Accepted value	Group contribution value	$\Delta /$ kJ·mol <sup>-1</sup>
Acetone	C <sub>3</sub> H <sub>6</sub> O	2.98 <sup>a</sup>	-7.89 <sup>b</sup> , -8.21 <sup>c</sup> , -8.14 <sup>d</sup> , -8.59 <sup>e</sup> , -8.01 <sup>f</sup> , -8.79 <sup>g</sup> , -8.02 <sup>h</sup> , -8.02 <sup>i</sup> , -7.93 <sup>j</sup> , -7.94 <sup>k</sup> , -8.00 <sup>l</sup> , -8.22 <sup>m</sup> , -8.29 <sup>n</sup> , -8.43 <sup>o</sup>	-8.18±0.30	-7.48	-0.70
2-Butanone	C <sub>4</sub> H <sub>8</sub> O	5.28 <sup>a</sup>	(-8.75) <sup>b</sup> , -7.18 <sup>p</sup> , -7.01 <sup>f</sup> , -7.40 <sup>g</sup> , (-5.06) <sup>q</sup> , -7.11 <sup>r</sup> , -6.97 <sup>s</sup> , -6.97 <sup>t</sup> , (-5.87) <sup>i</sup> , -6.99 <sup>j</sup> , -7.28 <sup>u</sup> , -7.41 <sup>v</sup> , -7.13 <sup>k</sup> , -7.58 <sup>l</sup>	-7.18±0.30	-6.76	-0.42
2-Pentanone	C <sub>5</sub> H <sub>10</sub> O	7.60 <sup>a</sup>	-6.12 <sup>w</sup> , -6.34 <sup>x</sup> , -6.19 <sup>y</sup> , -6.09 <sup>f</sup> , -6.17 <sup>z</sup> , -6.14 <sup>j</sup> , -6.42 <sup>u</sup> , -6.52 <sup>v</sup> , -6.21 <sup>aa</sup> , -6.80 <sup>l</sup> , -5.96 <sup>bb</sup>	-6.27±0.40	-6.05	-0.22
3-Pentanone	C <sub>5</sub> H <sub>10</sub> O	7.59 <sup>a</sup>	-5.82 <sup>y</sup> , -5.83 <sup>f</sup> , -5.81 <sup>j</sup> , -6.76 <sup>v</sup> , -5.81 <sup>aa</sup>	-6.01±0.40	-6.05	0.04
3-Methyl-2- butanone	C <sub>5</sub> H <sub>10</sub> O	6.63 <sup>a</sup>	-5.42 <sup>y</sup> , -5.61 <sup>cc</sup> , -5.56 <sup>z</sup> , -5.29 <sup>aa</sup>	-5.47±0.30	-5.60	0.13
2-Hexanone	C <sub>6</sub> H <sub>12</sub> O	10.35 <sup>dd</sup>	-5.67 <sup>y</sup> , -5.64 <sup>j</sup> , -5.48 <sup>u</sup> , -5.67 <sup>v</sup> , -5.87 <sup>aa</sup>	-5.67±0.30	-5.34	-0.33
3-Hexanone	C <sub>6</sub> H <sub>12</sub> O	9.92 <sup>dd</sup>	(0.63) <sup>ee</sup> , -4.95 <sup>j</sup> , -5.14 <sup>aa</sup>	-5.01±0.30	-5.34	0.33
4-Methyl-2- pentanone	C <sub>6</sub> H <sub>12</sub> O	9.11 <sup>dd</sup>	-4.64 <sup>ff</sup> , -4.81 <sup>y</sup> , (-2.33) <sup>q</sup> , -4.74 <sup>v</sup> , -4.91 <sup>aa</sup>	-4.78±0.30	-4.88	0.10
2-Methyl-3- pentanone	C <sub>6</sub> H <sub>12</sub> O	8.80 <sup>dd</sup>	-4.12 <sup>aa</sup>	-4.12±0.60	-4.88	0.76

3-Methyl-2-pentanone	C <sub>6</sub> H <sub>12</sub> O	9.24 <sup>dd</sup>	-5.28 <sup>aa</sup>	-5.28±0.60	-4.88	-0.40
3,3-Dimethyl-2-butanone	C <sub>6</sub> H <sub>12</sub> O	7.83 <sup>dd</sup>	-3.68 <sup>y</sup> , -3.83 <sup>u</sup> , -3.63 <sup>aa</sup>	-3.71±0.40	-4.64	0.93
2-Heptanone	C <sub>7</sub> H <sub>14</sub> O	13.04 <sup>gg</sup>	-4.38 <sup>w</sup> , -4.83 <sup>y</sup> , -4.81 <sup>u</sup> , -5.45 <sup>v</sup> , -5.02 <sup>aa</sup> , -4.77 <sup>l</sup>	-4.88±0.40	-4.63	-0.26
4-Heptanone	C <sub>7</sub> H <sub>14</sub> O	12.54 <sup>dd</sup>	-4.50 <sup>y</sup>	-4.50±0.60	-4.63	0.13
2,4-Dimethyl-3-pentanone	C <sub>7</sub> H <sub>14</sub> O	9.79 <sup>dd</sup>	-1.89 <sup>y</sup> , -2.37 <sup>aa</sup>	-2.13±0.50	-3.72	1.59
2-Octanone	C <sub>8</sub> H <sub>16</sub> O	15.84 <sup>gg</sup>	-4.70 <sup>y</sup> , -4.28 <sup>hh</sup> , -4.11 <sup>l</sup>	-4.36±0.40	-3.91	-0.45
2-Nonanone	C <sub>9</sub> H <sub>18</sub> O	18.46 <sup>gg</sup>	-3.53 <sup>kk</sup> , -3.76 <sup>y</sup> , -2.45 <sup>l</sup>	-3.25±0.50	-3.20	-0.05
2,6-Dimethyl-4-heptanone	C <sub>9</sub> H <sub>18</sub> O	15.07 <sup>dd</sup>	-0.73 <sup>y</sup>	-0.73±1.00	-2.29	1.56
2-Undecanone	C <sub>11</sub> H <sub>22</sub> O	24.28 <sup>dd</sup>	-1.09 <sup>l</sup> , -2.1 <sup>l</sup>	-1.6±0.6	-1.78	0.18

<sup>a</sup> Reid et al.<sup>7</sup>; <sup>b</sup> Iraci et al.<sup>12</sup>; <sup>c</sup> Benkelberg et al.; <sup>d</sup> Hoff et al.<sup>14</sup>; <sup>e</sup> Betterton<sup>15</sup>; <sup>f</sup> Landau et al.<sup>16</sup>; <sup>g</sup> Zhou and Mopper<sup>17</sup>; <sup>h</sup> Lichtenbelt and Schram<sup>18</sup>; <sup>i</sup> Snider and Dawson<sup>19</sup>; <sup>j</sup> Mash and Pemberton<sup>20</sup>; <sup>k</sup> Vitenberg et al.<sup>21</sup>; <sup>l</sup> Buttery et al.<sup>22</sup>; <sup>m</sup> Burnett<sup>23</sup>; <sup>n</sup> Burnett and Swoboda<sup>24</sup>; <sup>o</sup> Butler and Ramchandani<sup>25</sup>; <sup>p</sup> Wong et al.<sup>11</sup>; <sup>q</sup> Ashworth et al.<sup>26</sup>; <sup>r</sup> Park et al.<sup>27</sup>; <sup>s</sup> Sorrentino et al.<sup>28</sup>; <sup>t</sup> Richon et al.<sup>29</sup>; <sup>u</sup> Aarna et al.<sup>30</sup>; <sup>v</sup> Sato and Nakajima<sup>31</sup>; <sup>w</sup> Shiu and Mackay<sup>32</sup>; <sup>x</sup> Arce et al.<sup>33</sup>; <sup>y</sup> Stephenson<sup>34</sup>; <sup>z</sup> Ferino et al.<sup>35</sup>; <sup>aa</sup> Sørensen and Arlt<sup>36</sup>; <sup>bb</sup> Nelson and Hoff<sup>37</sup>; <sup>cc</sup> Correa et al.<sup>38</sup>; <sup>dd</sup> Stephenson and Malanowski<sup>39</sup>; <sup>ee</sup> Dewulf et al.<sup>40</sup>; <sup>ff</sup> Feki et al.<sup>41</sup>; <sup>gg</sup> Guetachew et al.<sup>42</sup>; <sup>kk</sup> Tewari et al.<sup>43</sup>; <sup>kk</sup> Li and Carr<sup>44</sup>.

Table 2. Values of the enthalpy of hydration of ketones at 298.15 K, 0.1 MPa

Compound	Formula	$\Delta_{\text{vap}}H^\circ /$ $\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_{\text{h}}H^\circ /$ $\text{kJ}\cdot\text{mol}^{-1}$	Accepted value	Group contribution value	$\Delta /$ $\text{kJ}\cdot\text{mol}^{-1}$
Acetone	$\text{C}_3\text{H}_6\text{O}$	31.27 <sup>a</sup>	-41.70 <sup>b</sup> , -41.57 <sup>c</sup> , -41.44 <sup>d</sup> , -41.44 <sup>e</sup> , -41.24 <sup>f</sup> , -41.48 <sup>g</sup> , -41.18 <sup>h</sup>	-41.5±0.3	-40.65	-0.85
2-Butanone	$\text{C}_4\text{H}_8\text{O}$	34.92 <sup>a</sup>	-45.64 <sup>e</sup> , -45.42 <sup>i</sup>	-45.5±0.5	-44.37	-1.13
2-Pentanone	$\text{C}_5\text{H}_{10}\text{O}$	38.46 <sup>a</sup>	-48.67 <sup>e</sup> , -49.98 <sup>j</sup>	-49.0±0.5	-48.11	-0.89
3-Pentanone	$\text{C}_5\text{H}_{10}\text{O}$	38.68 <sup>a</sup>	-49.58 <sup>e</sup> , -49.56 <sup>j</sup>	-49.6±0.5	-48.11	-1.49
3-Methyl-2- butanone	$\text{C}_5\text{H}_{10}\text{O}$	36.87 <sup>a</sup>	-47.50 <sup>e</sup>	-47.6±1.0	-48.26	0.66
2-Hexanone	$\text{C}_6\text{H}_{12}\text{O}$	43.15 <sup>a</sup>	-52.61 <sup>e</sup>	-52.6±1.0	-51.86	-0.74
4-Methyl-2- pentanone	$\text{C}_6\text{H}_{12}\text{O}$	40.65 <sup>a</sup>	-50.15 <sup>e</sup>	-50.2±1.0	-52.00	1.80
3,3-Dimethyl- 2-butanone	$\text{C}_6\text{H}_{12}\text{O}$	38.00 <sup>a</sup>	-47.50 <sup>e</sup>	-47.5±1.0	-51.34	3.84
2-Heptanone	$\text{C}_7\text{H}_{14}\text{O}$	47.24 <sup>a</sup>	-56.19 <sup>e</sup> , -56.86 <sup>j</sup>	-56.4±0.6	-55.60	-0.80
4-Heptanone	$\text{C}_7\text{H}_{14}\text{O}$	47.2 <sup>k</sup>	-58.1 <sup>j</sup>	-58.1±2.0	-55.60	-2.50
2,4-Dimethyl- 3-pentanone	$\text{C}_7\text{H}_{14}\text{O}$	41.57 <sup>a</sup>	-51.2 <sup>e</sup> , -57.1 <sup>j</sup>	-54.0±3.0	-55.88	1.88
2-Nonanone	$\text{C}_9\text{H}_{18}\text{O}$	56.44 <sup>a</sup>	-62.7 <sup>j</sup>	-62.7±2.0	-63.08	0.38

<sup>a</sup> Majer and Svoboda<sup>45</sup>; <sup>b</sup> Pfeffer et al.<sup>46</sup>; <sup>c</sup> Dohnal et al.<sup>47</sup>; <sup>d</sup> French<sup>48</sup>; <sup>e</sup> Della Gatta et al.<sup>49</sup>; <sup>f</sup> Duer and Bertrand<sup>50</sup>; <sup>g</sup> Arnett et al.<sup>51</sup>; <sup>h</sup> Arnett and McKelvey<sup>52</sup>; <sup>i</sup> Hanson and Winkle<sup>53</sup>; <sup>j</sup> Bury et al.<sup>54</sup>; <sup>k</sup> Stephenson and Malanowski<sup>39</sup>.

Table 3. Values of the heat capacity of hydration of ketones at 298.15 K, 0.1 MPa

Compound	Formula	$C_{p,ig}/$ $J \cdot K^{-1} \cdot mol^{-1}$	$\Delta_h C_p^o /$ $J \cdot K^{-1} \cdot mol^{-1}$	Accepted value	Group contribution value	$\Delta /$ $J \cdot K^{-1} \cdot mol^{-1}$
Acetone	$C_3H_6O$	74.5 <sup>a</sup>	150 <sup>b</sup> , 166 <sup>c</sup>	158±10	163	-5
2-Butanone	$C_4H_8O$	103.3 <sup>a</sup>	234 <sup>d</sup> ; 233 <sup>e</sup>	234±5	230	4
3-Pentanone	$C_5H_{10}O$	129.9 <sup>a</sup>	298 <sup>e</sup>	298±10	297	1

<sup>a</sup> Frenkel et al.<sup>3</sup>; <sup>b</sup> Tasker et al.<sup>55</sup>; <sup>c</sup> Desnoyers et al.<sup>56</sup>; <sup>d</sup> Hovorka et al.<sup>57</sup>; <sup>e</sup> Roux et al.<sup>58</sup>

Table 4. Values of  $V_2^0$  of ketones in water at 298.15 K, 0.1 MPa

Compound	Formula	$V_2^0 /$ $\text{cm}^3 \cdot \text{mol}^{-1}$	Accepted value	Group contribution value	$\Delta /$ $\text{cm}^3 \cdot \text{mol}^{-1}$
Acetone	$\text{C}_3\text{H}_6\text{O}$	66.92 <sup>a</sup> , 66.8 <sup>b</sup> , 66.92 <sup>c</sup> , 67.0 <sup>d</sup>	66.9±0.3	66.80	0.10
2-Butanone	$\text{C}_4\text{H}_8\text{O}$	82.44 <sup>e</sup> , 82.56 <sup>f</sup> , 82.52 <sup>g</sup> , 82.9 <sup>b</sup> , 82.5 <sup>d</sup>	82.5±0.3	82.51	-0.01
2-Pentanone	$\text{C}_5\text{H}_{10}\text{O}$	98.0 <sup>b</sup>	98.0±2.0	98.21	-0.21
3-Pentanone	$\text{C}_5\text{H}_{10}\text{O}$	98.08 <sup>g</sup>	98.1±1.0	98.21	-0.11
3-Methyl-2- butanone	$\text{C}_5\text{H}_{10}\text{O}$	95.0 <sup>b</sup>	95.0±2.0	98.41	-3.41

<sup>a</sup> Tasker et al.<sup>59</sup>; <sup>b</sup> Edward et al.<sup>60</sup>; <sup>c</sup> Kiyohara et al.<sup>61</sup>; <sup>d</sup> Boje and Hvidt<sup>62</sup>; <sup>e</sup> Hovorka et al.<sup>57</sup>; <sup>f</sup> Davies et al.<sup>63</sup>; <sup>g</sup> Roux et al.<sup>58</sup>

Table 5. Numerical values of the group contributions to each thermodynamic functions of hydration at 298.15 K, 0.1 MPa together with their uncertainties at the 0.95 confidence level. The number of compounds containing the selected groups for each of the properties is given in parentheses

Group	$\Delta_{\text{h}}G^{\circ}/$ kJ·mol <sup>-1</sup>	$\Delta_{\text{h}}H^{\circ}/$ kJ·mol <sup>-1</sup>	$\Delta_{\text{h}}Cp^{\circ}/$ J·K <sup>-1</sup> ·mol <sup>-1</sup>	$V_2^{\circ}/$ cm <sup>3</sup> ·mol <sup>-1</sup>
CH <sub>3</sub>	3.62±0.15 (79)	-7.55±0.58 (40)	128±5 (26)	25.46±0.89 (30)
CH <sub>2</sub>	0.71±0.07 (66)	-3.74±0.29 (29)	67±2 (19)	15.70±0.15 (22)
CH	-1.74±0.30 (43)	-0.08±1.44 (13)	9±11 (6)	6.15±0.98 (12)
C	-4.41±0.54 (12)	4.39±2.30 (4)	-42±15 (4)	-3.46±1.85 (4)
OH	-25.34±0.23 (32)	-40.47±1.09 (16)	1±7 (16)	12.63±0.97 (20)
CO	-22.68±0.31 (18)	-23.24±1.25 (12)	-93±11 (3)	14.76±1.82 (5)
Y <sub>o</sub>	7.96	-2.29	0	1.12