

# Supporting Information

## Vapor Pressures and Thermophysical Properties of 1-Heptanol, 1-Octanol, 1-Nonanol, and 1-Decanol: Data Reconciliation and PC-SAFT Modeling

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### 1. Description of SimCor method

Simultaneous correlation of vapor pressures and related thermal properties (SimCor) was suggested (in a simplified form) by King and Al-Najjar in 1974.<sup>1, 2</sup> The method was later sporadically used by several authors (e.g. by Ambrose and Davies,<sup>3</sup> Mosselman et al.,<sup>4</sup> Rogalski,<sup>5</sup> King and Mahmud,<sup>6</sup> Vetere<sup>7</sup> (who used simplified SimCor version with enthalpies of vaporization but without considering heat capacities), Bertucco et al.,<sup>9</sup> Craven and de Reuck,<sup>10</sup> Poling,<sup>11</sup> Varushchenko et al.,<sup>12</sup> Huber et al.,<sup>13</sup> Hogge et al.<sup>14, 15</sup>) and systematically in our laboratory.<sup>16-47</sup> The SimCor is based on exact thermodynamic relationships and the procedure must therefore yield reliable results providing that the input data are of reasonable accuracy. A great advantage of this approach is that a single equation can furnish a description of the temperature dependences of several thermodynamic properties and the SimCor thus also provides a test on the consistency of different experimental data.

A full description of the SimCor Method was presented previously by Růžička and Majer,<sup>20</sup> however it is repeated here for reader's convenience.

Let us define auxiliary quantities  $\Delta H'$  and  $\Delta C'$ :

$$\Delta H' \equiv \Delta_{cd}^g H_m / \Delta_{cd}^g z \quad (S1)$$

$$\Delta C' \equiv (d\Delta H'/dT)_{sat} = \left[ \Delta_{cd}^g C_{p,m} - 2\Delta H' \left( \frac{\partial \Delta_{cd}^g z}{\partial T} \right)_p - \frac{p}{RT} \Delta H'^2 \left( \frac{\partial \Delta_{cd}^g z}{\partial p} \right)_T \right] / \Delta_{cd}^g z \quad (S2)$$

where  $\Delta_{cd}^g z$  stands for the difference between the compressibility factors of the coexisting condensed and gas phases,  $\Delta_{cd}^g H_m$  is the vaporization/sublimation enthalpy and  $\Delta_{cd}^g C_{p,m} = C_{p,m}^g - C_{p,m}^{cd}$  is the difference between isobaric heat capacity of gas and that of condensed phase at the saturation curve, i.e. at the vapor pressure  $p$  (the subscript ‘sat’ denotes a derivative along the saturation line;  $R$  is the molar gas constant).

The SimCor than starts from the Clapeyron equation in the form

$$\Delta H' = RT^2 (d \ln p / dT)_{sat} \quad (S3)$$

which relates the vapor pressure  $p$  to  $\Delta_{cd}^g H_m$  and the  $pVT$  behavior of the coexisting phases. The differentiation yields an equation relating vapor pressures to heat capacities

$$\Delta C' = R \left\{ d \left[ T^2 (d \ln p / dT) \right] / dT \right\}_{sat}. \quad (S4)$$

It is apparent that quantities  $\Delta H'$  and  $\Delta C'$  can be calculated exclusively from vapor pressure equation (eqs S3 and S4) or from thermal properties ( $\Delta_{cd}^g H_m$  and  $\Delta_{cd}^g C_{p,m}^0$ ) and appropriate  $pVT$  corrections (eqs S1 and S2). This means that after selecting a suitable vapor pressure equation it is possible to correlate simultaneously experimental values of  $p_{sat}$ ,  $\Delta_{cd}^g H_m$ , and  $\Delta_{cd}^g C_{p,m}^0$  as a function of temperature, resulting in a set of vapor pressure equation parameters which are valid in a combined temperature range of all input experimental values.

While calorimetry is a source of  $\Delta_{cd}^g H_m$  and  $C_{p,m}^{cd}$ , the heat capacity of real gas is obtained using

$$C_{p,m}^g = C_{p,m}^{g0} - T \int_0^{p_{sat}} \left( \frac{\partial^2 V_m^g}{\partial T^2} \right) dp \quad (S5)$$

where  $C_{p,m}^{g0}$  is isobaric heat capacity of ideal gas, evaluated usually from spectroscopic (or *ab initio*) vibrational frequencies by means of statistical thermodynamics, and  $V_m^g$  is molar volume of gas phase.

Generally, the  $pVT$  term in eq S1 (i.e. term  $\Delta_{cd}^g z$ ) represents correction around (3 to 7) percent to  $\Delta_{cd}^g H_m$  at the normal boiling point temperature  $T_b$ , while  $pVT$  terms in eq S2 can amount up to 40 percent of  $\Delta_{cd}^g C_{p,m}$  value (see Fig. 1 on page 28 in Růžička and Majer<sup>20</sup>). Since data for exact

evaluation of  $pVT$  corrections are generally not available, all authors using the SimCor method had to select either of the two possible solutions:

- i) To neglect the  $pVT$  correction in eqs S1 and S2 at all. This implies that enthalpies of vaporization/sublimation  $\Delta_{cd}^g H_m$  can be included in the SimCor at saturated pressures smaller than 1 kPa and heat capacity difference  $\Delta_{cd}^g C_{p,m}$  at saturated pressures less than 10 Pa. For example in the case of naphthalene<sup>16</sup> this corresponds to temperature of triple point temperature  $T_{tr}=353.37$  K ( $p=993.5$  Pa,  $pVT$  correction in eq S1 represents 0.19 %) and  $T=280$  K ( $p=1.6$  Pa,  $pVT$  correction in eq S2 represents 0.17 %).
- ii) To express the  $pVT$  correction by means of second virial coefficients (and molar volumes of liquid/solid phase). As experimental second virial coefficients are typically not available for temperatures well below the normal boiling temperature  $T_{nbp}$ , estimation methods must be used. This means that the uncertainty of  $pVT$  corrections is high and limits inclusion of thermal properties in the SimCor. Thus to avoid the distortion of SimCor by errors in  $pVT$  description,  $\Delta_{cd}^g H_m$  can be included in the SimCor at saturated pressures smaller than approximately 10 kPa and heat capacity difference  $\Delta_{cd}^g C_{p,m}$  at saturated pressures less than approximately 1 kPa; in case of hydrogen-bonding compounds as in this work, the upper pressure limit was set to 500 Pa only.

When the volume of gaseous phase is expressed as  $V_m^g = \frac{RT}{p} + B$ , eq S1 can be written as

$$\Delta H' = \frac{\Delta_{cd}^g H_m}{1 + \frac{P_{sat}}{RT} (B - V_m^{cd})} \quad (S6)$$

and eq S4 can be converted (after neglecting the pressure dependence of  $V_m^{cd}$ ) to the form<sup>1</sup>

$$\Delta C' = \Delta_{cd}^g C_{p,m}^0 - T \frac{d^2 B}{dT^2} P_{sat} - 2T \frac{d(B - V_m^{cd})}{dT} \left( \frac{dp}{dT} \right)_{sat} - T (B - V_m^{cd}) \left( \frac{d^2 p}{dT^2} \right)_{sat} \quad (S7)$$

The molar volume of saturated condensed phase  $V_m^{cd}$  and its temperature derivative play negligible role at temperatures well below the normal boiling temperature, where eqs S6 and S7 are applied.

Several estimation methods for the second virial coefficient can be found in the literature. We prefer the method suggested by Tsonopoulos,<sup>48</sup> as it provides also (empirical) corrections for polar compounds. Input parameters for this estimation method are given in Table S1. Note that in the limits suggested for applying  $pVT$  correction ( $P_{sat} < 10$  kPa in eq S6 and  $P_{sat} < 1$  kPa in eq S7) even large change of input parameters would not influence resulting vapor pressures and

enthalpies of vaporization. The molar volumes of the liquid phase along the saturation line play a negligible role in the temperature range considered and were therefore neglected.

**Table S1** Input Parameters Used for Evaluation of the Second Virial Coefficients by Tsonopoulos' Method<sup>48</sup>

compound	T <sub>c</sub> / K <sup>a</sup>	p <sub>c</sub> /MPa <sup>a</sup>	ω <sup>b</sup>	μ / D <sup>c</sup>
1-heptanol	632.6	3.058	0.568	1.76
1-octanol	652.5	2.777	0.580	1.78
1-nonal	670.7	2.528	0.599	1.80
1-decanol	687.3	2.315	0.625	1.82

<sup>a</sup> critical temperature and pressure recommended by Gude and Teja.<sup>49</sup>

<sup>b</sup> acentric factor calculated by the SimCor.

<sup>c</sup> dipole moment calculated at the DFT B3LYP/6-311+G(df,p) level of theory for 1-heptanol. For 1-octanol, 1-nonal, and 1-decanol, it was estimated based on shorter chained alcohols (from 1-pentanol to 1-heptanol, the dipole moment is 1.72, 1.74 and 1.76, so we can reasonably expect the trend to still be the same).

Any vapor pressure equation can be used in the SimCor method providing it is flexible enough to describe input properties within their assumed uncertainties. Different equations were tested by Růžička and Majer.<sup>50</sup> The Cox equation<sup>51</sup> (eq 3 in this paper) was used in most of our works as it is flexible and (in contrast to Wagner equation, which otherwise performs also quite well) does not require critical temperature and critical pressure.

The parameters of the vapor pressure equation are obtained by minimizing an objective function *S*, which is defined as

$$S = \sum_{i=1}^{m_p} \frac{(\ln p_{\text{sat}}^{\text{exp}} - \ln p_{\text{sat}}^{\text{calc}})_i^2}{\sigma_i^2 \ln p_{\text{sat}}} + K_H^2 \sum_{i=1}^{m_H} \frac{(\Delta H'_{\text{exp}} - \Delta H'_{\text{calc}})_i^2}{\sigma_i^2 \Delta H'} + K_C^2 \sum_{i=1}^{m_C} \frac{(\Delta C'_{\text{exp}} - \Delta C'_{\text{calc}})_i^2}{\sigma_i^2 \Delta C'}. \quad (\text{S8})$$

The quantities with the superscript “exp” relate to the experimental data ( $\Delta H'_{\text{exp}}$  are calculated by means of eq S6 and  $\Delta C'_{\text{exp}}$  by means of eq S7). The quantities with the superscript “calc” are expressed from the Cox equation (eq 3) and eqs S3 and S4. The individual data points are weighted using the expected uncertainties of the experimental data. As a starting point, uncertainties claimed in the original data source are used. Very often, the original uncertainties are too optimistic and they are raised during SimCor or the whole dataset is even excluded from the correlation, when inconsistency with other types of data is observed. The quantity  $\sigma_i^2 \ln p_{\text{sat}}$  is obtained from errors in temperature ( $\sigma T$ ) and pressure ( $\sigma p$ )

$$\sigma_i^2 \ln p_{\text{sat}} = \left( \frac{\sigma p}{p} \right)^2 + \left( \frac{d \ln p}{dT} \right)^2 (\sigma T)^2. \quad (\text{S9})$$

In this work,  $\sigma p$  in “medium” pressure range was more or less comparable (20 Pa,<sup>52,53</sup> 40 Pa,<sup>54</sup> 100 Pa<sup>55</sup>), however  $\sigma T$  for vapor pressures obtained by DTA technique<sup>55</sup> is significantly higher

(0.1 K) than  $\sigma T$  for ebulliometric measurements<sup>52, 53 54</sup> (0.01 K).  $\sigma_i^2 \Delta H'$  is evaluated from the uncertainty in the enthalpy of vaporization/sublimation as  $\sigma_i^2 \Delta H' = (\sigma \Delta_{cd}^g H_m)^2$ . It is usually set to 5 percent for vaporization enthalpy obtained by drop calorimetry and 1 percent for vaporization enthalpy measured in Lund laboratory (using the Wadsö<sup>56</sup> or the Morawetz calorimeter<sup>57</sup>) which is included in SimCor (given in bold in Table 5).

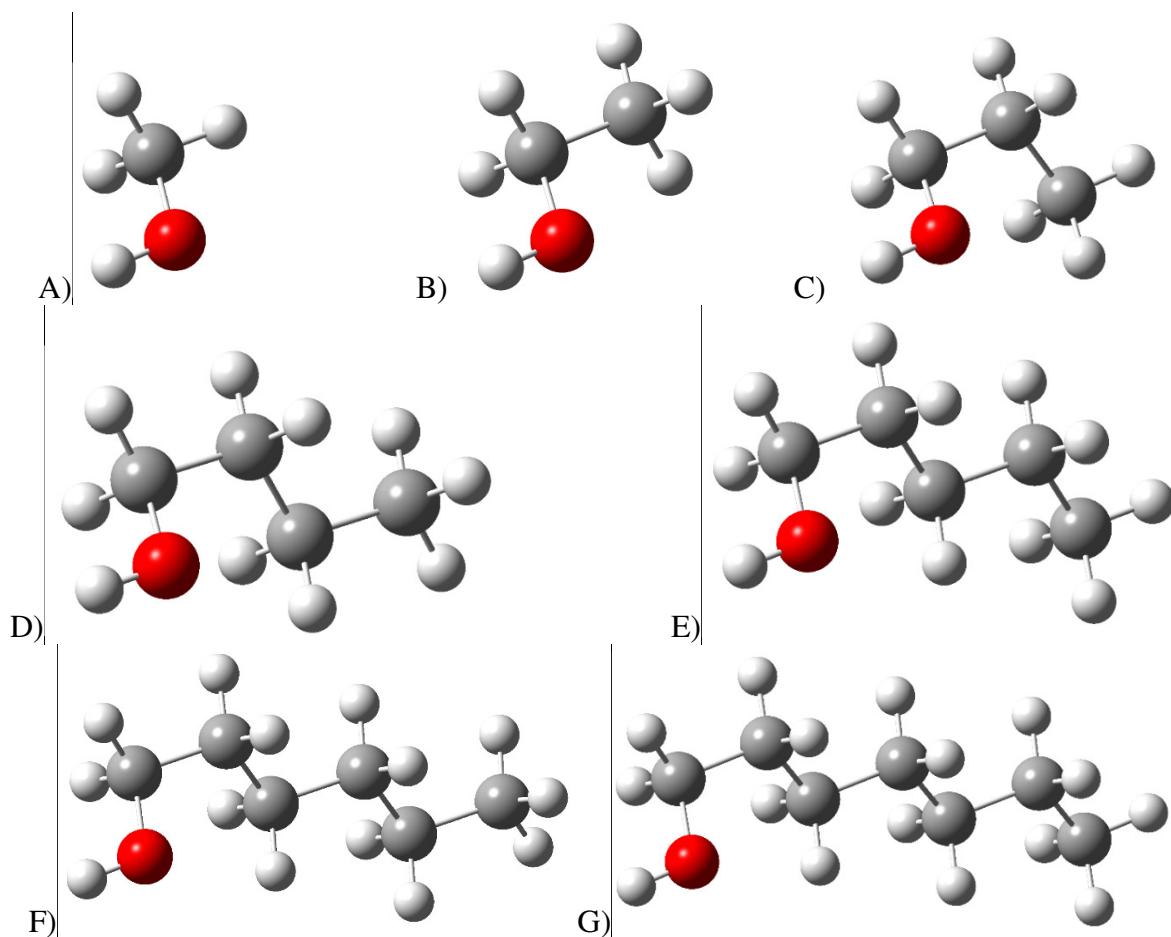
Finally,  $\sigma_i^2 \Delta C'$  is estimated from the expected uncertainties in heat capacities of respective phases

$$\sigma_i^2 \Delta C' = (\sigma C_{p,m}^g)^2 + (\sigma C_{p,m}^{cd})^2 \quad (S10)$$

$\sigma C_{p,m}^{cd}$  for values included in SimCor (given in bold in Table 7) calculated from eq 1 with parameters from Table 8 was set to 1 percent for data from Tian-Calvet calorimeters and 0.3 percent for data from adiabatic calorimeters.  $\sigma C_{p,m}^g$  is tabulated set to 0.5 to 0.9 percent (see Table 10 and Table S5) for  $C_{p,m}^g$ . Weighing factors  $K_H^2$  and  $K_C^2$  are set to unity unless inconsistency between the different types of data is observed. Whenever possible, the inconsistency is resolved by new measurements instead of by changing  $K_H^2$  and  $K_C^2$ .

## 2. Details on DFT calculations

For all molecules, calculations of optimized molecular geometry, fundamental vibrational frequencies and potential energy surfaces of internal rotations were performed using the density functional theory (DFT) at the B3LYP/6-311+G(d,p) level of theory. The results of conformational study are summed in Table S2, which lists stable conformers (the most stable conformers are shown in Figure S1), their relative energies, symmetries, dipole moments, products of inertia  $I_{ABC}^{\text{calc}}$ . The parameters of methyl rotations are listed in Table S3.



**Figure S1** Lowest-energy conformers for each of the seven molecules. (A) methanol; (B) ethanol t; (C) 1-propanol tg; (D) 1-butanol tgt; (E) 1-pentanol tgtt; (F) 1-hexanol tgttt; (G) 1-heptanol tgtttt.

**Table S2** Conformational Study of Methanol, Ethanol, 1-Propanol, 1-Butanol, 1-Pentanol, 1-Hexanol, and 1-Heptanol. Stable Conformers Treated in the R1TM Approach (Described in Section 3.4 of the Main Article) at the B3LYP/6-311+G(2df,p) Level of Theory and Their Relative Energies, Symmetries, Dipole Moments  $\mu$ , and Products of Inertia  $I_{ABC}^{\text{calc}}$

Conformer	symmetry <sup>a</sup>	$\Delta_r H_{ij}^0 /$ kJ mol <sup>-1</sup>	$\mu /$ $D$	$I_{ABC}^{\text{calc}} /$ $10^{-135}$ $\text{kg}\cdot\text{m}^2$	Conformer	symmetry <sup>a</sup>	$\Delta_r H_{ij}^0 /$ kJ mol <sup>-1</sup>	$\mu /$ $D$	$I_{ABC}^{\text{calc}} /$ $10^{-135}$ $\text{kg}\cdot\text{m}^2$
methanol					gggtg	$C_1$	5.277	1.660	105.76
	$C_S$	0.000	1.770	0.0078349	gg'tg'g'	$C_1$	5.312	1.857	104.81
ethanol					ggtg'g'	$C_1$	5.388	1.717	97.958
t	$C_S$	0.000	1.663	0.22083	gttgg	$C_1$	5.589	1.904	119.88
1-propanol					gggtg'	$C_1$	5.646	1.592	99.435
tg	$C_1$	0.000	1.568	1.8632	gtg'g't	$C_1$	5.964	1.839	122.75
gt	$C_1$	0.238	1.825	1.7078	gtg'tg'	$C_1$	6.369	1.852	109.33
1-butanol					gd'gtt	$C_1$	6.422	2.074	117.20
tgt	$C_1$	0.000	1.561	9.1468	tgg'g't	$C_1$	6.707	1.748	87.637
gtt	$C_1$	0.616	1.840	8.7355	gtg'tg	$C_1$	6.763	1.844	96.281
ggg	$C_1$	2.459	1.702	9.0722	ggggg	$C_1$	7.282	1.587	80.210
gtg'	$C_1$	3.687	1.892	9.6754	ggg'tg'	$C_1$	7.911	1.660	101.65
ggg'	$C_1$	5.469	1.689	8.8134	gtg'g'g'	$C_1$	8.186	1.794	101.23
gd'g	$C_1$	7.444	2.012	8.9253	ggg'tg	$C_1$	8.417	1.573	97.352
1-pentanol					gd'gt	$C_1$	9.341	2.044	102.33
tgtt	$C_1$	0.000	1.549	35.752	tgg'g'g'	$C_1$	9.460	1.720	75.779
tg'tg	$C_1$	0.449	1.861	30.067	gg'g'dt	$C_1$	9.479	1.956	96.745
tgg'g'	$C_1$	2.409	1.667	34.385	gd'gtg'	$C_1$	10.03	2.058	99.310
gtg't	$C_1$	2.828	1.475	35.801	ggdg't	$C_1$	10.75	1.639	105.94
gtg'd	$C_1$	3.341	1.908	32.034	gtd'gt	$C_1$	10.92	1.813	125.76
ggdg'	$C_1$	3.350	1.887	27.951	gtg'dt	$C_1$	11.44	1.883	125.94
ggg't	$C_1$	3.459	1.807	35.383	tgtdg'	$C_1$	11.65	1.524	100.04
g'ttt	$C_1$	4.929	1.656	34.922	gg'dtg'	$C_1$	11.67	1.733	97.840
g'ttg'	$C_1$	5.084	1.615	31.696	ggdg'g'	$C_1$	11.82	1.672	76.920
g'tgg	$C_1$	5.975	1.866	27.102	ggdg'g	$C_1$	12.14	1.619	102.53
g'tdg'	$C_1$	6.757	1.974	36.885	tgtg'd	$C_1$	12.19	1.430	98.838
g'gtg	$C_1$	7.027	1.694	36.413	gttdg'	$C_1$	12.40	1.884	125.68
g'ggd'	$C_1$	10.36	2.015	30.480	gg'tg'd	$C_1$	12.41	1.866	107.23
g'g'g't	$C_1$	11.18	1.688	37.584	gttdg'	$C_1$	12.53	1.937	120.17
g'g'g'g'	$C_1$	11.33	1.883	28.868	gggd'g'	$C_1$	12.60	1.663	81.366
g'dg't	$C_1$	11.91	1.891	36.839	tgg'dt	$C_1$	12.86	1.641	85.281
g'g'gd'	$C_1$	13.91	1.783	38.626	gtd'gg	$C_1$	13.09	1.822	102.09
1-hexanol					ggggd'	$C_1$	14.11	1.631	84.653
tgttt	$C_1$	0.000	1.556	106.52	gggdg'	$C_1$	14.28	1.613	89.617
gtttt	$C_1$	0.460	1.867	91.629	gtg'g'd	$C_1$	14.49	1.871	98.636
gggtt	$C_1$	2.313	1.673	117.13	gtg'dg	$C_1$	14.54	1.813	109.51
tgttg'	$C_1$	2.902	1.553	120.44	gtg'd'g	$C_1$	15.28	1.857	109.91
ggtg't	$C_1$	3.055	1.654	94.929	tgg'dg	$C_1$	16.67	1.540	80.866
gg'ttg'	$C_1$	3.140	1.877	119.45	ggg'g'd	$C_1$	17.03	1.589	74.426
gg'tg't	$C_1$	3.285	1.799	107.56	tgg'd'g	$C_1$	17.29	1.624	85.394
gttgt	$C_1$	3.347	1.820	120.82	tgg'd'g	$C_1$	17.34	1.698	76.232
gtg'tt	$C_1$	3.394	1.890	121.41	tgg'g'd	$C_1$	17.96	1.750	73.748
gtttg	$C_1$	3.461	1.887	111.19	gg'ddg'	$C_1$	18.59	1.760	88.911
ggg'tt	$C_1$	4.886	1.658	114.71	gtd'gd'	$C_1$	20.03	1.851	97.397
ggggt	$C_1$	4.994	1.689	99.729	ggdg'd	$C_1$	20.53	1.603	87.333
1-heptanol									
					tgtttt	$C_1$	0.000	1.549	289.79
					gttttt	$C_1$	0.411	1.881	228.76
					gggttt	$C_1$	2.244	1.649	311.47
					tgttg't	$C_1$	2.846	1.558	342.85
					ggtg'tt	$C_1$	2.927	1.650	271.34

Conformer	symmetry <sup>a</sup>	$\Delta_r H_{ij}^0 /$ kJ mol <sup>-1</sup>	$\mu / D$	$I_{ABC}^{\text{calc}}$ $10^{-135}$	/ kg·m <sup>2</sup>
gg'ttg't	C <sub>1</sub>	3.087	1.878	336.60	
gg'ttg	C <sub>1</sub>	3.103	1.882	281.25	
gg'ttg'	C <sub>1</sub>	3.124	1.932	303.77	
gg'tg'tt	C <sub>1</sub>	3.186	1.883	327.70	
gttgtt	C <sub>1</sub>	3.234	1.905	377.55	
gtttgt	C <sub>1</sub>	3.340	1.883	304.01	
gtg'ttt	C <sub>1</sub>	3.345	1.808	300.60	
gttttg'	C <sub>1</sub>	3.393	1.891	298.47	
ggggtt	C <sub>1</sub>	4.807	1.600	280.90	
ggg'ttt	C <sub>1</sub>	4.820	1.644	304.71	
tgttg'g'	C <sub>1</sub>	5.006	1.568	300.62	
gg'tg'g't	C <sub>1</sub>	5.091	1.824	308.25	
gggtgt	C <sub>1</sub>	5.143	1.640	294.13	
gggttg'	C <sub>1</sub>	5.171	1.669	311.83	
gggttg	C <sub>1</sub>	5.202	1.593	296.92	
gg'ttg'g'	C <sub>1</sub>	5.291	1.896	299.75	
ggtg'g't	C <sub>1</sub>	5.322	1.620	281.98	
gttggt	C <sub>1</sub>	5.371	1.867	360.55	
gtttg'g'	C <sub>1</sub>	5.587	1.929	321.05	
gggtgt	C <sub>1</sub>	5.612	1.682	264.74	
gtg'g'tt	C <sub>1</sub>	5.677	1.844	357.69	
ggtg'tg'	C <sub>1</sub>	5.929	1.662	270.62	
gg'tg'tg'	C <sub>1</sub>	6.120	1.843	271.29	
gttgtg	C <sub>1</sub>	6.212	1.863	330.68	
gtg'tg't	C <sub>1</sub>	6.240	1.843	283.01	
gtg'tg'	C <sub>1</sub>	6.269	1.875	341.91	
gtg'tg	C <sub>1</sub>	6.291	1.886	356.38	
ggtg'tg	C <sub>1</sub>	6.343	1.723	242.91	
tgg'g'tt	C <sub>1</sub>	6.348	1.790	250.33	
gd'gtt	C <sub>1</sub>	6.359	2.015	309.35	
gg'tg'tg	C <sub>1</sub>	6.499	1.838	267.49	
gttgtg'	C <sub>1</sub>	6.513	1.864	274.54	
gggtgg	C <sub>1</sub>	6.614	1.672	235.37	
gtg'tgt	C <sub>1</sub>	6.733	1.850	234.67	
gggggt	C <sub>1</sub>	7.026	1.625	226.33	
gg'tg'g'g'	C <sub>1</sub>	7.404	1.785	256.24	
ggtg'g'g'	C <sub>1</sub>	7.505	1.716	249.68	
ggggtg	C <sub>1</sub>	7.505	1.658	256.85	
ggg'ttg	C <sub>1</sub>	7.534	1.673	290.80	
gttggg	C <sub>1</sub>	7.631	1.841	287.07	
ggg'g't	C <sub>1</sub>	7.740	1.634	277.46	
ggg'ttg	C <sub>1</sub>	7.751	1.578	293.07	
gtg'g'g't	C <sub>1</sub>	7.840	1.870	297.61	
gggtg'g'	C <sub>1</sub>	7.894	1.598	240.36	
ggggtg'	C <sub>1</sub>	8.159	1.634	249.62	
gtg'tg'g'	C <sub>1</sub>	8.365	1.917	296.07	
ggg'tgt	C <sub>1</sub>	8.366	1.663	253.62	
gtg'g'tg'	C <sub>1</sub>	8.442	1.842	310.89	
gtg'tgg	C <sub>1</sub>	9.048	1.912	265.75	
gtg'g'tg	C <sub>1</sub>	9.100	1.773	287.12	
gd'gtgt	C <sub>1</sub>	9.126	2.043	272.65	
gg'g'dtt	C <sub>1</sub>	9.133	2.038	273.26	
gd'gttg	C <sub>1</sub>	9.164	2.082	298.65	
tgg'g'g't	C <sub>1</sub>	9.166	1.768	221.04	
tgg'g'tg'	C <sub>1</sub>	9.176	1.715	207.54	
gd'gttg'	C <sub>1</sub>	9.239	2.101	298.46	

Conformer	symmetry <sup>a</sup>	$\Delta_r H_{ij}^0 /$ kJ mol <sup>-1</sup>	$\mu / D$	$I_{ABC}^{\text{calc}}$ $10^{-135}$	/ kg·m <sup>2</sup>
gggggg	C <sub>1</sub>	9.329	1.646	191.23	
ggg'tg'g'	C <sub>1</sub>	9.601	1.663	237.41	
gd'gtg't	C <sub>1</sub>	9.979	2.049	256.51	
tgg'g'tg	C <sub>1</sub>	10.00	1.760	222.94	
gtg'g'g'g'	C <sub>1</sub>	10.17	1.785	228.27	
ggdg'tt	C <sub>1</sub>	10.56	1.663	312.90	
ggg'tgg	C <sub>1</sub>	10.63	1.574	240.74	
gtd'gtt	C <sub>1</sub>	10.68	1.852	368.78	
tgtdg't	C <sub>1</sub>	11.12	1.618	296.24	
ggdg'g't	C <sub>1</sub>	11.18	1.687	210.74	
gtg'dtt	C <sub>1</sub>	11.25	1.865	363.31	
gd'gtgg	C <sub>1</sub>	11.28	2.130	249.49	
tgg'g'g'g'	C <sub>1</sub>	11.47	1.734	181.59	
ggtg'dt	C <sub>1</sub>	11.55	1.638	296.35	
gg'dtg't	C <sub>1</sub>	11.58	1.763	260.81	
tgttg'd	C <sub>1</sub>	11.66	1.495	304.76	
gg'ttdg'	C <sub>1</sub>	11.69	1.957	301.47	
gttg'dt	C <sub>1</sub>	11.74	1.893	372.76	
gg'tg'dt	C <sub>1</sub>	11.74	1.869	316.04	
tgtd'gt	C <sub>1</sub>	11.75	1.464	288.51	
gg'ttd'g	C <sub>1</sub>	11.99	1.959	299.67	
gg'g'dtg	C <sub>1</sub>	11.99	2.026	239.70	
gttdg't	C <sub>1</sub>	12.01	1.876	366.79	
gg'ttg'd	C <sub>1</sub>	12.06	1.957	314.73	
gg'g'dgt	C <sub>1</sub>	12.19	2.028	217.13	
gd'gtg'g'	C <sub>1</sub>	12.30	2.133	248.97	
gttdt'dg	C <sub>1</sub>	12.30	1.972	321.36	
gtd'ggt	C <sub>1</sub>	12.39	1.874	284.26	
gtttg'd	C <sub>1</sub>	12.41	1.924	333.47	
tgg'dtt	C <sub>1</sub>	12.57	1.550	238.94	
gg'g'dtg'	C <sub>1</sub>	12.76	1.996	242.82	
gggtgd'	C <sub>1</sub>	12.84	1.645	222.72	
ggtggd'	C <sub>1</sub>	13.06	1.667	217.61	
tgtdg'g'	C <sub>1</sub>	13.21	1.501	241.46	
ggggd't	C <sub>1</sub>	13.24	1.587	244.73	
tgtg'g'd	C <sub>1</sub>	13.59	1.407	243.50	
gtg'g'dt	C <sub>1</sub>	13.63	1.805	286.30	
ggdg'tg'	C <sub>1</sub>	13.64	1.581	259.65	
ggdg'g'g'	C <sub>1</sub>	13.68	1.653	186.18	
gggdg't	C <sub>1</sub>	13.77	1.634	247.03	
gtd'gtg	C <sub>1</sub>	13.78	1.808	316.20	
gttg'g'd	C <sub>1</sub>	13.79	2.003	279.56	
tgtd'gg	C <sub>1</sub>	13.79	1.495	248.77	
gg'dtg'g'	C <sub>1</sub>	13.79	1.798	236.37	
gttdg'g'	C <sub>1</sub>	13.96	1.860	293.03	
ggdg'tg	C <sub>1</sub>	14.07	1.656	267.61	
gggtgd'	C <sub>1</sub>	14.08	1.574	260.37	
gtg'dtg	C <sub>1</sub>	14.15	1.890	312.07	
gtd'gtg'	C <sub>1</sub>	14.16	1.767	299.29	
gtg'dgt	C <sub>1</sub>	14.33	1.894	321.46	
gggtgd'g	C <sub>1</sub>	14.63	1.562	242.11	
ggtg'dg	C <sub>1</sub>	14.72	1.653	271.88	
gtg'dtg'	C <sub>1</sub>	14.72	1.816	296.49	
gg'tg'd'g	C <sub>1</sub>	14.74	1.877	270.91	
gggtg'd	C <sub>1</sub>	14.79	1.624	263.04	
gtg'd'gt	C <sub>1</sub>	14.80	1.809	321.66	

Conformer	symmetry <sup>a</sup>	$\Delta_r H_{ij}^0 /$ kJ mol <sup>-1</sup>	$\mu / D$	$I_{ABC}^{\text{calc}}$ $10^{-135}$	/ kg·m <sup>2</sup>
gg'tg'dg	<i>C</i> <sub>1</sub>	14.90	1.789	265.59	
gttg'd'g'	<i>C</i> <sub>1</sub>	14.94	1.814	325.71	
gtg'td'g	<i>C</i> <sub>1</sub>	15.05	1.870	297.76	
gg'g'dgg	<i>C</i> <sub>1</sub>	15.09	2.012	193.33	
gg'tgdg'	<i>C</i> <sub>1</sub>	15.11	1.961	273.33	
gtd'ggg	<i>C</i> <sub>1</sub>	15.11	1.789	244.41	
gttgdg'	<i>C</i> <sub>1</sub>	15.16	1.917	308.08	
ggg'dtg	<i>C</i> <sub>1</sub>	15.26	1.734	199.30	
gtg'tg'd	<i>C</i> <sub>1</sub>	15.28	1.821	288.33	
gggdg'g'	<i>C</i> <sub>1</sub>	15.64	1.678	213.76	
gtg'tdg'	<i>C</i> <sub>1</sub>	15.65	1.872	273.24	
gggggd'	<i>C</i> <sub>1</sub>	15.88	1.572	199.94	
ggggd'g'	<i>C</i> <sub>1</sub>	15.98	1.666	207.66	
gtg'tgd'	<i>C</i> <sub>1</sub>	16.04	1.830	268.69	
tgg'dtg'	<i>C</i> <sub>1</sub>	16.06	1.651	216.33	
ggg'g'dt	<i>C</i> <sub>1</sub>	16.15	1.554	216.99	
gtg'g'dg	<i>C</i> <sub>1</sub>	16.20	1.799	235.46	
ggg'td'g	<i>C</i> <sub>1</sub>	16.38	1.625	233.03	
tgg'dgt	<i>C</i> <sub>1</sub>	16.41	1.495	233.09	
gtg'd'gg	<i>C</i> <sub>1</sub>	16.43	1.851	238.68	
tgg'd'gt	<i>C</i> <sub>1</sub>	16.73	1.730	245.78	
tgg'd'gt	<i>C</i> <sub>1</sub>	16.79	1.829	222.84	
ggg'tg'd	<i>C</i> <sub>1</sub>	16.87	1.582	250.90	
gtg'g'g'd	<i>C</i> <sub>1</sub>	16.99	1.814	244.57	
tgg'g'dt	<i>C</i> <sub>1</sub>	17.03	1.872	213.12	
tgg'd'gg	<i>C</i> <sub>1</sub>	17.24	1.798	176.89	
ggg'tdg'	<i>C</i> <sub>1</sub>	17.36	1.547	243.19	
ggg'tgd'	<i>C</i> <sub>1</sub>	17.82	1.605	243.28	
gg'g'g'd'g	<i>C</i> <sub>1</sub>	18.00	1.988	210.23	
gg'ddg't	<i>C</i> <sub>1</sub>	18.09	1.703	252.19	
tgg'g'g'd	<i>C</i> <sub>1</sub>	18.15	1.649	182.68	
ggg'g'dg	<i>C</i> <sub>1</sub>	18.30	1.556	170.10	
gd'gtgd'	<i>C</i> <sub>1</sub>	18.37	2.039	251.21	
gd'gtdg'	<i>C</i> <sub>1</sub>	18.52	2.114	252.15	
gd'gtd'g	<i>C</i> <sub>1</sub>	18.60	2.079	247.22	
gtd'gd't	<i>C</i> <sub>1</sub>	18.70	1.838	263.86	
ggdg'dt	<i>C</i> <sub>1</sub>	19.12	1.674	239.23	
gggd'd'g	<i>C</i> <sub>1</sub>	19.26	1.611	196.78	
tgtdg'd	<i>C</i> <sub>1</sub>	19.34	1.637	209.41	
ggg'g'd'g	<i>C</i> <sub>1</sub>	19.51	1.543	203.17	
ggg'dgg	<i>C</i> <sub>1</sub>	19.57	1.707	195.32	
gd'gtg'd	<i>C</i> <sub>1</sub>	19.78	2.073	242.18	
gg'ggd'g'	<i>C</i> <sub>1</sub>	20.45	1.765	178.60	
gg'dtg'd	<i>C</i> <sub>1</sub>	20.66	1.731	249.97	
gd'gd'g'g'	<i>C</i> <sub>1</sub>	20.67	2.055	212.47	
gttd'gd'	<i>C</i> <sub>1</sub>	20.73	1.996	272.16	
gg'tdg'd	<i>C</i> <sub>1</sub>	21.14	1.953	246.45	
gtg'ddg'	<i>C</i> <sub>1</sub>	21.76	1.827	259.00	
gtd'gd'g'	<i>C</i> <sub>1</sub>	22.46	1.773	249.82	
tgdg'g'd	<i>C</i> <sub>1</sub>	22.46	1.378	179.58	
gg'd'ggg'	<i>C</i> <sub>1</sub>	22.90	2.072	186.47	
ggdg'dg	<i>C</i> <sub>1</sub>	22.94	1.590	220.21	
gg'dgdg'	<i>C</i> <sub>1</sub>	23.16	1.714	220.17	
gggdg'd	<i>C</i> <sub>1</sub>	23.31	1.591	223.20	
ggdg'd'g	<i>C</i> <sub>1</sub>	23.38	1.643	192.41	
gtd'gdg'	<i>C</i> <sub>1</sub>	23.97	1.802	248.80	

Conformer	symmetry <sup>a</sup>	$\Delta_r H_{ij}^0 /$ kJ mol <sup>-1</sup>	$\mu / D$	$I_{ABC}^{\text{calc}}$ $10^{-135}$	/ kg·m <sup>2</sup>
gtg'd'gd'	<i>C</i> <sub>1</sub>	24.11	1.777	261.92	
gtd'ggd'	<i>C</i> <sub>1</sub>	24.18	1.839	239.39	
gg'gd'd'g	<i>C</i> <sub>1</sub>	24.19	2.040	204.01	
ttgd'g'd	<i>C</i> <sub>1</sub>	24.73	1.677	246.47	
tgg'd'gd'	<i>C</i> <sub>1</sub>	26.44	1.737	179.17	
ggg'dgd'	<i>C</i> <sub>1</sub>	26.90	1.656	178.77	
gg'ddg'd	<i>C</i> <sub>1</sub>	27.47	1.684	211.32	

<sup>a</sup> conformers with a mirror plane are included once in the mixing model, conformers without a mirror plane have two isomorphs, both of them are to be included.

**Table S3** Parameters of Top Rotations in Studied Compounds

Compound	Type of top	Internal symmetry number	Reduced moment of inertia <sup>a</sup> $I_r / 10^{-47} \text{ kg m}^2$	Fourier expansion parameters <sup>a,b</sup> $/ \text{J mol}^{-1}$
methanol	methyl	3	1.06474	$V_0 = 2115, V_3^{\cos} = -2115$
	methyl	3	4.35373	$V_0 = 6573, V_3^{\cos} = -6573$
	hydroxyl	1	1.27873	$V_0 = 2338, V_1^{\cos} = -302,$ $V_2^{\cos} = 116, V_3^{\cos} = -2294,$ $V_4^{\cos} = 131$
ethanol	methyl	3	4.96357	$V_0 = 5570, V_3^{\cos} = -5570$
	hydroxyl	1	1.30431	$V_0 = 2367,$ $V_1^{\cos} = -984, V_1^{\sin} = -137,$ $V_2^{\cos} = 733, V_2^{\sin} = -350,$ $V_3^{\cos} = -2191, V_3^{\sin} = 313$
1-propanol	methyl	3	4.84913	$V_0 = 6262, V_3^{\cos} = -6262$
	hydroxyl	1	1.31556	$V_0 = 2373,$ $V_1^{\cos} = -931, V_1^{\sin} = -154,$ $V_2^{\cos} = 682, V_2^{\sin} = -237,$ $V_3^{\cos} = -2191, V_3^{\sin} = 69$
1-butanol	methyl	3	5.02814	$V_0 = 6190, V_3^{\cos} = -6190$
	hydroxyl	1	1.32334	$V_0 = 2306,$ $V_1^{\cos} = -861, V_1^{\sin} = -227,$ $V_2^{\cos} = 685, V_2^{\sin} = -200,$ $V_3^{\cos} = -2191, V_3^{\sin} = 77$
1-pentanol	methyl	3	4.98678	$V_0 = 6165, V_3^{\cos} = -6165$
	hydroxyl	1	1.32757	$V_0 = 2311,$ $V_1^{\cos} = -839, V_1^{\sin} = -229,$ $V_2^{\cos} = 681, V_2^{\sin} = -201,$ $V_3^{\cos} = -2187, V_3^{\sin} = 77$
1-hexanol	methyl	3	5.06406	$V_0 = 6166, V_3^{\cos} = -6166$
	hydroxyl	1	1.33170	$V_0 = 2343,$ $V_1^{\cos} = -825, V_1^{\sin} = -245,$ $V_2^{\cos} = 683, V_2^{\sin} = -194,$ $V_3^{\cos} = -2189, V_3^{\sin} = 79$
1-heptanol	methyl	3		
	hydroxyl	1		

<sup>a</sup> for the lowest-energy conformer.

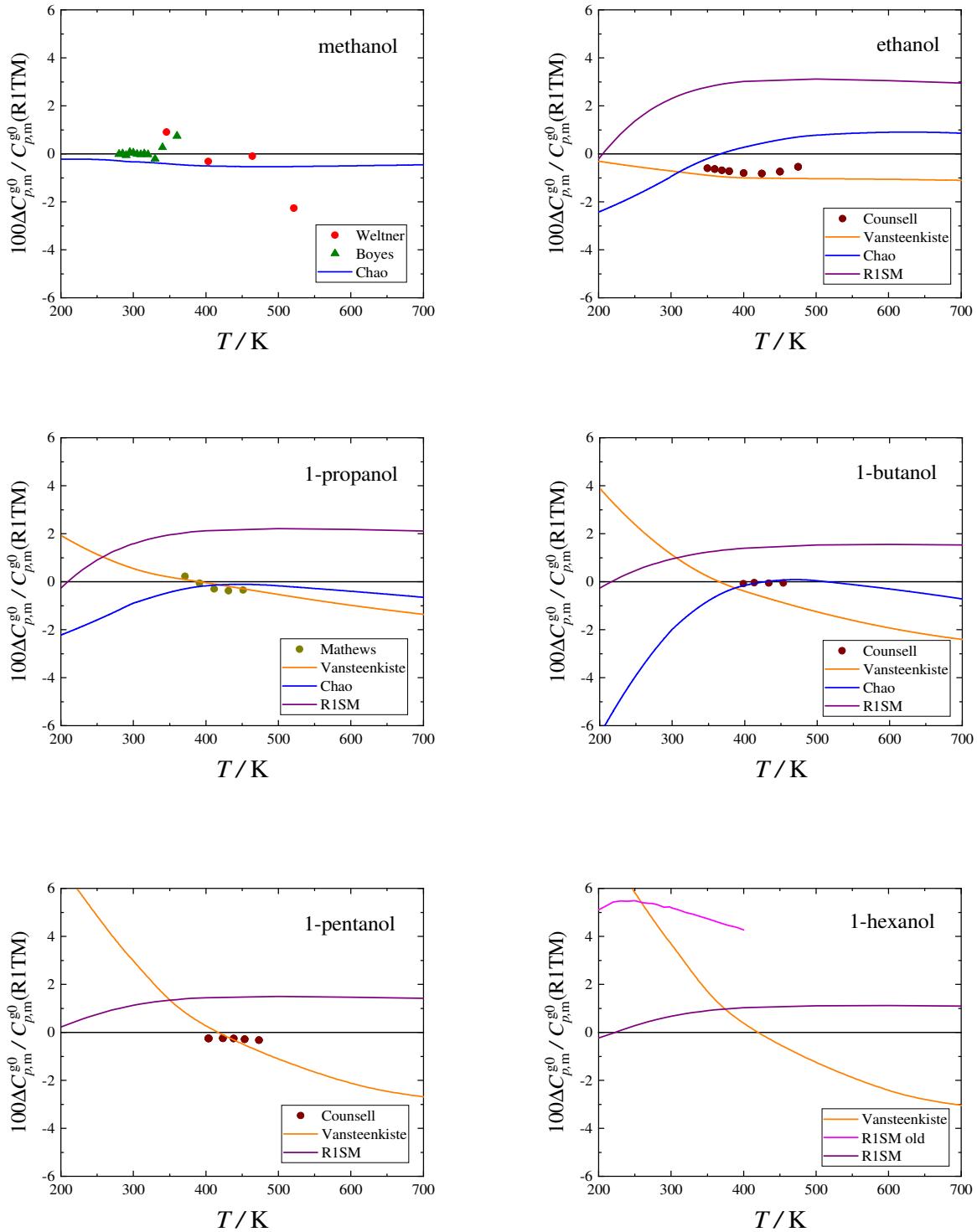
$$\begin{aligned} b \quad V = & V_0 + V_1^{\cos} \cdot \cos(x) + V_1^{\sin} \cdot \sin(x) + V_2^{\cos} \cdot \cos(2x) + V_2^{\sin} \cdot \sin(2x) + V_3^{\cos} \cdot \cos(3x) + V_3^{\sin} \cdot \sin(3x) \\ & + V_4^{\cos} \cdot \cos(4x) \end{aligned}$$

**Table S4** Standard Molar Thermodynamic Functions (in  $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ) of Methanol, Ethanol and 1-Propanol in the Ideal Gaseous State at  $p = 10^5 \text{ Pa}^{\text{a}}$

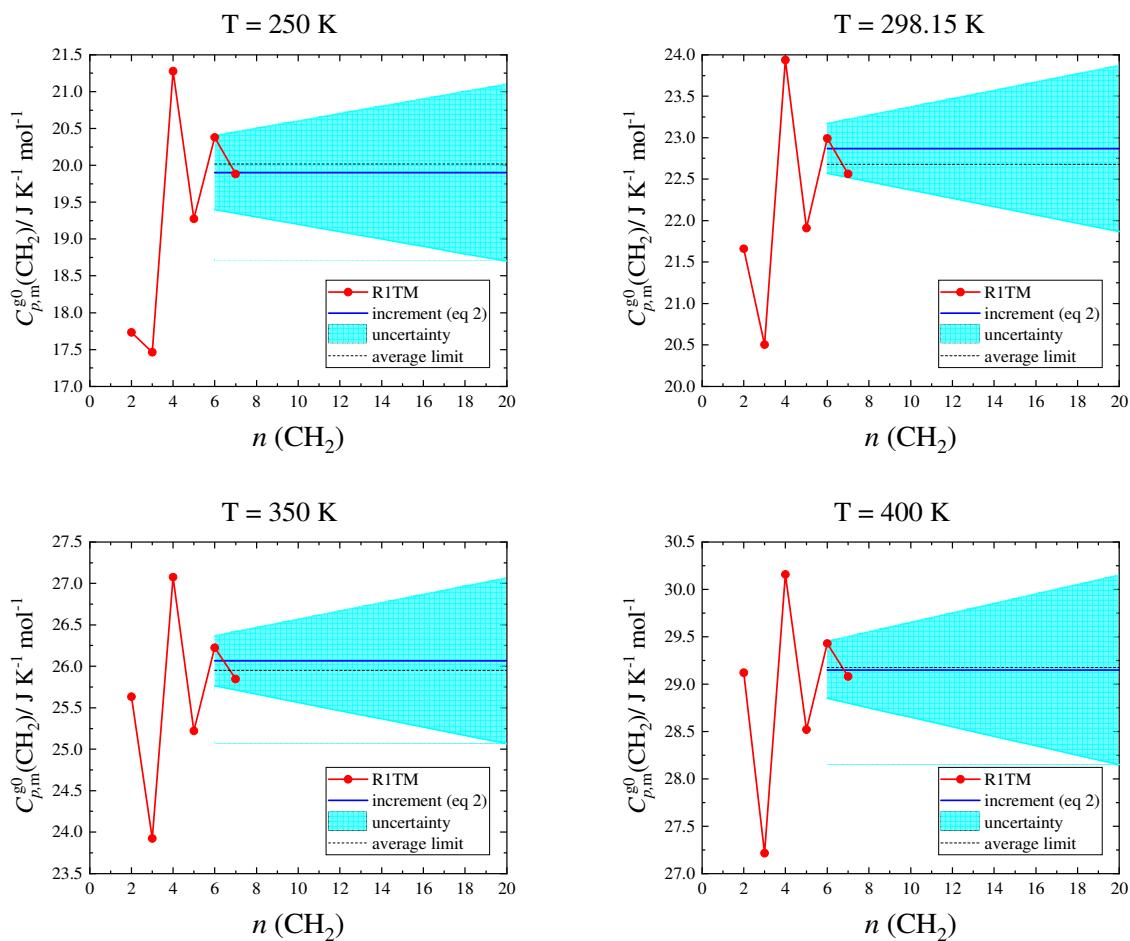
T/K	methanol		1-ethanol		1-propanol	
	$C_{p,\text{m}}^{\text{g}0}$	$S_{\text{m}}^{\text{g}0}$	$C_{p,\text{m}}^{\text{g}0}$	$S_{\text{m}}^{\text{g}0}$	$C_{p,\text{m}}^{\text{g}0}$	$S_{\text{m}}^{\text{g}0}$
200	39.77	223.6	53.31	258.7	67.88	294.9
210	40.04	225.6	54.42	261.3	69.55	298.2
220	40.34	227.4	55.57	263.9	71.26	301.5
230	40.69	229.2	56.75	266.4	73.02	304.7
240	41.08	231.0	57.98	268.8	74.84	307.9
250	41.52	232.7	59.25	271.2	76.71	311.0
260	41.99	234.3	60.55	273.6	78.63	314.0
270	42.51	235.9	61.90	275.9	80.60	317.0
273.15	42.69	236.4	62.33	276.6	81.23	317.9
280	43.08	237.4	63.28	278.1	82.61	320.0
290	43.67	239.0	64.68	280.4	84.66	322.9
298.15	44.19	240.2	65.85	282.2	86.35	325.3
300	44.31	240.5	66.12	282.6	86.74	325.8
310	44.97	241.9	67.57	284.8	88.85	328.7
320	45.67	243.4	69.04	287.0	90.98	331.5
330	46.39	244.8	70.53	289.1	93.13	334.4
340	47.13	246.2	72.02	291.2	95.28	337.2
350	47.89	247.6	73.52	293.4	97.45	340.0
360	48.67	248.9	75.03	295.4	99.61	342.8
370	49.46	250.3	76.53	297.5	101.8	345.5
380	50.26	251.6	78.03	299.6	103.9	348.3
390	51.07	252.9	79.52	301.6	106.1	351.0
400	51.88	254.2	81.00	303.7	108.2	353.7
500	60.02	266.7	95.04	323.3	128.4	380.1
600	67.53	278.3	107.28	341.7	146.0	405.1
700	74.20	289.2	117.82	359.1	161.1	428.7
$u_r^{\text{b}}$	0.8%	0.3%	0.7%	0.4%	0.8%	0.5%

<sup>a</sup> Values were calculated combining R1TM approach with B3LYP-D3/6-311+G(df,p) quantum-chemical calculations. Calculated fundamental frequencies were scaled by a double-linear scaling factor SF ( $\nu > 2000 \text{ cm}^{-1}$ ) = 0.960; SF ( $\nu < 2000 \text{ cm}^{-1}$ ) =  $0.9948 - 1.35 \cdot 10^{-5} \nu_i$ .<sup>58</sup>

<sup>b</sup> Standard relative uncertainty estimated according to the scheme presented in ref<sup>58</sup>.



**Figure S2** Relative deviations of ideal-gas heat capacities from the values obtained in this work by the means of the R1TM approach. Experimental data points (Weltner and Pitzer,<sup>59</sup> Boyes et al.,<sup>60</sup> Counsell et al.,<sup>61-63</sup> Mathews and McKetta<sup>64</sup>) are displayed as symbols and theoretical calculations (Vansteenkiste,<sup>65</sup> Chao and Hall,<sup>66</sup> R1SM old (Štejfa et al.),<sup>35</sup> R1SM approach from this work) are displayed as lines.



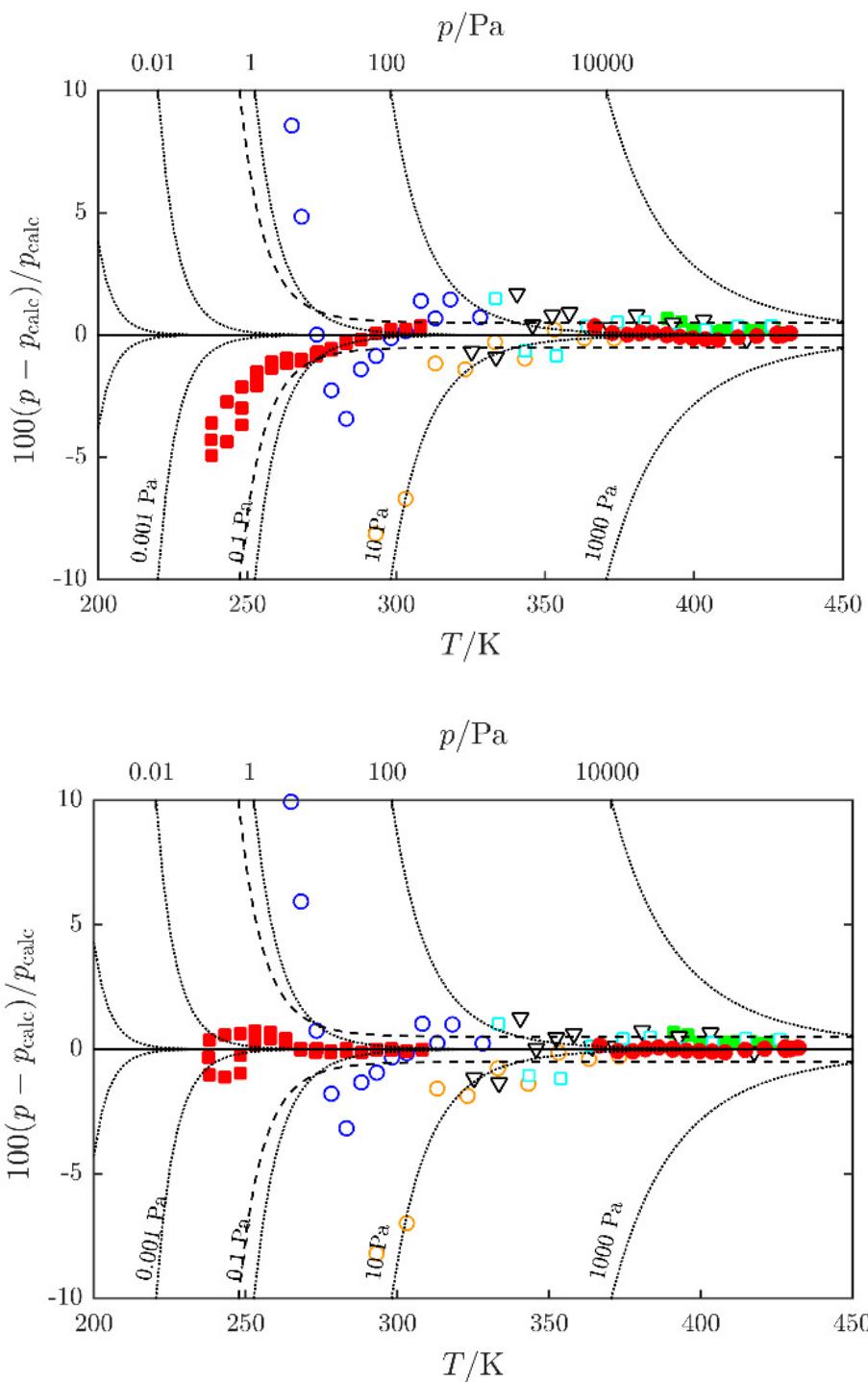
**Figure S3** Contribution of the CH<sub>2</sub> increment  $C_{p,m}^{g0}(\text{CH}_2) = C_{p,m}^{g0}(\text{C}_n\text{OH}) - C_{p,m}^{g0}(\text{C}_{n-1}\text{OH})$  to the molar heat capacity of linear aliphatic alcohols: dependence on the number of carbon atoms (with extrapolation towards longer-chained aliphatic alcohols: blue —, based on eq 2 with parameters from Table 12; ...., obtained by averaging the two previous values) at different temperatures (250 K, 298.15 K, 350 K, 400 K).

**Table S5.** Standard Molar Thermodynamic Functions (in  $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ) of 1-Octanol, 1-Nonanol, and 1-Decanol in the Ideal Gaseous State at  $p = 10^5 \text{ Pa}^{\text{a}}$

$T/\text{K}$	1-octanol		1-nonanol		1-decanol	
	$C_{p,\text{m}}^{\text{g}0}$	$S_{\text{m}}^{\text{g}0}$	$C_{p,\text{m}}^{\text{g}0}$	$S_{\text{m}}^{\text{g}0}$	$C_{p,\text{m}}^{\text{g}0}$	$S_{\text{m}}^{\text{g}0}$
250	178.1	480.6	198.4	514.8	218.7	548.9
260	182.7	487.6	203.5	522.6	224.4	557.5
270	187.4	494.6	208.8	530.3	230.3	566.0
273.15	188.9	496.8	210.5	532.7	232.1	568.6
280	192.2	501.5	214.2	537.9	236.2	574.4
290	197.1	508.3	219.7	545.5	242.3	582.8
298.15	201.2	513.8	224.2	551.7	247.3	589.6
300	202.1	515.1	225.2	553.1	248.4	591.1
310	207.1	521.8	230.9	560.6	254.6	599.3
320	212.3	528.4	236.6	568.0	260.9	607.6
330	217.4	535.1	242.3	575.4	267.2	615.7
340	222.6	541.7	248.1	582.8	273.5	623.9
350	227.9	548.2	253.9	590.1	279.9	632.0
360	233.1	554.8	259.7	597.4	286.3	640.1
370	238.3	561.3	265.5	604.7	292.7	648.2
380	243.6	567.8	271.3	612.0	299.0	656.2
390	248.8	574.4	277.1	619.3	305.4	664.3
400	253.9	580.9	282.8	626.6	311.7	672.4
$ur^{\text{b}}$	0.6%	0.7%	0.7%	0.8%	0.8%	0.9%

<sup>a</sup> Calculated using Eq 2 optimized based on  $C_{p,\text{m}}^{\text{g}0}$  for 1-pentanol, 1-hexanol, and 1-heptanol and tested on 1-butanol (see chapter 3.4) with parameters from Table 13.

<sup>b</sup> Standard relative uncertainty estimated according to the scheme presented in ref<sup>58</sup> increased by the uncertainty of the  $\text{CH}_2$  increment (see figure S3)



**Figure S4** Comparison of vapor pressures of 1-hexanol obtained by SimCor when using previously published  $C_{p,m}^{g0}$  (Štejfa et al.,<sup>35</sup> top) and new  $C_{p,m}^{g0}$  calculated in this work using the R1TM approach with B3LYP-D3/6-311+G(df,p) quantum-chemical calculations (bottom). Cyan □, Butler et al.,<sup>67</sup> ▽, Kemme and Kreps;<sup>55</sup> orange ○, Wolff and Shadiakhy,<sup>68</sup> blue ○, Kulikov et al.,<sup>69</sup> green ■, Schmitt and Hasse;<sup>70</sup> red ●, Čenský et al.;<sup>54</sup> red ■, Štejfa et al.<sup>35</sup>

### 3. Recommended Vaporization Enthalpies

The enthalpy of vaporization can be calculated using the Cox equation, eq 3, with parameters given in Table 13 and  $pVT$  behavior using eq S6. This requires the knowledge of the second virial coefficient  $B$ , which was estimated using the Tsonopoulos method.<sup>48</sup> For the reader's convenience, recommended values of  $\Delta_1^g H_m$  are tabulated in Table S6 at discrete temperatures together with their estimated uncertainties.

**Table S6** Recommended Enthalpies of Vaporization of 1-Hexanol, 1-Heptanol, 1-Octanol, 1-Nonanol, and 1-Decanol.<sup>a</sup>

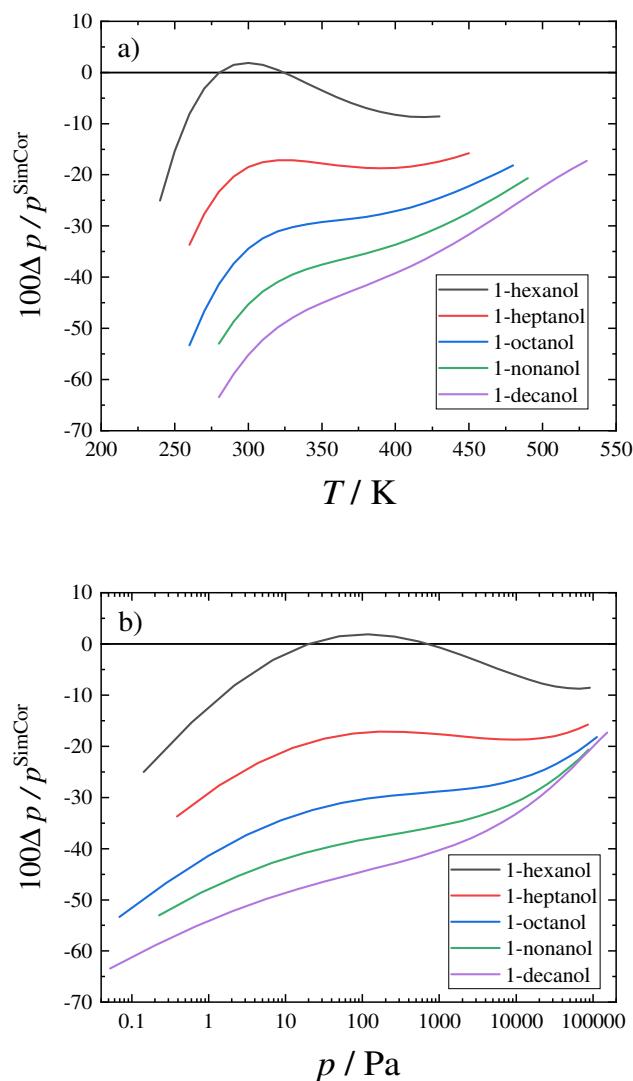
T / K	$\Delta_1^g H_m$ / kJ·mol <sup>-1</sup>				
	1-Hexanol	1-Heptanol	1-Octanol	1-Nonanol	1-Decanol
240	65.88 ± 0.79				
250	65.28 ± 0.72				
260	64.63 ± 0.66	69.79 ± 0.84	74.37 ± 0.89		
270	63.93 ± 0.61	69.02 ± 0.75	73.69 ± 0.80		
280	63.17 ± 0.57	68.19 ± 0.67	72.89 ± 0.71	78.31 ± 1.29	83.37 ± 0.82
290	62.36 ± 0.54	67.29 ± 0.61	72.00 ± 0.65	77.26 ± 1.00	82.23 ± 0.74
300	61.49 ± 0.52	66.32 ± 0.56	71.02 ± 0.60	76.13 ± 0.84	81.00 ± 0.69
310	60.58 ± 0.52	65.30 ± 0.56	69.95 ± 0.59	74.92 ± 0.83	79.68 ± 0.68
320	59.61 ± 0.52	64.22 ± 0.55	68.80 ± 0.59	73.64 ± 0.82	78.29 ± 0.66
330	58.60 ± 0.53	63.09 ± 0.55	67.59 ± 0.58	72.29 ± 0.82	76.83 ± 0.65
340	57.54 ± 0.54	61.92 ± 0.55	66.32 ± 0.58	70.90 ± 0.82	75.32 ± 0.64
350	56.43 ± 0.56	60.70 ± 0.56	64.99 ± 0.59	69.46 ± 0.82	73.76 ± 0.63
360	55.28 ± 0.57	59.45 ± 0.57	63.62 ± 0.60	67.98 ± 0.84	72.16 ± 0.63
370	54.08 ± 0.59	58.16 ± 0.59	62.22 ± 0.61	66.47 ± 0.87	70.54 ± 0.64
380	52.83 ± 0.61	56.84 ± 0.60	60.79 ± 0.63	64.94 ± 0.91	68.90 ± 0.65
390	51.55 ± 0.63	55.49 ± 0.62	59.34 ± 0.64	63.39 ± 0.95	67.25 ± 0.66
400	50.22 ± 0.64	54.12 ± 0.64	57.88 ± 0.65	61.84 ± 0.99	65.61 ± 0.66
410	48.86 ± 0.66	52.73 ± 0.66	56.42 ± 0.67	60.29 ± 1.02	63.98 ± 0.67
420	47.46 ± 0.68	51.33 ± 0.67	54.96 ± 0.68	58.75 ± 1.07	62.36 ± 0.69
430	46.04 ± 0.69	49.92 ± 0.68	53.52 ± 0.69	57.22 ± 1.09	60.78 ± 0.70
440		48.50 ± 0.70	52.10 ± 0.70	55.71 ± 1.14	59.23 ± 0.71
450		47.09 ± 0.71	50.72 ± 0.71	54.23 ± 1.17	57.73 ± 0.72
460			49.37 ± 0.72	52.79 ± 1.19	56.28 ± 0.73
470			48.08 ± 0.72	51.40 ± 1.21	54.90 ± 0.74
480			46.85 ± 0.73	50.06 ± 1.21	53.59 ± 0.75
490				48.79 ± 1.22	52.37 ± 0.76
500					51.23 ± 0.77
510					50.20 ± 0.78
520					49.28 ± 0.79
530					48.49 ± 0.80

<sup>a</sup> The stated uncertainties reflect the uncertainties of the input data. The SimCor method has been used several times while varying the input data by their uncertainties. The stated expanded uncertainties (0.95 level of confidence) are the resulting variations of the fitted values for  $\Delta_1^g H_m$ .

## 4. Comparison of experimental and estimated vapor pressures

Estimation methods are not very successful when applied to vapor pressures of alkanols. Rarey and coworkers had to use additional term in their estimation method,<sup>71</sup> yet the average relative deviation for alcohols in the “medium” pressure range (5.5 %) were significantly worse than for hydrocarbons (1.9 %). Updated method<sup>72</sup> improved average relative deviation to 4.1 %, thus confirming that estimation of vapor pressure of alcohols is challenging.

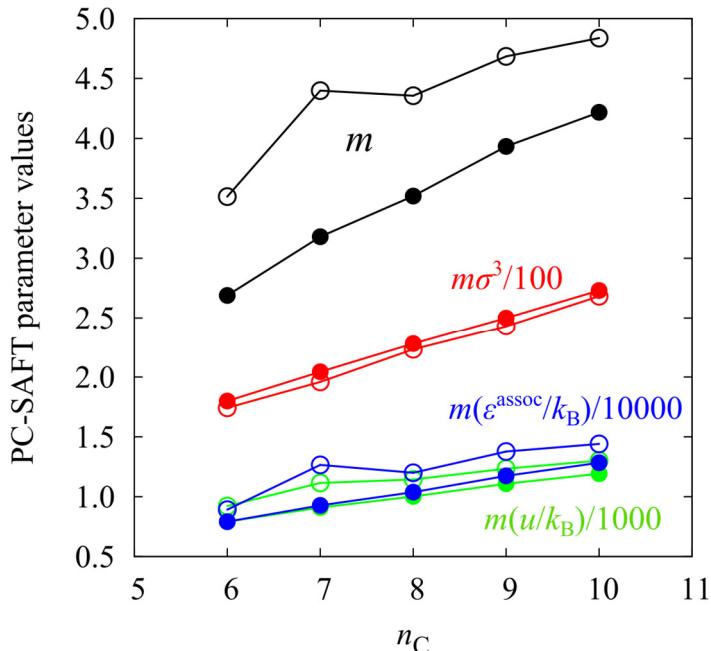
Figure S5 shows deviations of estimated vapor pressures (Moller et al.,<sup>72</sup> as implemented in the Artist software package<sup>73</sup>) from values recommended in this work as a function of temperature (top) and pressure (bottom). Differences are increasing with decreasing temperature/pressure.



**Figure S5.** Comparison of vapor pressure obtained by the estimation method of Rarey and Moller<sup>72</sup> (as implemented in the Artist software package<sup>73</sup>) with vapor pressure recommended in this work ( $p^{\text{SimCor}}$ )  $\Delta p = p^{\text{Rarey}} - p^{\text{SimCor}}$ . a) dependence on temperature, b) dependence on pressure ( $p^{\text{SimCor}}$ ) in the logarithmic scale. The estimation method of Rarey and Moller<sup>72</sup> requires the normal boiling point as an input. For this purpose, normal boiling point temperature estimated using the method by Rarey and coworkers<sup>74</sup> was used.

## 5. Dependence of PC-SAFT Parameters on the Number of Carbon Atoms

Figure S6 shows the dependence of both the previously reported<sup>75 76</sup> PC-SAFT parameters and those developed in this work (Table 14) on the number of carbon atoms for the homologous series 1-hexanol to 1-decanol.



**Figure S6.** Dependence of the PC-SAFT parameters of 1-alkanols on the number of carbon atoms: ○, previously reported PC-SAFT parameter sets;<sup>75 76</sup> ●, PC-SAFT parameter sets determined in this work. The lines are to guide the eyes. The linear equations for the parameters from this work are:  $m = 0.3809n_C + 0.4605$ ;  $m\sigma^3/100 = 0.2318n_C + 0.4158$ ;  $m(u/k_B)/1000 = 0.0997n_C + 0.2039$ ; and  $m(\epsilon_{assoc}/k_B)/10000 = 0.1230n_C + 0.0584$ .

Note that the previously reported<sup>75</sup> PC-SAFT parameters are based on values extracted from the DIPPR database.<sup>77</sup> This industrially oriented database is reporting parameters of smoothing equation and also data used to derive these parameters. Table S7 shows references quoted by DIPPR for 1-heptanol (all of them contain smoothed data) and corresponding references containing experimental vapor pressures.

**Table S7** 1-Heptanol: sources of literature vapor pressures used in the DIPPR database

DIPPR reference	Reference to original data
Stull (1947) <sup>78</sup>	Anschütz and Reitter (1895) <sup>79</sup> Butler et al. (1935) <sup>67</sup>
Boublík et al. (1973) <sup>80</sup>	Kemme and Kreps (1969) <sup>55</sup>
Wilhoit and Zwolonski (1973) <sup>81</sup>	Butler et al. (1935) <sup>67</sup> Thomas and Meatyard (1963) <sup>82</sup> Kemme and Kreps (1969) <sup>55</sup>
TRC Tables (1980) <sup>83</sup>	Butler et al. (1935) <sup>67</sup> Thomas and Meatyard (1963) <sup>82</sup> Kemme and Kreps (1969) <sup>55</sup>
Smith and Srivastava (1986) <sup>84</sup>	Kemme and Kreps (1969) <sup>55</sup> Deffet (1931, only $T_{\text{nbp}}$ ) <sup>85</sup>

Such “multilevel referencing” (criticized e.g. by Li and Wania<sup>86</sup>) leads DIPPR users to a conclusion, that there is mutual agreement between five “independent” sources,<sup>78, 80, 81, 83, 84</sup> and therefore utilization of such data is safe. In fact, only three sources of original vapor pressures were used,<sup>55, 67, 82</sup> and the first two sources were rejected in the frame of this work (as well as by Ambrose and Walton<sup>87</sup>). The situation for remaining alkanols is similar.

One should be also careful when using freely accessible database NIST WebBook<sup>88</sup>, which is updated much less frequently than its professional counterpart;<sup>89</sup> the most recent reference containing vapor pressures for the title compound was published in 1975.<sup>90</sup>

To conclude, data sources can be roughly divided into three categories (see also section *Sources of Data for the Reference/Calibration Compounds* in Růžička et al.:<sup>91</sup>): bibliographic sources, sources suitable for engineering use (DIPPR database,<sup>77</sup> and NIST WebBook<sup>88</sup> belong to this category), and sources suitable for scientific use (typically review papers or collections of **critically assessed data**).

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