Supporting Information

Air-water partitioning of C5 and C6 alkanones. Measurement, Critical Compilation, Correlation, and Recommended Data

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Table S1. Parameters for Estimation of the Second Virial Coefficients by the Hayden-O'Connell Method: Critical Temperature T_c, Critical Pressure P_c, Radius of Gyration R_D, Dipole Moment μ, Association Constant η_{ii}, and Solvation Constant $\eta_{i,water}$

Liquid	T_c / K[a]	P_c / MPa[a]	R_D / Å[b]	μ / D[c]	η_{ii}[d]	$\eta_{i,water}$[d]
pentan-2-one	561	3.70	3.618	2.77	0.9	1.0
pentan-3-one	562	3.73	3.583	2.82	0.9	1.0
3-methylbutan-2-one	555	3.79	3.465	2.76	0.9	1.0
hexan-2-one	587	3.32	4.093	2.68	0.9	1.0
hexan-3-one	583	3.32	4.009	2.87	0.9	1.0
3-methylpentan-2-one	573[f]	3.32[f]	3.828	2.77	0.9	1.0
4-methylpentan-2-one	575[g]	3.27[g]	3.572	2.69	0.9	1.0
2-methylpentan-3-one	567[f]	3.32[f]	3.892	3.12	0.9	1.0
3,3-dimethylbutan-2-one	567	3.47	3.800	2.75	0.9	1.0
water	647.14	21.491	0.615	1.83	1.7[e]	–

[a] From reference 1.

[b] From reference 2.

[c] From reference 3.

[d] From reference 4, the value assumed to be the same as for butan-2-one.

[e] From reference 4.

[f] From reference 5.

[g] From reference 6.

Table S2. Experimental Values of Air-Water Partition Coefficient and Activity Coefficient of Alkanones at Infinite Dilution in Water Reported in the Literature[a] along with Their Estimated Standard Uncertainties[b] and Experimental Method[c]

T/ K	$1000 \cdot K_{aw}$	$u_{rel}(K_{aw})$	γ_1^{∞}	$u_{rel}(\gamma_1^{\infty})$	method	ref
pentan-2-one						
301.15	**4.4**	0.1	111	0.1	EPICS	68NEL/HOF[7]
298.15	**2.6**	0.2	75.8	0.2	HSA	69BUT/LIN[8]
303.15	**4.1**	0.1	93.8	0.1	HSA	71NAW[9]
310.15	**6.02**	0.1	99.8	0.1	PRV	79SAT/NAK[10]
298.15	3.39	0.03	**98.9**	0.03	GLC	80MAS/PEM[11]
310.2	**7.24**	0.05	120	0.05	IGS	81KUH/BOC[12]
298.15	4.63	0.2	**135.1**	0.2	GLC/LLC	86JAN/QAD[13]
303.15	5.46	0.2	**125.0**	0.2	GLC/LLC	86JAN/QAD[13]
308.15	7.15	0.2	**129.7**	0.2	GLC/LLC	86JAN/QAD[13]
298.15	3.52	0.05	**102.5**	0.05	GLC/LLC	88DJE/LAU[14]
298.15	3.50	0.05	**102**	0.05	NSGLC	91LAN/BEL[15]
298.15	3.23	0.03	**94.3**	0.02	HSA	93DAL[16]
298.15	**3.42**	0.03	99.7	0.03	IGS	97SHI/MAC[17]
303.25	4.61	0.03	**105**	0.03	IGS	04ATI/GRU[18]
313.25	8.30	0.03	**120**	0.03	IGS	04ATI/GRU[18]
323.25	13.5	0.03	**128**	0.03	IGS	04ATI/GRU[18]

333.25	21.0	0.03	**135**	0.03	IGS	04ATI/GRU[18]
297.85	4.36	0.2	**129**	0.2	RGLC	05STR/DEL[19]
298.15	5.08	0.5	**148**	0.2	RGLC	05STR/DEL[19]
298.15	**3.41**	0.03	99.4	0.03	MHE	05BRA/CHA[20]
323.15	**12.3**	0.05	117	0.05	RHSA	05CHA/FAL[21]
333.15	**18.7**	0.05	121	0.05	RHSA	05CHA/FAL [21]
343.15	**27.8**	0.05	125	0.05	RHSA	05CHA/FAL [21]
353.15	**39.7**	0.03	127	0.03	RHSA	05CHA/FAL [21]
278.15	**0.67**	0.2	57.5	0.2	HSA	07JI/EVA[22]
283.15	**0.95**	0.2	61.1	0.2	HSA	07JI/EVA[22]
288.15	**1.30**	0.2	63.5	0.2	HSA	07JI/EVA[22]
293.15	**1.82**	0.2	68.3	0.2	HSA	07JI/EVA[22]
298.15	**2.45**	0.2	71.4	0.2	HSA	07JI/EVA[22]
pentan-3-one						
310.15	**5.53**	0.2	91.5	0.2	PRV	79SAT/NAK[10]
298.15	3.87	0.03	**113**	0.03	GLC	80MAS/PEM[11]
310.2	**8.32**	0.03	137	0.03	IGS	81KUH/BOC[12]
298.15	4.62	0.2	**134.8**	0.2	GLC/LLC	86JAN/QAD[13]
303.15	6.10	0.2	**139.6**	0.2	GLC/LLC	86JAN/QAD[13]
308.15	9.94	0.2	**180**	0.2	GLC/LLC	86JAN/QAD[13]

298.15	3.87	0.03	**113**	0.03	NSGLC	91LAN/BEL[15]
298.15	3.68	0.03	**107.4**	0.03	HSA	93DAL[16]
278.15	**0.72**	0.2	62.1	0.2	RHSA	07JI/EVA[22]
283.15	**0.99**	0.2	64.0	0.2	RHSA	07JI/EVA[22]
288.15	**1.39**	0.2	68.1	0.2	RHSA	07JI/EVA[22]
293.15	**1.93**	0.2	72.5	0.2	RHSA	07JI/EVA[22]
298.15	**2.56**	0.5	74.7	0.2	RHSA	07JI/EVA[22]
293.2	**1.93**[d]	0.2	72.2	0.2	TENS	10OFA/WAG[23]
3-methylbutan-2-one						
298.15	4.20	0.05	**84**	0.05	HSA	93DAL[16]
hexan-2-one						
303.15	**5.3**	0.1	359	0.1	HSA	71NAW[9]
310.15	**9.0**	0.1	425	0.1	PRV	79SAT/NAK[10]
298.15	4.14	0.03	**368**	0.03	GLC	80MAS/PEM[11]
310.2	**9.33**	0.02	439	0.02	IGS	81KUH/BOC[12]
298	3.67	0.1	**329**	0.1	GLC/LLC	88DJE/LAU[14]
298.15	4.00	0.05	**355.7**	0.03	HSA	93DAL[16]
298.15	2.98	0.2	**265**	0.2	RGLC	05STR/DEL[19]
297.85	3.53	0.2	**319**	0.2	RGLC	05STR/DEL[19]
323.15	**16.5**	0.1	419	0.1	RHSA	05CHA/FAL[21]

333.15	**25.3**	0.1	416	0.1	RHSA	05CHA/FAL[21]
343.15	**37.0**	0.1	406	0.1	RHSA	05CHA/FAL[21]
353.15	**59.2**	0.05	446	0.05	RHSA	05CHA/FAL[21]
298.15	**4.3**	0.03	382	0.03	MHE	05BRA/CHA[20]
hexan-3-one						
298.15	5.66	0.03	**412**	0.03	GLC	80MAS/PEM[11]
310.2	**12.9**	0.01	507	0.03	IGS	81KUH/BOC[12]
275.15	**39**	– [e]	11000	– [e]	EPICS	99DEW/LAN[24]
279.15	**55**	– [e]	12030	– [e]	EPICS	99DEW/LAN[24]
283.15	**54**	– [e]	9230	– [e]	EPICS	99DEW/LAN[24]
291.15	**50**	– [e]	5350	– [e]	EPICS	99DEW/LAN[24]
298.15	**52**	– [e]	3780	– [e]	EPICS	99DEW/LAN[24]
4-methylpentan-2-one						
310.15	12.7	0.05	358	0.05	PRV	79SAT/NAK[10]
310.2	**14.1**	0.02	396	0.02	IGS	81KUH/BOC[12]
283.15	**28.4**[f]	– [e]	3350	– [e]	EPICS	88ASH[25]
288.15	**15.6**	1	1380	1	EPICS	88ASH[25]
293.15	**12.1**	1	804	1	EPICS	88ASH[25]
298.15	**15.9**	1	814	1	EPICS	88ASH[25]
303.15	**27.3**	1	1080	1	EPICS	88ASH[25]

313.15	**18.4**	0.1	451	0.1	HSA	92KOL/WEL[26]
333.15	**43.9**	0.05	459	0.05	HSA	92KOL/WEL[26]
343.15	**61.7**	0.05	441	0.05	HSA	92KOL/WEL[26]
353.15	**84.7**	0.05	424	0.05	HSA	92KOL/WEL[26]
298.15	**10.4**[g]	0.5	531	0.5	EPICS	14KIM/KIM[27]

[a] The property value reported in the original literature is given in bold, the other one was obtained from the interconversion formula $K_{\mathrm{aw}} = \gamma_1^{\infty} p_1^{\mathrm{s}} v_2^{\mathrm{L}} / (RT)$ assuming the ideal behavior of gas phase.

[b] The uncertainties were assigned in this work.

[c] EPICS, equilibrium partitioning in closed system; HSA, headspace analysis; RHSA, relative headspace analysis; PRV, phase ratio variation; GLC gas-liquid chromatography; RGLC relative gas-liquid chromatography; LLC liquid-liquid chromatography; NSGLC non-steady state gas-liquid chromatography; IGS, inert gas stripping; MHE, multiple headspace extraction; TENS, tensimetry.

[d] The original source reports the Henry's law constant $H_{12} = p_1 / x_1$ which was converted here to K_{aw} by $K_{\mathrm{aw}} = H_{12} v_2^{\mathrm{L}} / (RT)$.

[e] Rejected wrong value.

[f] The original source reports the Henry's law constant $H_c = p_1 / c_1$ which was converted here to K_{aw} by $K_{\mathrm{aw}} = H_c / (RT)$.

[g] The original source reports the inverse Henry's law constant $1/H_c = c_1 / p_1$ which was converted here to K_{aw} by $K_{\mathrm{aw}} = H_c / (RT)$.

Table S3. Values of Infinite Dilution Partial Molar Excess Enthalpy $\bar{H}_1^{E,\infty}$ [a] and Hydration Enthalpy $\Delta_{hyd}H_1$ [b] Used in the Simultaneous Correlation with Data on Limiting Activity Coefficient and Air-Water Partition Coefficient, Respectively, along with Their Estimated Standard Uncertainties (in Parentheses)

alkanone	T / K	$\frac{\bar{H}_1^{E,\infty}}{kJ \cdot mol^{-1}}$ [a]	ref	$\frac{\Delta_{hyd}H_1}{kJ \cdot mol^{-1}}$ [b]
pentan-2-one	298.15	-10.21 (0.15)	81DEL/STR[28]	-46.38 (0.5)
	288.15	-12.76 (0.05)	17DOH/REH[29]	
	298.15	-10.42 (0.05)	17DOH/REH[29]	-46.59 (0.5)
	308.15	-8.20 (0.03)	17DOH/REH[29]	
	318.15	-5.95 (0.02)	17DOH/REH[29]	
pentan-3-one	298.15	-10.9 (0.1)	81DEL/STR[28]	-47.29 (0.4)
	288.15	-13.01 (0.08)	17DOH/REH[29]	
	298.15	-10.68 (0.06)	17DOH/REH[29]	-47.07 (0.4)
	308.15	-8.37 (0.06)	17DOH/REH[29]	
	318.15	-6.09 (0.05)	17DOH/REH[29]	
3-methylbutan-2-one	298.15	-10.63 (0.1)	81DEL/STR[28]	-45.21 (0.4)
	288.15	-12.61 (0.05)	17DOH/REH[29]	
	298.15	-10.47 (0.04)	17DOH/REH[29]	-45.05 (0.4)
	308.15	-8.25 (0.03)	17DOH/REH[29]	
	318.15	-6.13 (0.03)	17DOH/REH[29]	
hexan-2-one	298.15	-9.46 (0.1)	81DEL/STR[28]	-50.32 (0.4)

	288.15	-12.23 (0.10)	17DOH/REH[29]	
	298.15	-9.46 (0.08)	17DOH/REH[29]	-50.32 (0.4)
	308.15	-6.58 (0.06)	17DOH/REH[29]	
	318.15	-3.92 (0.05)	17DOH/REH[29]	
4-methylpentan-2-one	288.15	-12.77 (0.08)	17DOH/REH[29]	
	298.15	-9.97 (0.08)	17DOH/REH[29]	-48.33 (0.4)
	308.15	-7.25 (0.05)	17DOH/REH[29]	
	318.15	-4.73 (0.04)	17DOH/REH[29]	
3,3-dimethylbutan-2-one	298.15	-9.5 (0.1)	81DEL/STR[28]	-45.08(0.5)

[a] Direct calorimetric measurements in the highly dilute region.

[b] Determined from $\Delta_{hyd}H_1 = \bar{H}_1^{E,\infty} - \Delta_{vap}H_1^0 + RT(1-\alpha_w T)$ where $\Delta_{vap}H_1^0$ is the pure solute standard vaporization enthalpy (taken from reference 30) and α_w is the thermal expansion coefficient of water.

Table S4. Values of Infinite Dilution Partial Molar Excess Heat Capacity $\bar{C}_{p,1}^{\mathrm{E},\infty}$ and Hydration Heat Capacity $\Delta_{\mathrm{hyd}}C_{p,1}$ at 298.15 K Used in the Simultaneous Correlation with Data on Limiting Activity Coefficient and Air-Water Partition Coefficient, Respectively, along with Their Estimated Standard Uncertainties (in Parentheses)

alkanone	$\frac{\bar{C}_{p,1}^{\mathrm{E},\infty}}{\mathrm{J\cdot K^{-1}\cdot mol^{-1}}}$		$\frac{\Delta_{\mathrm{hyd}}C_{p,1}}{\mathrm{J\cdot K^{-1}\cdot mol^{-1}}}$	ref
pentan-2-one			290 (10)[a]	17DOH/REH[29]
pentan-3-one	237[b] (6)	78ROU/PER[31] 96ZAB/RUZ[32]	301 (25)[c]	78ROU/PER[31] 81BUR[33]
			292 (15)[a]	17DOH/REH[29]
3-methylbutan-2-one			273 (10)[a]	17DOH/REH[29]
hexan-2-one			348 (10)[a]	17DOH/REH[29]
hexan-3-one	289[d] (29)	04PLY/PLY[34] 96ZAB/RUZ[32] 81BUR[33]	356[e] (36)	04PLY/PLY[34]
3-methylpentan-2-one	296[d] (30)	04PLY/PLY[34] 08KOL/KUK[35] 81BUR[33]	357[e] (36)	04PLY/PLY[34]
4-methylpentan-2-one			337 (10)[a]	17DOH/REH[29]
2-methylpentan-3-one	292[d]	04PLY/PLY[34] 08KOL/KUK[35] 81BUR[33]	357[e] (36)	04PLY/PLY[34]
3,3-dimethylbutan-2-one	277[d]	04PLY/PLY[34] 96ZAB/RUZ[32] 81BUR[33]	336[e] (34)	04PLY/PLY[34]

[a] The value of $\Delta_{\mathrm{hyd}}C_{p,1}$ reported here was taken from ref 29.

[b] The value of $\bar{C}_{p,1}^{\mathrm{E},\infty}$ reported here was calculated from $\bar{C}_{p,1}^{\mathrm{E},\infty} = \bar{C}_{p,1}^{\infty} - C_{p,1}^{\bullet}$ where $\bar{C}_{p,1}^{\infty}$ is the solute partial molar heat capacity at infinite dilution determined by direct calorimetric measurements in ref 31 and $C_{p,1}^{\bullet}$ is the solute heat capacity in the pure liquid state taken from ref 32.

[c] The value of $\Delta_{\mathrm{hyd}}C_{p,1}$ reported here was calculated from $\Delta_{\mathrm{hyd}}C_{p,1} = \bar{C}_{p,1}^{\infty} - C_{p,1}^{0}$ where $\bar{C}_{p,1}^{\infty}$ is the solute partial molar heat capacity at infinite dilution determined by direct calorimetric

measurements in ref 31 and $C_{p,1}^{0}$ is the pure solute heat capacity in the ideal gas state taken from ref 33.

[d] The value of $\bar{C}_{p,1}^{\mathrm{E},\infty}$ reported here was calculated from $\bar{C}_{p,1}^{\mathrm{E},\infty} = \Delta_{\mathrm{hyd}} C_{p,1} + (C_{p,1}^{0} - C_{p,1}^{\bullet})$ where $\Delta_{\mathrm{hyd}} C_{p,1}$ is the hydration heat capacity as estimated by the first order group contribution method of Plyasunov et al.[34], and $C_{p,1}^{0}$, and $C_{p,1}^{\bullet}$ are the pure solute heat capacity in the ideal gas state, and that in the liquid state, respectively. The $C_{p,1}^{\bullet}$ data were taken from ref 32 or estimated by the method of Kolská et al.[35] and $C_{p,1}^{0}$ data were taken from ref 33.

[e] Estimated by the first order group contribution method of Plyasunov et al.[34]

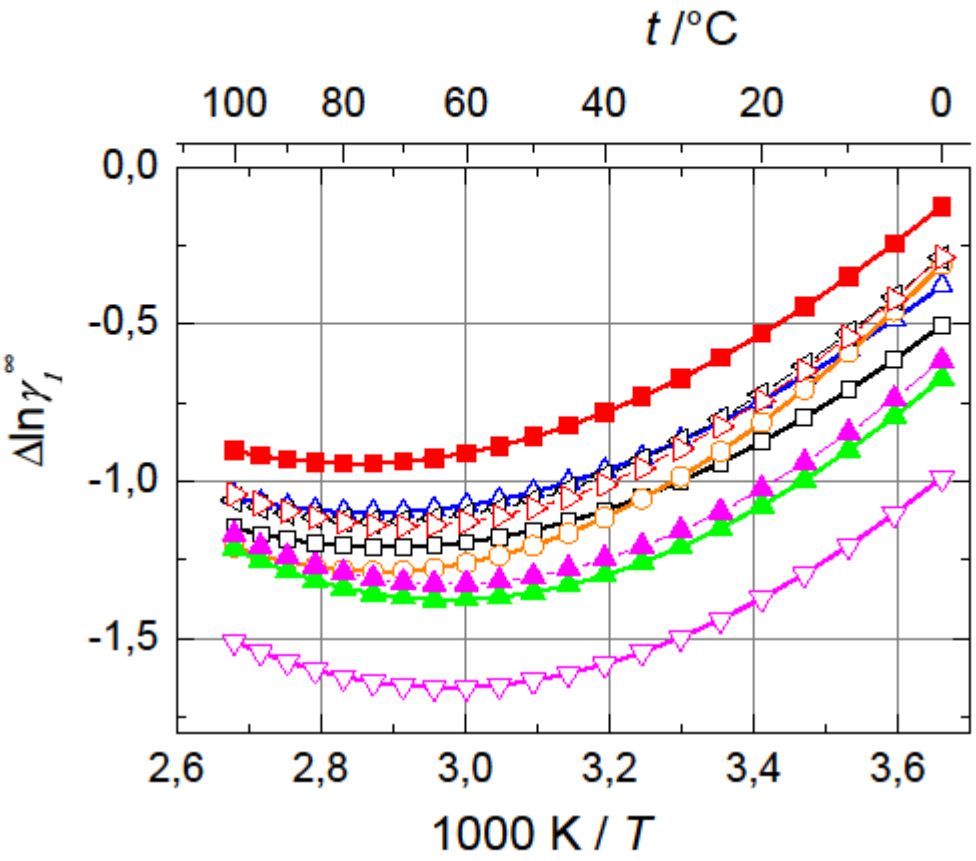

Figure S1. Deviation $\Delta \ln \gamma_1^{\infty} = \ln \gamma_1^{\infty}(\text{predicted}) - \ln \gamma_1^{\infty}(\text{recommended})$ as a function of temperature for the COSMO-SAC method: (□), pentan-2-one; (■), pentan-3-one; (△), 3-methylbutan-2-one; (▽), hexan-2-one; (○), hexan-3-one; (▲), 3-methylpentan-2-one; (◁), 4-methylpentan-2-one; (▷), 2-methylpentan-3-one; (▲), 3,3-dimethylbutan-2-one.

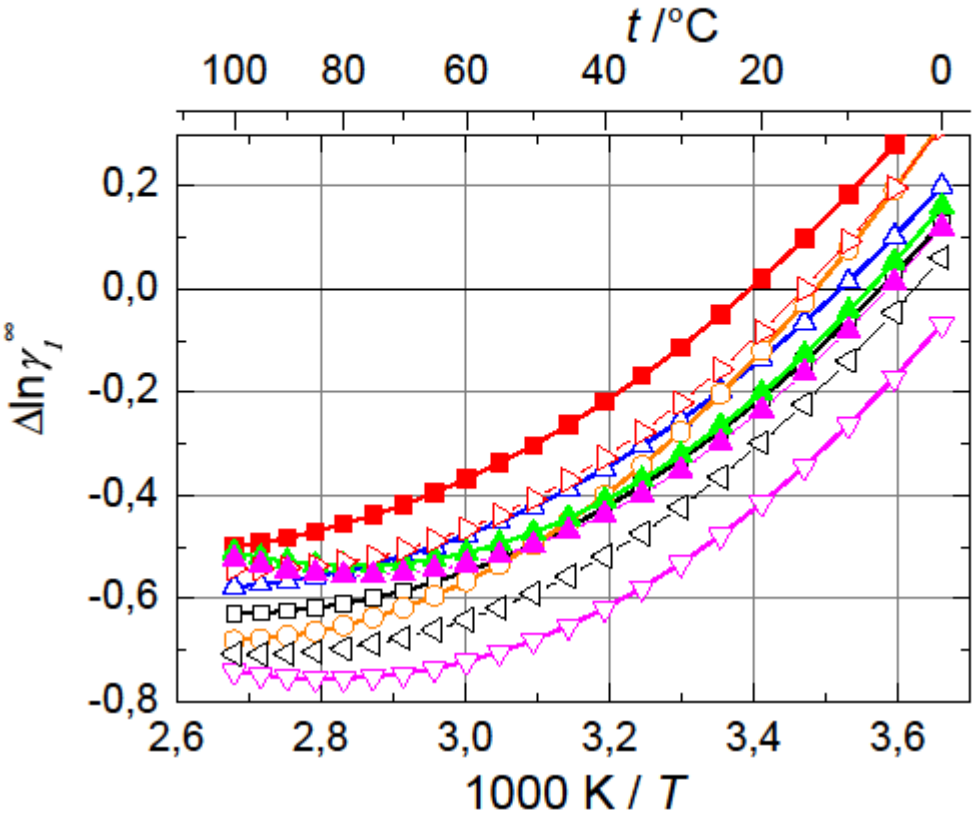

Figure S2. Deviation $\Delta \ln \gamma_1^{\infty} = \ln \gamma_1^{\infty}(\text{predicted}) - \ln \gamma_1^{\infty}(\text{recommended})$ as a function of temperature for the modified UNIFAC (Dortmund): (□), pentan-2-one; (■), pentan-3-one; (△), 3-methylbutan-2-one; (▽), hexan-2-one; (○), hexan-3-one; (▲), 3-methylpentan-2-one; (◁), 4-methylpentan-2-one; (▷), 2-methylpentan-3-one; (▲), 3,3-dimethylbutan-2-one.

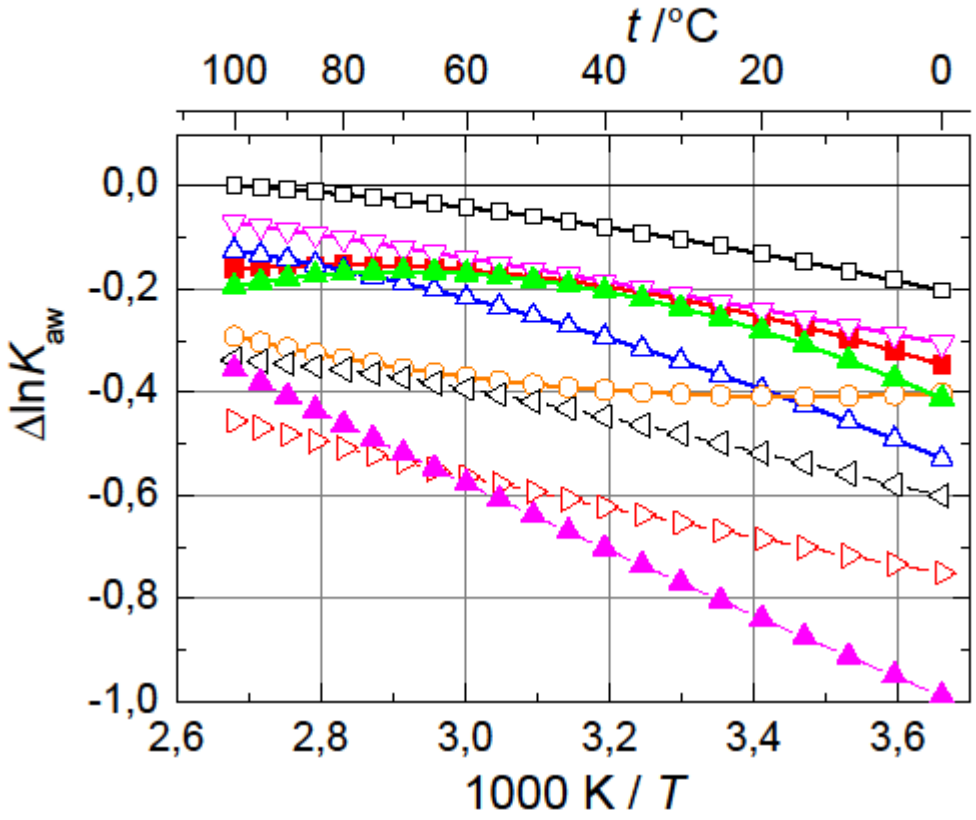

Figure S3. Deviation $\Delta \ln K_{aw} = \ln K_{aw}(\text{predicted}) - \ln K_{aw}(\text{recommended})$ as a function of temperature for the Abraham LFER-L method: (□), pentan-2-one; (■), pentan-3-one; (△), 3-methylbutan-2-one; (▽), hexan-2-one; (○), hexan-3-one; (▲), 3-methylpentan-2-one; (◁), 4-methylpentan-2-one; (▷), 2-methylpentan-3-one; (▲), 3,3-dimethylbutan-2-one.

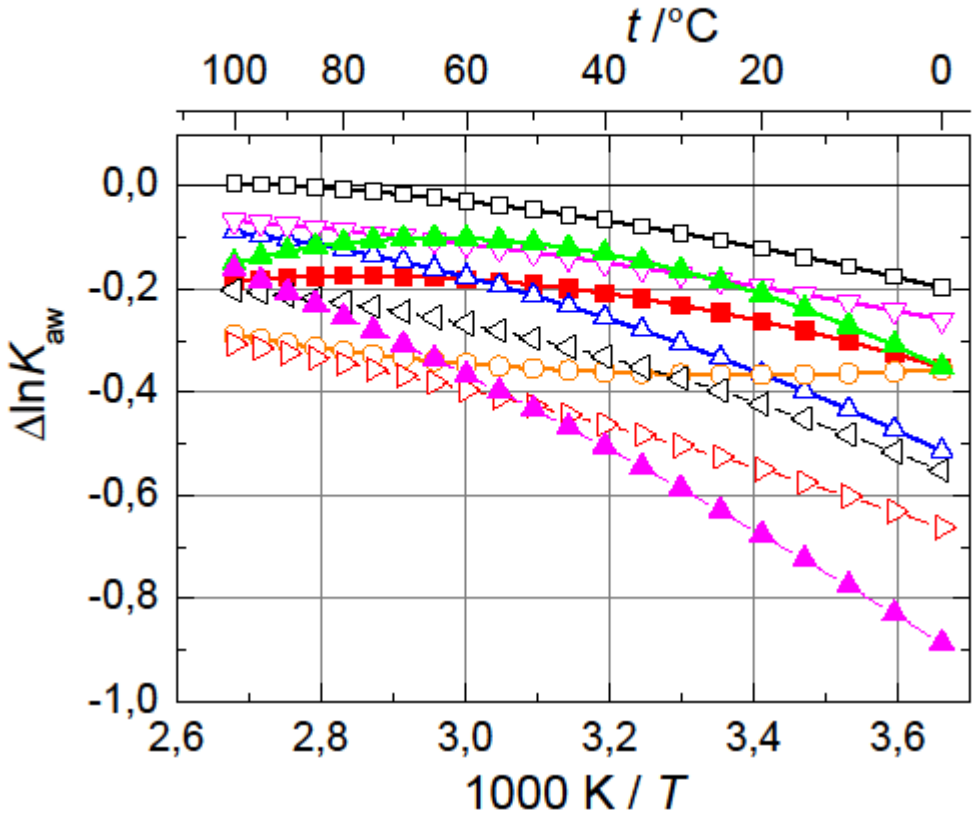

Figure S4. Deviation $\Delta \ln K_{aw} = \ln K_{aw}(\text{predicted}) - \ln K_{aw}(\text{recommended})$ as a function of temperature for the Abraham LFER-V method: (□), pentan-2-one; (■), pentan-3-one; (△), 3-methylbutan-2-one; (▽), hexan-2-one; (○), hexan-3-one; (▲), 3-methylpentan-2-one; (◁), 4-methylpentan-2-one; (▷), 2-methylpentan-3-one; (▲), 3,3-dimethylbutan-2-one.

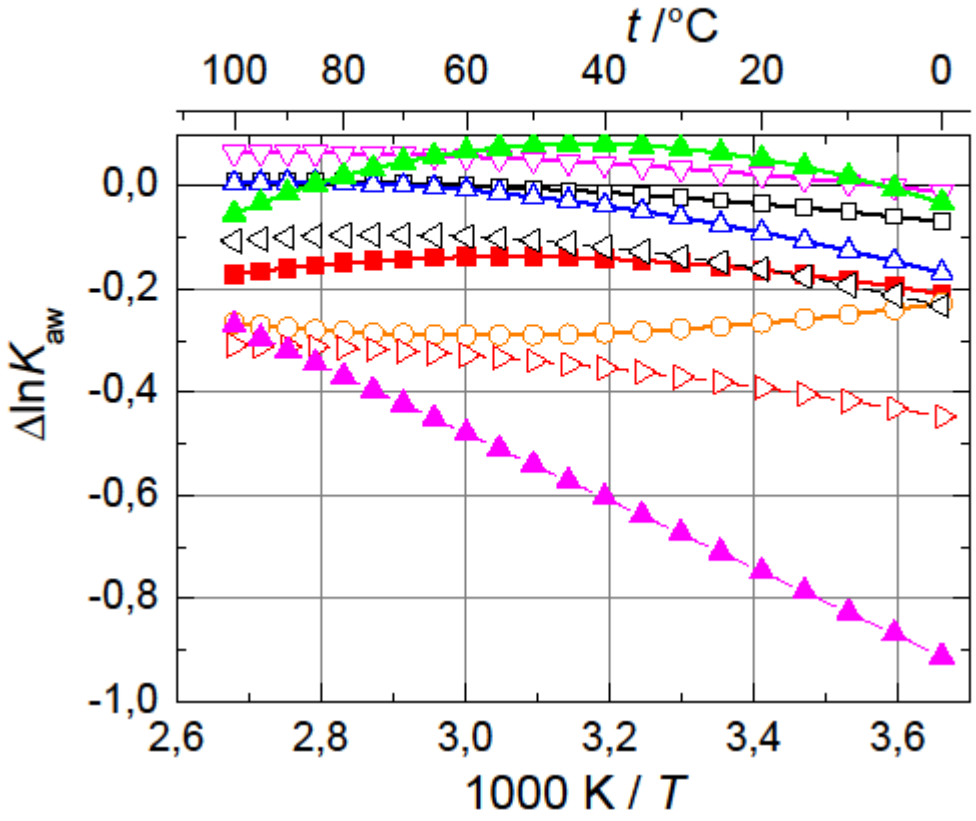

Figure S5. Deviation $\Delta \ln K_{aw} = \ln K_{aw}(\text{predicted}) - \ln K_{aw}(\text{recommended})$ as a function of temperature for the Cabani group contribution method: (□), pentan-2-one; (■), pentan-3-one; (△), 3-methylbutan-2-one; (▽), hexan-2-one; (○), hexan-3-one; (▲), 3-methylpentan-2-one; (◁), 4-methylpentan-2-one; (▷), 2-methylpentan-3-one; (▲), 3,3-dimethylbutan-2-one.

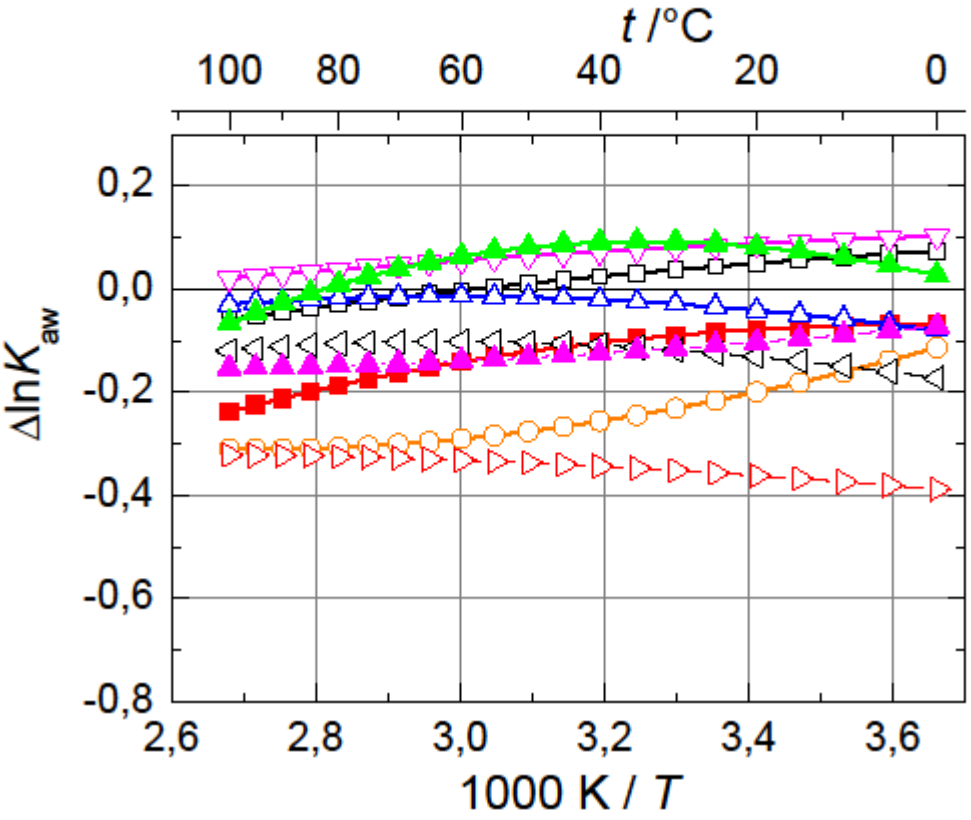

Figure S6. Deviation $\Delta \ln K_{aw} = \ln K_{aw}(\text{predicted}) - \ln K_{aw}(\text{recommended})$ as a function of temperature for the Plyasunov first-order group contribution method: (□), pentan-2-one; (■), pentan-3-one; (△), 3-methylbutan-2-one; (▽), hexan-2-one; (○), hexan-3-one; (▲), 3-methylpentan-2-one; (◁), 4-methylpentan-2-one; (▷), 2-methylpentan-3-one; (▲), 3,3-dimethylbutan-2-one.

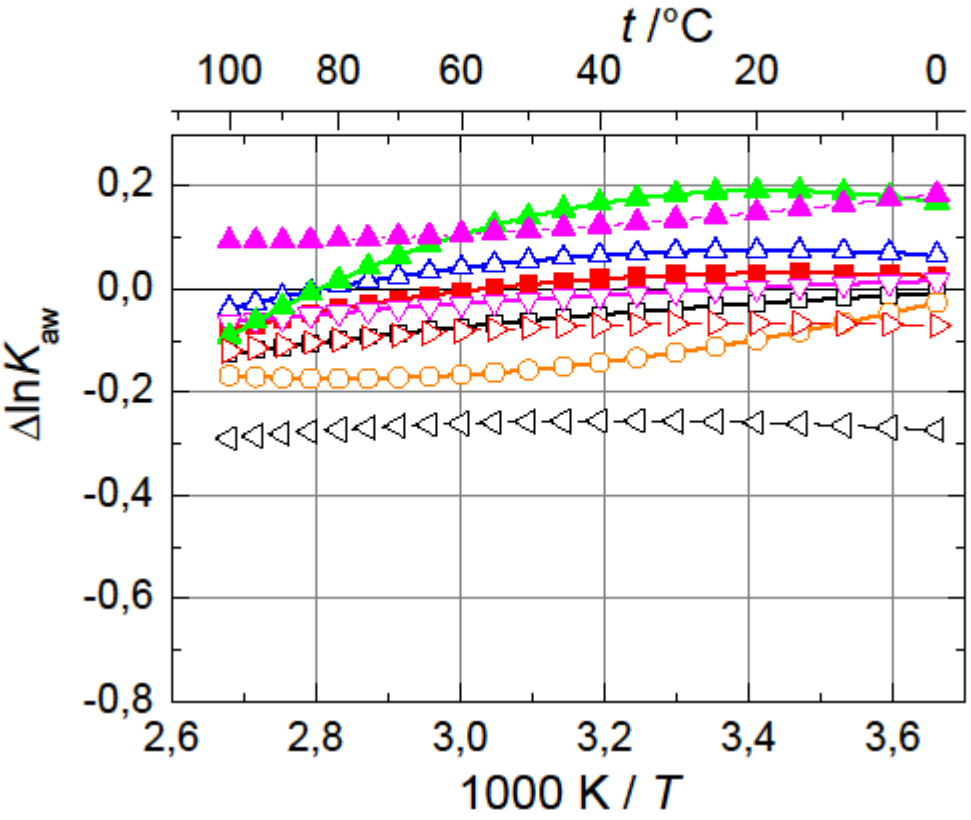

Figure S7. Deviation $\Delta \ln K_{aw} = \ln K_{aw}(\text{predicted}) - \ln K_{aw}(\text{recommended})$ as a function of temperature for the Plyasunov second-order group contribution method: (☐), pentan-2-one; (■), pentan-3-one; (△), 3-methylbutan-2-one; (▽), hexan-2-one; (○), hexan-3-one; (▲), 3-methylpentan-2-one; (◁), 4-methylpentan-2-one; (▷), 2-methylpentan-3-one; (▲), 3,3-dimethylbutan-2-one.

References

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