

Electronic Supporting Information:

Non-Covalent Interactions in Molecular Systems: Thermodynamic Evaluation of the Hydrogen Bond Strength in Aminoalcohols

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Table S1. Comparison of the Intra-Molecular Hydrogen Bond Strength in Amino-Alcohols Derived from Different Thermodynamic Methods (in kJ·mol⁻¹)

Compound and type of bond	Solvent	Method	ΔH_{HB}	Ref.
2-amino-ethanol (OH-N)	C ₂ Cl ₄	FTIR	-11.1±3.0	this work
	C ₂ Cl ₄	IR	-2.9±0.4	1
	CCl ₄	IR	-6.7±0.2	2
	gas	SCF	-7.3	3
	gas	RHF	-11.3	4
	gas	MP2	-15.4	5
	gas	DFT	-12.9	6
	gas	CCSD(T)	-7.9	7
2-amino-ethanol (NH-O)	C ₂ Cl ₄	FTIR	-8.9±4.1	this work
	gas	MP2	-3.2	5
2-(dimethyl-amino)-1-ethanol (OH-N)	C ₂ Cl ₄	FTIR	-15.1±1.2	this work
	C ₂ Cl ₄	IR	-11.7±0.8	1
	CCl ₄	IR	-21.5±2.5	2
	C ₂ Cl ₄	IR	-17.7	8

Table S2. Provenance and Purity of Sample Used in this Work

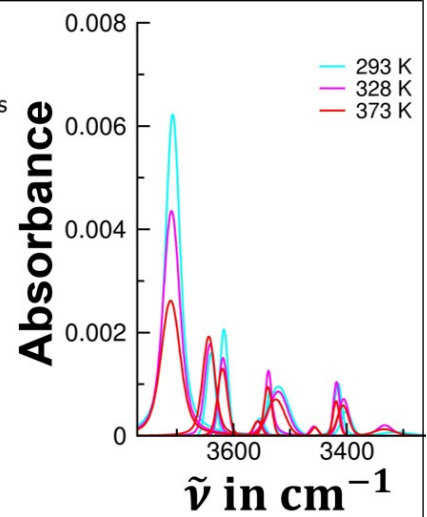
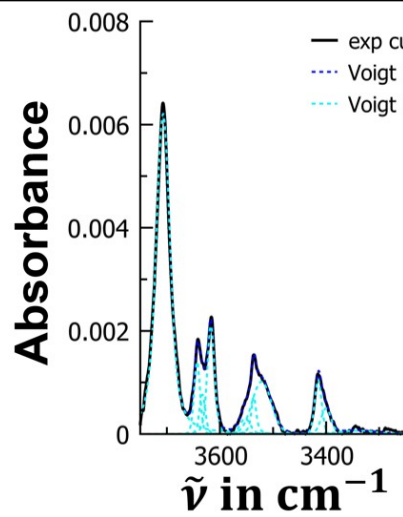
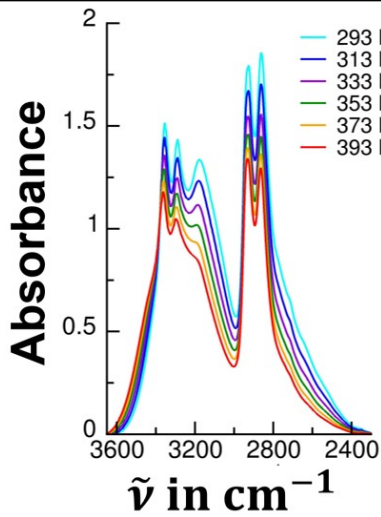
Compound	CAS	Source	Purity given by supplier	Final purity ^a
2-aminoethanol	141-43-5	Aldrich	0.995	0.9998
DL-1-amino-2-propanol	7896-6	Alfa Aesar	0.93	0.9811
DL-2-amino-1-propanol	6168-72-5	TCI	0.98	0.9956
DL-2-amino-1-butanol	13054-87-0	TCI	0.98	0.9955
2-amino-1-pentanol	22724-81-8	Sigma-Aldrich	0.97	0.9896
2-amino-1-hexanol	80696-28-2	Sigma-Aldrich	0.97	0.9866
2-(dimethylamino)ethanol	108-01-0	Aldrich	0.995	0.9997
2-methoxyethylamine	109-85-3	Aldrich	0.99	0.9989

^a Mass fraction impurity determined by the gas chromatography before sample use.

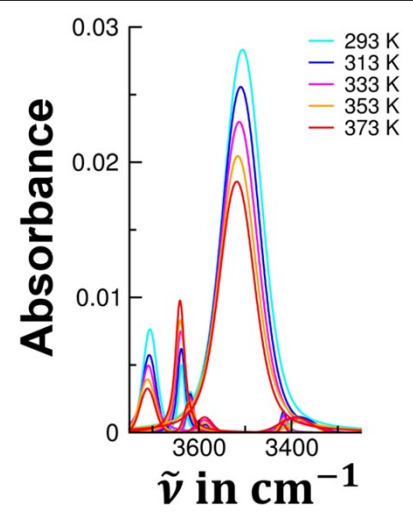
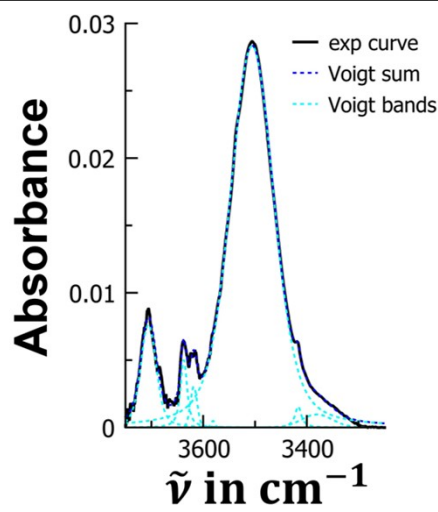
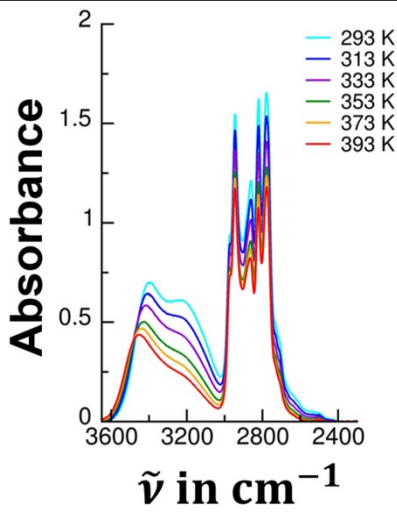
Table S3. Frequencies $\tilde{\nu}$ at 298 K in cm^{-1}

compound		$\nu(\text{OH-N})$	$\nu(\text{NH-O})$	(OH free)	Ref
2-amino-ethanol	C_2Cl_4	3526	3618	3641	this work
	C_2Cl_4	3526		3640	1
	CCl_4	3509		3610	9
	CCl_4	3513		3634	9
	CCl_4	3300		3600	9
	CCl_4	3230		3570	9
	CCl_4	3517	3620	3640	10
	gas	3555		3666	11
	gas	3557		3665	12
	gas	3549			13
gas	3570			14	
1-amino-2-propanol	C_2Cl_4	3511	3613	3631	this work
	gas	3544		3667	12
	gas	3556		3653	15
2-(dimethyl-amino)-1-ethanol	C_2Cl_4	3507	-	3637	this work
	C_2Cl_4	3506		3638	1
	C_2Cl_4	3510		3640	8
	CCl_4	3500		3638	10
	gas	3540		3654	12
	gas	3534		3656	12
2-(diethyl-amino)-1-ethanol	C_2Cl_4	3472		3630	1
	CCl_4	3470		3640	16
	gas	3515		3660	12

aminoethanol



2-(dimethyl-amino)-1-ethanol



methoxyethylamine

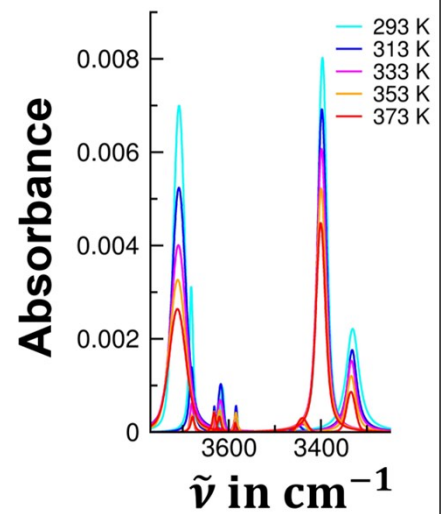


Figure S1. FTIR-spectra of 2-aminoethanol, 2-(dimethyl-amino)-1-ethanol and methoxyethylamine: The left spectrum shows pure compound at different temperatures. The middle spectrum shows the formation of integrals with the Voigtinator software at 293 K for 0.1 mole percent aminoalcohol in C₂Cl₄. In the right spectrum, the temperature dependency of integrals for diluted aminoalcohol is shown.

For 2-aminoethanol, the peak in the region of $\tilde{\nu} = 3516 \text{ cm}^{-1}$ to $\tilde{\nu} = 3556 \text{ cm}^{-1}$ appears to be deformed. It looks like there are at least two vibrations in that range. Therefore, monomer+water frequencies were calculated in addition to the monomer frequencies. The trans-aminoethanol-water cluster has a frequency in this region, which is the hydroxyl stretching frequency at $\tilde{\nu} = 3539 \text{ cm}^{-1}$. Therefore, the peak of the OHN-conformer in the region of $\tilde{\nu} = 3516 \text{ cm}^{-1}$ to $\tilde{\nu} = 3556 \text{ cm}^{-1}$ is interrupted by the peak at $\tilde{\nu} = 3537 \text{ cm}^{-1}$ of the trans-conformer-water cluster. For the Van 't Hoff plot only the integral values of the OHN-conformer were used.

Table S4.

Anharmonic Transition Energies (E)^a in cm^{-1} and Dipole Strengths (DS)^b in $10^{-40} \text{ esu}^2 \text{ cm}^2$

compound	E (OH \cdots N)	DS (OH \cdots N)	E (NH \cdots O)	DS (NH \cdots O)	E (trans)	DS (trans)
2-aminoethanol	3527.663	58.89536842	3673.485	19.83477033	3670.504	17.81696592
2-amino-1-propanol	3516.347	64.32903830	3660.531	20.35727926	3668.066	10.54279919
2-amino-1-butanol	3509.883	64.37772106	3670.235	20.35031719	3660.951	8.54717878
2-amino-1-pentanol	3509.729	66.07242596	3660.941	20.77768470	3663.813	18.16773210
2-amino-1-hexanol	3507.185	63.79430531	3651.138	20.52543937	3662.034	12.58891279
1-amino-2-propanol	3507.864	74.21218493	3609.555	8.29987577	3618.757	8.37661206
2-(dimethylamino)ethanol	3522.051	65.95985315	---	---	3669.469	18.10825200

^a Anharmonic transition energies (E) are equal to vibration frequencies

^b Dipole strengths (DS) are used to correct integral values for Van't Hoff plots.

Table S5. Equilibrium Constants K_{eq} for Van't Hoff Plots

T in K	AE ^a	AE ^b	2AP ^a	2AP ^b	2AB ^a	2AB ^b	2APe ^a	2APe ^b	2AH ^a	2AH ^b	A2P ^a	A2P ^b	DMAE ^a
293	0.48	1.08	0.41	0.21	0.44	0.086	1.06	0.25	0.79	0.187	0.95	0.40	
298	0.35	0.79	0.41	0.17	0.42	0.091	0.95	0.37	0.75	0.194	0.82	0.36	
303	0.37	0.67	0.39	0.16	0.40	0.089	0.88	---	0.75	0.147	0.68	0.32	
308	0.34	0.55	0.32	0.17	0.39	0.084	0.76	0.23	0.67	0.141	0.58	0.29	
313	0.31	0.68	0.33	0.14	0.36	0.081	0.75	0.24	0.65	0.161	0.56	0.29	
318	0.38	1.03	---	---	0.36	0.088	---	---	---	---	0.49	0.27	3.84
323	0.36	0.69	0.29	0.16	0.33	0.081	0.72	0.23	0.62	0.133	0.60	0.36	-
324	---	---	---	---	0.34	---	---	---	---	---	---	---	3.49
328	0.28	0.58	---	---	0.31	0.077	---	---	---	---	0.62	0.40	---
329	---	---	---	---	---	---	---	---	---	---	---	---	3.21
333	0.38	0.79	0.27	0.17	0.31	0.072	0.70	0.21	0.50	0.110	0.46	0.32	2.98
338	0.32	0.65	---	---	0.27	0.067	---	---	---	---	0.37	0.27	2.67
343	---	---	0.26	0.12	0.26	0.063	0.60	0.20	0.47	0.112	0.34	0.26	2.46
344	0.22	0.38	---	---	---	---	---	---	---	---	---	---	---
348	0.22	0.51	---	---	---	---	---	---	---	---	0.33	0.26	---
349	---	---	---	---	0.25	0.060	---	---	---	---	---	---	2.38
353	0.19	0.36	0.23	0.11	---	---	0.56	0.20	0.45	0.128	0.34	0.30	---
354	---	---	---	---	0.22	0.068	---	---	---	---	---	---	2.37
360	0.19	0.52	---	---	0.21	0.055	---	---	---	---	0.31	0.28	1.90
366	0.17	0.44	---	---	0.19	0.049	---	---	---	---	0.25	0.26	1.81
373	0.16	0.44	---	---	0.19	0.057	---	---	---	---	0.24	0.25	1.65

Abbreviations for Aminoalcohols: AE (2-aminoethanol), 2AP (2-amino-1-propanol), 2AB (2-amino-1-butanol), 2APe (2-amino-1-pentanol), 2AH (2-amino-1-hexanol), A2P (1-amino-2-propanol), DMAE (2-(dimethyl-amino)-1-ethanol)

^a OH-N hydrogen bond

^b NH-O hydrogen bond

Table S6a. The G4 Calculated Gas Phase Standard Molar Enthalpies of Formation of Aminoalcohols Stable Conformers at $p^\circ=0.1$ MPa and $T=298$ K (in $\text{kJ}\cdot\text{mol}^{-1}$)^a

compound	$\Delta_f H_m^\circ(\text{g})_{\text{OH-}}$ N ^a	$\Delta_f H_m^\circ(\text{g})_{\text{NH-}}$ O ^b	$\Delta_f H_m^\circ(\text{g})_{\text{trans}}$ c	$\Delta_f H_m^\circ(\text{g})_{\text{cis}}$ d	Σ increments ^c	
	1	2	3	4	5	6
2-amino-ethanol		-207.4	-201.7	-195.7	-189.3	-200.7
2-amino-1-propanol		-242.7	-237.9	-231.3	-222.5	-235.6
2-amino-1-butanol		-263.1	-257.9	-251.7	-242.6	-257.1
2-amino-1-pentanol		-284.3	-279.3	-272.8	-263.7	-278.5
2-amino-1-hexanol		-305.9	-300.9	-294.5	-285.2	-300.0
1-amino-2-propanol		-248.4	-239.7	-235.6	-227.1	-238.2
1-amino-2-butanol		-269.8	-258.3	-256.0	-248.0	-259.7
2-(dimethyl-amino)-1-ethanol		-209.7	-	-195.8	-192.4	-201.0
2-(diethyl-amino)-1-ethanol		-254.8	-	-241.1	-237.3	-254.7

^a Calculated by the G4 method according to the standard atomization procedure. The expanded uncertainty assessed to be $\pm 3.5 \text{ kJ}\cdot\text{mol}^{-1}$.¹⁷

^b Calculated

Table S6b. Raw Enthalpy H_{298} Data in Hartree from G4 Calculations for Different Conformers

Compound	Conformation ^a			
	Intra HB OH-N	Intra HB NH-O	trans	cis
2-aminoethanol	-210.252120	-210.249953	-210.247670	-210.245211
2-amino-1-propanol	-249.534367	-249.533260	-249.531670	-249.526679
2-amino-1-butanol	-288.810989	-288.809001	-288.806638	-288.803177
2-amino-1-pentanol	-328.087900	-328.085969	-328.083519	-328.080019
2-amino-1-hexanol	-367.364946	-367.363030	-367.360582	-367.357072
1-amino-2-propanol	-249.536567	-249.532553	-249.531040	-249.528440
1-amino-2-butanol	-288.813529	-288.809149	-288.808270	-288.805225
dimethylaminoethanol	-288.790632	---	-288.785338	-288.784048
diethylaminoethanol	-367.345461	---	-367.340259	-367.338827

^aFor definition see Fig. S2

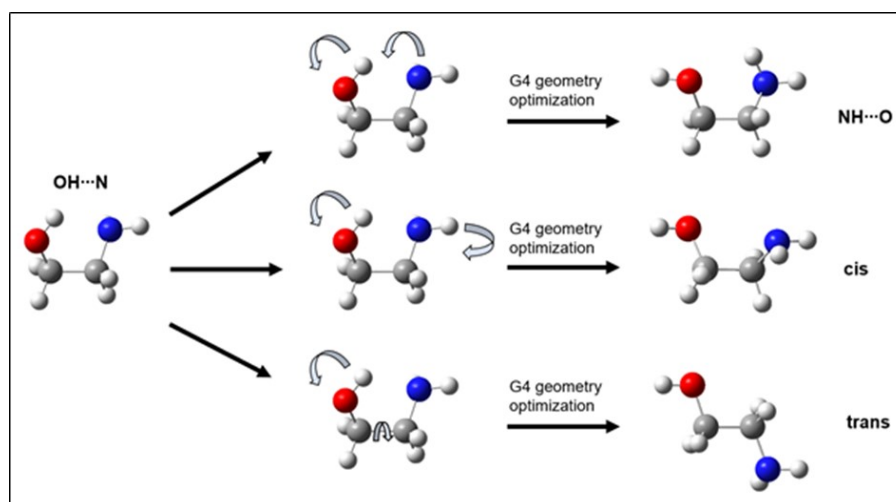


Figure S2. Definition of 2-amino-ethanol conformers discussed in this work

Table S6c. Comparison of Measures of the *Intra*-HB Strength in Aminoalcohols at $p^{\circ}=0.1$ MPa and $T=298$ K (in $\text{kJ}\cdot\text{mol}^{-1}$)

Compound (type of bond)	ΔH_{HB}^a	H_S^b	$\Delta_f H_m^o(g)_{QC}^c$
2-amino-ethanol (OH \cdots N)	-11.1 \pm 3.0	-6.2	-11.7
2-amino-ethanol (NH \cdots O)	-8.9 \pm 4.1		-6.0
2-amino-1-propanol (OH \cdots N)	-8.4 \pm 1.5	-7.1	-11.4
2-amino-1-propanol (NH \cdots O)	-6.8 \pm 3.3		-6.6
2-amino-1-butanol (OH \cdots N)	-10.1 \pm 0.8	-6.0	-11.4
2-amino-1-butanol (NH \cdots O)	-6.6 \pm 1.4		-6.2
2-amino-1-pentanol (OH \cdots N)	-8.3 \pm 1.6	-5.8	-11.5
2-amino-1-pentanol (NH \cdots O)	-5.9 \pm 4.1		-6.5
2-amino-1-hexanol (OH \cdots N)	-8.8 \pm 1.2	-5.9	-11.4
2-amino-1-hexanol (NH \cdots O)	-7.1 \pm 3.3		-6.4
1-amino-2-propanol (OH \cdots N)	-14.7 \pm 2.2	-9.9	-12.8
1-amino-2-propanol (NH \cdots O)	-3.7 \pm 2.2		-4.1
1-amino-2-butanol (OH \cdots N)	-	-10.1	-13.8
1-amino-2-butanol (NH \cdots O)	-		-2.3
2-(dimethyl-amino)-1-ethanol (OH \cdots N)	-15.1 \pm 1.2	-6.6	-13.9
2-(diethyl-amino)-1-ethanol (OH \cdots N)	-	-3.5	-13.7

^a Spectroscopic measure of the *intra*-HB strength from Table 2.

^b The strain enthalpies $H_S = \Delta_f H_m^o(g)_{\text{exp}} - \Sigma(\text{increments})$ of the amino alcohols (see main text) without correction for strain.

^c Quantum-chemical measure of the true *intra*-HB strength, calculated as the differences $[\Delta_f H_m^o(g)_{\text{OH}\cdots\text{N}} - \Delta_f H_m^o(g)_{\text{trans}}]$ and $[\Delta_f H_m^o(g)_{\text{NH}\cdots\text{O}} - \Delta_f H_m^o(g)_{\text{trans}}]$ from G4-values collected in Table S6a with the expanded uncertainty taken as ± 3.5 $\text{kJ}\cdot\text{mol}^{-1}$.

Table S7. Compilation of the Standard Molar Enthalpies of Vaporization $\Delta_l^q H_m^o$ of Amino-Alcohols and Gaseous Standard Molar Enthalpies of Formation $\Delta_f H_m^o(g)$ at 298 K (in $\text{kJ}\cdot\text{mol}^{-1}$)

Compound	$\Delta_l^q H_m^o$ ^{18,19}	$\Delta_f H_m^o(g)$
1-amino-2-propanol [78-96-6]	59.3 \pm 0.4 (this work)	-248.1 \pm 2.1 ^{18,19}
1-amino-2-butanol [13552-21-1]	64.9 \pm 0.3	-269.8 ^a
1-amino-2-pentanol [5343-35-1]	69.1 \pm 0.7	
1-amino-2-hexanol [72799-62-3]	73.8 \pm 1.0	
2-amino-ethanol [141-43-5]	59.2 \pm 0.4	-206.9 \pm 1.3 ^{18,19}
2-amino-1-propanol [6168-72-5]	59.7 \pm 0.6	-242.7 ^a
2-amino-1-butanol [96-20-8]	64.5 \pm 0.4 (this work)	-263.1 ^a
2-amino-1-pentanol [16369-14-5]	68.3 \pm 0.7	-284.8 ^a
2-amino-1-hexanol [5665-74-7]	73.2 \pm 0.7	-305.9 ^a
2-(dimethyl-amino)-ethanol [108-01-0]	47.1 \pm 0.1 ^{18,19}	-207.6 \pm 1.7 ^{18,19}
2-(diethyl-amino)-ethanol [100-37-8]	52.6 \pm 0.2 ^{18,19}	-258.2 \pm 1.2 ^{18,19}

^a The most stable conformer from Table S6a

Table S8. Group-Additivity Values Γ_i for Calculation of Enthalpies of Vaporization, $\Delta_l^g H_m^o(298\text{ K})$ and Enthalpies of Formation, $\Delta_f H_m^o(\text{g}, 298\text{ K})$, of Alkanes, Amines, and Amino-Alcohols (in kJ mol^{-1})²⁰⁻²²

Groups ^a	$\Delta_l^g H_m^o(298\text{ K})$ Γ_i	$\Delta_f H_m^o(\text{g}, 298\text{ K})$ Γ_i
Alkanes		
C-(C)(H) ₃	6.33	-42.05
C-(C) ₂ (H) ₂	4.52	-21.46
C-(C) ₃ (H)	1.24	-9.04
C-(C) ₄	-2.69	-1.26
Amines		
C-(N)(H) ₃	6.33	-42.05
C-(N)(C)(H) ₂	2.9	-26.9
C-(N)(C) ₂ (H)	-2.0	-20.0
C-(N)(C) ₃	-7.7	-16.1
N-(C)(H) ₂	18.0	19.4
N-(C) ₂ (H)	12.6	62.2
N-(C) ₃	4.9	103.2
N-(Cb)(C)(H)	10.9	65.4
Cb-(N)	9.5	2.1
Alcohols		
C-(O)(H) ₃	6.33	-42.05
C-(O)(C)(H) ₂	4.7	-33.7
C-(O)(C) ₂ (H)	1.3	-29.2
C-(O)(C) ₃	-3.8	-26.9
HO-(C)	31.5	-159.45

Static method: vapor pressure measurements

The vapor pressures of 1-amino-2-propanol in the temperature range 327-373 K were measured with the static method by using the self-made experimental setup.²³ The stainless still cylindrical cell with the sample was kept at a constant temperature within ± 0.02 K. The sample cell was connected to the high temperature capacitance manometers covering the working range of (0.1 to 10^5) Pa. Uncertainties of 0.5 % for the pressure readings for both manometers were stated by the manufacturer. The temperature of tubing connections between the measuring cell and pressure gauges was kept higher by 30-50 K than those in the sample cell in order to avoid condensation of sample vapors in the tubing system. The uncertainty of absolute temperature determination was ± 0.05 K over the working temperature interval of the system of (291 – 345) K. The detailed description of the experimental apparatus, procedure, and uncertainty analysis, is given elsewhere.²³

Table S9. Absolute Vapor Pressures p , Standard ($p^o = 0.1$ MPa) Molar Vaporization Enthalpies, $\Delta_l^g H_m^o$, and Standard ($p^o = 0.1$ MPa) Molar Vaporization Entropies, $\Delta_l^g S_m^o$ Obtained by the Static Method

$T/$ K	$p/$ Pa	$u(p)^a /$ Pa	$\Delta_l^g H_m^o(T)_b /$ kJ·mol ⁻¹	$\Delta_l^g S_m^o(T) /$ J·K ⁻¹ ·mol ⁻¹
1-amino-2-propanol [78-96-6] $\Delta_l^g H_m^o(298 \text{ K}) = (59.3 \pm 0.4) \text{ kJ} \cdot \text{mol}^{-1}$				
$\ln(p/p_0) = \frac{300.5}{R} - \frac{78270.5}{RT} - \frac{63.5}{R} \ln \frac{T}{298.15}; p_0 = 1 \text{ Pa}$				
326.82	759	-4	57.5	135.4
326.96	769	-1	57.5	135.4
327.03	769	-4	57.5	135.4
327.09	776	0	57.5	135.4
327.18	777	-4	57.5	135.3
327.40	786	-6	57.5	135.3
327.57	798	-3	57.5	135.3
327.68	805	-1	57.5	135.3
327.77	801	-10	57.5	135.2
327.96	819	-2	57.4	135.2
328.71	867	6	57.4	135.1
328.90	882	10	57.4	135.1
329.02	885	6	57.4	135.1
329.08	890	8	57.4	135.1
329.69	920	3	57.3	134.9
329.82	922	-2	57.3	134.8
330.07	940	1	57.3	134.8
330.24	946	-3	57.3	134.8
330.52	967	1	57.3	134.7
330.55	967	-1	57.3	134.7
330.96	988	-5	57.3	134.6
331.12	1014	11	57.2	134.7
331.16	1002	-4	57.2	134.6
332.07	1053	-12	57.2	134.3
332.18	1068	-4	57.2	134.4
332.44	1095	5	57.2	134.4
332.61	1103	2	57.1	134.3

332.93	1125	2	57.1	134.3
333.00	1118	-10	57.1	134.2
333.50	1172	8	57.1	134.2
333.58	1176	7	57.1	134.2
333.62	1170	-2	57.1	134.1
333.74	1179	-2	57.1	134.1
334.94	1277	6	57.0	133.9
335.02	1277	0	57.0	133.9
335.74	1341	6	57.0	133.8
335.89	1346	-1	56.9	133.7
335.95	1346	-6	56.9	133.7
336.02	1359	1	56.9	133.7
336.03	1355	-3	56.9	133.7
336.93	1438	4	56.9	133.5
337.30	1465	-2	56.9	133.4
338.32	1569	10	56.8	133.3
339.39	1669	8	56.7	133.1
339.65	1693	6	56.7	133.0
339.76	1702	4	56.7	133.0
340.51	1767	-8	56.6	132.8
340.60	1769	-15	56.6	132.8
340.73	1799	1	56.6	132.8
341.60	1895	3	56.6	132.7
343.07	2083	23	56.5	132.5
344.12	2187	-2	56.4	132.2
344.37	2231	11	56.4	132.2
344.44	2229	0	56.4	132.1
345.07	2337	26	56.4	132.1
345.18	2338	13	56.4	132.0
345.20	2349	21	56.4	132.1
345.42	2349	-8	56.3	131.9
349.74	3000	-2	56.1	131.1
351.74	3340	-9	55.9	130.8
351.84	3362	-5	55.9	130.8
352.14	3419	-3	55.9	130.7
352.37	3459	-6	55.9	130.7
352.48	3509	23	55.9	130.7
352.55	3509	10	55.9	130.7
352.74	3518	-17	55.9	130.6
352.92	3562	-8	55.9	130.6
353.19	3626	4	55.8	130.5
353.25	3622	-12	55.8	130.5
353.30	3644	0	55.8	130.5
353.38	3650	-9	55.8	130.5
354.46	3871	-6	55.8	130.3
354.80	3940	-8	55.7	130.2
355.02	3999	4	55.7	130.2

355.04	3995	-4	55.7	130.2
355.15	4017	-5	55.7	130.2
355.35	4058	-7	55.7	130.1
355.38	4066	-6	55.7	130.1
355.43	4074	-9	55.7	130.1
356.03	4200	-14	55.7	130.0
356.19	4231	-19	55.7	129.9
356.69	4349	-15	55.6	129.9
356.78	4372	-12	55.6	129.9
356.84	4406	8	55.6	129.9
357.28	4474	-27	55.6	129.7
357.45	4541	0	55.6	129.8
357.69	4578	-20	55.6	129.7
357.70	4609	8	55.6	129.7
357.82	4638	8	55.5	129.7
357.92	4661	7	55.5	129.7
358.35	4737	-22	55.5	129.6
358.44	4768	-14	55.5	129.6
359.21	4971	-5	55.5	129.4
360.15	5235	12	55.4	129.3
360.21	5221	-18	55.4	129.2
360.54	5368	39	55.4	129.3
360.62	5373	22	55.4	129.2
360.94	5431	-8	55.4	129.1
361.01	5465	7	55.3	129.1
361.09	5472	-9	55.3	129.1
362.09	5740	-27	55.3	128.9
363.59	6275	55	55.2	128.8
363.95	6340	6	55.2	128.6
364.98	6658	-10	55.1	128.4
365.74	6927	3	55.0	128.3
365.77	6907	-27	55.0	128.3
366.85	7286	-28	55.0	128.1
368.25	7871	39	54.9	127.9
368.65	7984	-2	54.9	127.8
369.62	8343	-26	54.8	127.6
370.51	8742	7	54.7	127.5
370.54	8787	39	54.7	127.5
371.08	8981	4	54.7	127.4
372.92	9820	23	54.6	127.1
372.93	9805	3	54.6	127.1

^a Experimental temperature measured with the standard uncertainty ($u(T) = 0.1$ K).

^b Standard uncertainties of experimental vapor pressures were calculated according to the following equations: $u(p/\text{Pa}) = 0.05 + 0.010(p/\text{Pa})$

^c Uncertainty of the vaporization enthalpy $U(\Delta_l^g H_m^o)$ is the expanded uncertainty (0.95 level of confidence). They were calculated according to a procedure described elsewhere.^{24,25} Uncertainties include uncertainties from the experimental conditions and the fitting equation, vapor pressures, and uncertainties from adjustment of vaporization/sublimation enthalpies to the reference temperature $T = 298$ K.

Transpiration method

Absolute vapor pressures were measured using the transpiration method.²³⁻²⁵ The main idea of this method is to saturate the gas stream flowing over the sample and to determine the amount of compound transferred by the gas within a given time. Approximately 0.5 to 0.8 g of the sample is mixed with glass beads (diameter 1 mm) and placed in the thermostatted U-shaped saturator. The glass beads are needed to enlarge the contact area between gas and sample. A stream of nitrogen at a well-defined flow rate was passed through the saturator at constant temperature (± 0.1 K), and the transported material was collected in a cold trap. The amount of the condensed substance was determined by GC. The saturation vapor pressure p_i at each temperature T_i was calculated from the amount of condensate collected within a definite period of time:

$$p_i = m_i \cdot R \cdot T_a / V \cdot M_i ; \quad V = (n_{N_2} + n_i) \cdot R \cdot T_a / P_a \quad (S1)$$

where V is the volume of the gas phase consisting of the n_{N_2} moles of the carrier gas and n_i mole of gaseous compound under study (with the molar mass M_i) at the atmospheric pressure P_a and the ambient temperature T_a . The volume of the carrier gas V_{N_2} was determined by the digital flow rate sensor from integration with a microcontroller. We used the Honeywell S&C - HAFBLF0200C2AX5 digital flow rate sensor with uncertainty at the level of 2.5 %. The flow rate of the nitrogen stream was also controlled by using a soap bubble flow meter (HP soap film flowmeter (model 0101-0113)) and optimized in order to reach the saturation equilibrium of the transporting gas at each temperature under study. The volume of the carrier gas V_{N_2} was readied from the digital flow rate sensor. The amount of the compound under investigation n_i in the carrier gas was estimated at each temperature using the ideal gas law.

Before starting the vapor pressure measurements, the sample was first pre-conditioned at 310-320 K (within about one hour) in order to remove possible traces of water. The saturator was then kept at 310-315 K (to remove possible traces of volatile compounds). In order to assure the competition of pre-conditioning at the selected temperature, three samples were taken during the sample flashing at and analysed by the GC. A constant vapor pressure at this temperature indicated that the transpiration experiments could begin. GC analysis of the transported material did not reveal any additional contamination. The absence of impurities and decomposition products was re-checked by GC analysis of the saturator content at the end of the entire series of experiments.

Table S10. Results of Transpiration Method: Absolute Vapor Pressures p , Standard ($p^\circ = 0.1$ MPa) Molar Vaporization Enthalpy and Standard ($p^\circ = 0.1$ MPa) Molar Vaporization Entropy

$T/$ K ^a	$m/$ mg ^b	$V(N_2)^c /$ dm ³	$T_a/$ K ^d	Flow/ dm ³ ·h ⁻¹	$p/$ Pa ^e	$u(p)/$ Pa ^f	$\Delta_l^g H_m^\circ(T)$ kJ·mol ⁻¹	$\Delta_l^g S_m^\circ(T)$ J·K ⁻¹ ·mol ⁻¹
2-amino-1-butanol [96-20-8]: $\Delta_l^g H_m^\circ(298 \text{ K}) = (64.5 \pm 0.4) \text{ kJ} \cdot \text{mol}^{-1}$								
$\ln(p/p_0) = \frac{314.4}{R} - \frac{85930.6}{RT} - \frac{71.8}{R} \ln \frac{T}{298.15} ; p_0 = 1 \text{ Pa}$								
278.3	1.83	14.42	294.9	1.26	3.55	0.09	66.0	151.8
280.7	1.09	6.620	294.9	1.26	4.59	0.12	65.8	151.3
283.3	3.02	13.901	294.9	1.26	6.04	0.18	65.6	150.8
283.7	1.09	4.834	294.9	1.26	6.26	0.18	65.6	150.7
286.8	1.11	3.794	294.9	1.26	8.15	0.23	65.3	149.6
289.7	1.09	2.721	294.9	1.26	11.07	0.30	65.1	149.1
292.7	1.11	2.051	294.9	1.26	14.89	0.40	64.9	148.6
295.4	0.94	1.464	294.9	1.27	17.75	0.47	64.7	147.3
298.5	0.94	1.124	294.9	1.27	23.09	0.60	64.5	146.5
302.5	1.04	0.870	294.9	1.27	32.84	0.85	64.2	145.6
303.5	0.42	0.325	294.9	0.89	35.37	0.91	64.1	145.3
303.5	1.68	1.303	294.9	1.28	35.56	0.91	64.1	145.3

305.7	1.05	0.649	294.9	1.26	44.36	1.13	64.0	145.1
306.6	1.85	1.079	294.9	1.28	47.16	1.20	63.9	144.8
307.6	1.17	0.615	294.9	1.27	52.20	1.33	63.8	144.8
308.6	1.06	0.530	294.9	1.27	55.15	1.40	63.8	144.3
309.6	2.24	0.994	294.9	1.28	62.04	1.58	63.7	144.4
310.6	1.00	0.440	294.9	1.26	62.73	1.59	63.6	143.6
311.6	1.08	0.424	294.9	1.27	70.03	1.78	63.6	143.6
312.6	2.35	0.865	294.9	1.28	74.56	1.89	63.5	143.3
313.7	1.04	0.345	294.9	1.26	82.57	2.09	63.4	143.1
315.7	2.51	0.730	294.9	1.27	94.56	2.39	63.3	142.5
318.7	2.50	0.561	294.9	1.27	122.31	3.08	63.1	142.1
321.8	2.57	0.445	294.9	1.27	158.93	4.00	62.8	141.7
324.7	2.72	0.381	294.9	1.27	196.19	4.93	62.6	141.1
327.8	2.65	0.296	294.9	1.27	245.13	6.15	62.4	140.4
330.8	2.59	0.243	294.9	1.27	291.48	7.31	62.2	139.5
333.9	2.38	0.180	294.9	1.27	361.94	9.07	62.0	138.9

^a Saturation temperature measured with the standard uncertainty ($u(T) = 0.1$ K).

^b Mass of transferred sample condensed at $T = 243$ K.

^c Volume of nitrogen ($u(V) = 0.005$ dm³) used to transfer m ($u(m) = 0.0001$ g) of the sample. Uncertainties are given as standard uncertainties.

^d T_a is the temperature of the soap bubble meter used for measurement of the gas flow.

^e Vapor pressure at temperature T , calculated from the m and the residual vapor pressure at the condensation temperature calculated by an iteration procedure.

^f Standard uncertainties were calculated with $u(p_i/\text{Pa}) = 0.005 + 0.025(p_i/\text{Pa})$ for pressures below 5 Pa and with $u(p_i/\text{Pa}) = 0.025 + 0.025(p_i/\text{Pa})$ for pressures from 5 to 3000 Pa. The standard uncertainties for T , V , p , m , are standard uncertainties with 0.683 confidence level. Uncertainties of the vaporization enthalpies are expressed as the expanded uncertainty (0.95 level of confidence, $k = 2$). They were calculated according to a procedure described elsewhere.^{24,25} Uncertainties include uncertainties from the experimental conditions and the fitting equation, vapor pressures, and uncertainties from adjustment of vaporization/sublimation enthalpies to the reference temperature $T = 298$ K.

Experimental vaporization enthalpies $\Delta_l^g H_m^o(298\text{ K})$

The experimental vapor pressures p_i temperature dependences measured in this work were fitted with the following equation^{24,25}:

$$R \ln(p_i/p_{ref}) = a + \frac{b}{T} + \Delta_l^g C_{p,m}^o \ln\left(\frac{T}{T_0}\right) \quad (\text{S2}),$$

where $R = 8.31446\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ is the molar gas constant, the reference pressure $p_{ref} = 1\text{ Pa}$, a and b are adjustable parameters, the arbitrary temperature T_0 applied in Eq. (S2) was chosen to be $T_0 = 298\text{ K}$ and $\Delta_l^g C_{p,m}^o$ is the difference of the molar heat capacities of the gas and the liquid phases respectively (see Table S11). Experimental vapor pressures measured in this work, have been used to obtain the enthalpies of vaporization of amino-alcohols using the following equation:

$$\Delta_l^g H_m^o(T) = -b + \Delta_l^g C_{p,m}^o \times T \quad (\text{S3})$$

Experimental vapor pressures temperature dependences were also used to derive the vaporization entropies at temperatures T by using the following equation:

$$\Delta_l^g S_m^o(T) = \Delta_l^g H_m^o/T + R \ln(p_i/p_{ref}) \quad (\text{S4})$$

Coefficients a and b of Eq. S2, $\Delta_l^g H_m^o(T)$ and $\Delta_l^g S_m^o(T)$ values are collected in Tables S9 and S10. The combined uncertainties of the vaporization enthalpies include uncertainties from the experimental conditions of transpiration, uncertainties in vapor pressure and uncertainties due to the temperature adjustment to $T = 298\text{ K}$ as described elsewhere.^{24,25}

Table S11. Compilation of Data on Molar Heat Capacities $C_{p,m}^o$ and Differences $\Delta_l^g C_{p,m}^o$ of Amino-Alcohols, at 298 K in $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

compound	$C_{p,m}^o(\text{liq})$	$-\Delta_l^g C_{p,m}^o$ ^a
1-amino-2-propanol [78-96-6]	205.0 ²⁶	63.5
2-amino-1-butanol [96-20-8]	235.4 ^b	71.8

^a Calculated according to the procedure developed by Chickos and Acree²⁷.

^b Calculated by the group-contribution procedure developed by Chickos *et al.*^{27,28}.

Table S12a. Compilation of Data Used for Evaluation of the Inter-Molecular Hydrogen Bonding in Linear Alcohols, Amines, and Alkanes (at 298 K, in kJ/mol)^a

Homomorph	$\Delta_l^g H_m^o(\text{exp})^{29}$	Homomorph	$\Delta_l^g H_m^o(\text{exp})^{29}$	$\text{HB}_{\text{inter}}^b$
<i>n-alcohols</i>				
methanol	37.8	ethane	9.76	-28.0
ethanol	42.5	n-propane	16.2	-26.3
1-propanol	47.5	n-butane	22.4	-25.1
1-butanol	52.4	n-pentane	26.7	-25.7
1-pentanol	56.9	n-hexane	31.7	-25.2
1-hexanol	61.1	n-heptane	36.5	-24.6
1-heptanol	66.8	n-octane	41.5	-25.3
1-octanol	70.1	n-nonane	46.5	-23.6
1-nonanol	76.9	n-decane	51.4	-25.5
1-decanol	80.9	n-undecane	56.3	-24.6
<i>n-amines</i>				
1-propanamine	31.3	n-butane	22.4	-8.9
1-butanamine	35.7	n-pentane	26.7	-9.0
1-pentanamine	40.5	n-hexane	31.7	-8.8
1-hexanamine	45.3	n-heptane	36.5	-8.8
1-heptanamine	50.1	n-octane	41.5	-8.6

^a Uncertainties are ± 0.2 kJ/mol (twice the standard deviation)

^b Measure of the inter-molecular hydrogen bonding (difference between column 2 and 4)

Table S12b. Compilation of Data Used for Evaluation of the Inter-Molecular Hydrogen Bonding in Branched Alcohols (at 298 K, in kJ/mol)^a

CAS	Homomorph	$\Delta_l^g H_m^o$	CAS	Homomorph	$\Delta_l^g H_m^o$	$\text{HB}_{\text{inter}}(\text{ROH})^b$
78-92-2	2-butanol	49.8 \pm 0.2 ²⁹	78-78-4	2-methylbutane	25.2 \pm 0.2 ²⁹	24.6 ^b
584-02-1	3-pentanol	54.0 \pm 0.2 ²⁹	96-14-0	3-methylpentane	30.5 \pm 0.2 ²⁹	23.5
623-37-0	3-hexanol	58.6 \pm 0.4 ³⁰	589-34-4	3-methylhexane	35.2 \pm 0.2 ²⁹	23.4
589-82-2	3-heptanol	63.1 \pm 0.7 ^c	589-81-1	3-methylheptane	39.9 \pm 0.2 ²⁹	23.2
589-98-0	3-octanol	67.6 \pm 0.7 ^c	2216-33-3	3-methyloctane	44.9 \pm 0.2 ²⁹	22.7
624-51-1	3-nonanol	70.9 \pm 0.3 ³¹	5911-04-6	3-methylnonane	49.7 \pm 0.2 ²⁹	21.2
78-83-1	2-methyl-propanol	50.9 \pm 0.2 ²⁹	78-78-4	2-methylbutane	25.2 \pm 0.2 ²⁹	25.7
137-32-6	2-methyl-1-butanol	54.6 \pm 1.3 ³²	96-14-0	3-methylpentane	30.5 \pm 0.2 ²⁹	24.1
105-30-6	2-methyl-1-pentanol	59.4 \pm 0.3 ³⁰	589-34-4	3-methylhexane	35.2 \pm 0.2 ²⁹	24.2
624-22-6	2-methyl-1-hexanol	63.9 \pm 0.7 ^c	589-81-1	3-methylheptane	39.9 \pm 0.2 ²⁹	24.0
60435-70-3	2-methyl-1-heptanol	68.4 \pm 0.7 ^c	2216-33-3	3-methyloctane	44.9 \pm 0.2 ²⁹	23.5
818-81-5	2-methyl-1-octanol	72.9 \pm 0.7 ^c	5911-04-6	3-methylnonane	49.7 \pm 0.2 ²⁹	23.2

^a Uncertainties are twice the standard deviation.

^b Measure of the inter-molecular hydrogen bonding (difference between column 3 and 6)

^c Derived by adding the $[\text{CH}_2] = 4.5$ kJ/mol contributions

Table S12c. Compilation of Data Used for Evaluation of the Inter-Molecular Hydrogen Bonding in Branched Amines (at 298 K, in kJ/mol)^a

CAS	Homomorph	$\Delta_f^q H_m^o$	CAS	Homomorph	$\Delta_f^q H_m^o$	HB _{inter} (ROH) ^b
78-81-9	2-Methyl-1-propanamine	34.0±0.2 ²⁹	78-78-4	2-methylbutane	25.2±0.2 ²⁹	8.8
96-15-1	2-Methyl-1-butanamine	38.9±0.5 ^c	96-14-0	3-methylpentane	30.5±0.2 ²⁹	8.4
13364-16-4	2-Methyl-1-pentanamine	43.7±0.5 ^c	589-34-4	3-methylhexane	35.2±0.2 ²⁹	8.5
44652-67-7	2-Methyl-1-hexanamine	48.5±0.5 ^c	589-81-1	3-methylheptane	39.9±0.2 ²⁹	8.6
101084-50-8	2-Methyl-1-heptanamine	53.4±0.7 ^d	2216-33-3	3-methyloctane	44.9±0.2 ²⁹	8.5
1081974-54-0	2-Methyl-1-octanamine	58.3±0.7 ^d	5911-04-6	3-methylnonane	49.7±0.2 ²⁹	8.6
13952-84-6	2-butanamine	32.7±0.2 ²⁹	78-78-4	2-methylbutane	25.2±0.2 ²⁹	7.5
616-24-0	3-pentanamine	37.9±0.7 ^c	96-14-0	3-methylpentane	30.5±0.2 ²⁹	7.4
16751-58-9	3-hexanamine	42.6±0.7 ^c	589-34-4	3-methylhexane	35.2±0.2 ²⁹	7.4
28292-42-4	3-heptanamine	47.3±0.7 ^c	589-81-1	3-methylheptane	39.9±0.2 ²⁹	7.4
24552-04-3	3-octanamine	51.3±0.7 ^b	2216-33-3	3-methyloctane	44.9±0.2 ²⁹	6.4
33787-95-0	3-nonanamine	55.3±0.7 ^c	5911-04-6	3-methylnonane	49.7±0.2 ²⁹	5.6

^a Uncertainties are twice the standard deviation.

^b Measure of the inter-molecular hydrogen bonding (difference between column 3 and 6)

^c From Table S13

^d From Table S14

Table S12d. Compilation of Data Used for Evaluation of the Inter-Molecular Hydrogen Bonding in Alcohols and Amines (at 298 K, in kJ/mol)^a

CAS	Homomorph	$\Delta_f^q H_m^o$	HB _{inter} (ROH) ^b	CAS	Homomorph	$\Delta_f^q H_m^o$	HB _{inter} (RNH2) ^c	HB _{inter} ^d
78-92-2	2-butanol	49.8±0.2 ²⁹	24.6	78-81-9	2-Methyl-1-propanamine	34.0±0.2 ²⁹	8.8	33.4
584-02-1	3-pentanol	54.0±0.2 ²⁹	23.5	96-15-1	2-Methyl-1-butanamine	38.9±0.5 ^f	8.4	31.9
623-37-0	3-hexanol	58.6±0.4 ³⁰	23.4	13364-16-4	2-Methyl-1-pentanamine	43.7±0.5 ^f	8.5	31.9
589-82-2	3-heptanol	63.1±0.7 ^e	23.2	44652-67-7	2-Methyl-1-hexanamine	48.5±0.5 ^f	8.6	31.8
589-98-0	3-octanol	67.6±0.7 ^e	22.7	101084-50-8	2-Methyl-1-heptanamine	53.4±0.7 ^g	8.5	31.2
624-51-1	3-nonanol	70.9±0.3 ³¹	21.2	1081974-54-0	2-Methyl-1-octanamine	58.3±0.7 ^g	8.6	29.8
78-83-1	2-methyl-propanol	50.9±0.2 ²⁹	25.7	13952-84-6	2-butanamine	32.7±0.2 ²⁹	7.5	33.2
137-32-6	2-methyl-1-butanol	54.6±1.3 ³²	24.1	616-24-0	3-pentanamine	37.9±0.5 ^f	7.4	31.5
105-30-6	2-methyl-1-pentanol	59.4±0.3 ³⁰	24.2	16751-58-9	3-hexanamine	42.6±0.5 ^f	7.4	31.6
624-22-6	2-methyl-1-hexanol	63.9±0.7 ^e	24.0	28292-42-4	3-heptanamine	47.3±0.5 ^f	7.4	31.4
60435-70-3	2-methyl-1-heptanol	68.4±0.7 ^e	23.5	24552-04-3	3-octanamine	51.3±0.5 ^f	6.4	29.9
818-81-5	2-methyl-1-octanol	72.9±0.7 ^e	23.2	33787-95-0	3-nonanamine	55.3±0.5 ^f	5.6	28.8

^a Uncertainties are twice the standard deviation.

^b From Table S12b.

^c From Table S12c.

^d Measure of the inter-molecular hydrogen bonding (difference between column 3 and 6)

^e Derived by adding the [CH₂] = 4.5 kJ/mol contributions

^f From Table S13.

^g From Table S14.

Table S13. Compilation of Data Used for Correlation of Normal Boiling Temperatures T_b and Experimental Standard Molar Vaporization Enthalpies, $\Delta_l^g H_m^o(\text{exp})$, of Amines (at 298 K, in kJ/mol)^a

CAS	Homomorph	T_b ³³	$\Delta_l^g H_m^o(\text{exp})$	$\Delta_l^g H_m^o(\text{calc})$ _b	Δ^c
78-81-9	2-methyl-1-propanamine	341	34.0±0.2 ²⁹		-0.2
96-15-1	2-methyl-1-butanamine	369		38.9±0.5	
13364-16-4	2-methyl-1-pentanamine	395		43.7±0.5	
44652-67-7	2-methyl-1-hexanamine	421		48.5±0.5	
101084-50-8	2-methyl-1-heptanamine	-			
1081974-54-0	2-methyl-1-octanamine	-			
13952-84-6	2-butanamine	336	32.7±0.2 ²⁹		0.1
616-24-0	3-pentanamine	363		37.9±0.5	
16751-58-9	3-hexanamine	389		42.6±0.5	
28292-42-4	3-heptanamine	414		47.3±0.5	
24552-04-3	3-octanamine	436		51.3±0.5	
33787-95-0	3-nonanamine	458		55.3±0.5	
109-73-9	1-butanamine	351	35.8±0.2 ²⁹		0.1
110-58-7	1-pentanamine	378	40.2±0.2 ²⁹		-0.4
111-26-2	1-hexanamine	403	45.1±0.2 ²⁹		-0.1
111-68-2	1-heptanamine	429	50.0±0.2 ²⁹		0.0
111-86-4	1-octanamine	452	54.6±0.2 ²⁹		0.4
104-75-6	2-ethyl-1-hexanamine	442	52.2±0.2 ²⁹		-0.2
112-20-9	1-nonanamine	475		58.4±0.5	
75-64-9	tert-butylamine	318	29.9±0.2 ²⁹		0.1

^a Uncertainties are twice the standard deviation.

^b Calculated according to the empirical equation, derived from the data collected in this table:

$$\Delta_l^g H_m^o(\text{calc}) = 0.1834 \times T_b - 28.7 \text{ with } R^2 = 0.9992$$

^c Difference exp. – calc.

Table S14. Compilation of Data Used for Correlation of Chain Length, N_C , and Experimental Standard Molar Vaporization Enthalpies, $\Delta_l^g H_m^o(\text{exp})$, of Amines (at 298 K, in kJ/mol)^a

CAS	Homomorph	N_C	$\Delta_l^g H_m^o(\text{empiric})$ ^b	$\Delta_l^g H_m^o(\text{calc})$ ^c	Δ^d
78-81-9	2-methyl-1-propanamine	3	33.9	34.0	-0.1
96-15-1	2-methyl-1-butanamine	4	38.9	38.8	0.1
13364-16-4	2-methyl-1-pentanamine	5	43.7	43.7	0.0
44652-67-7	2-methyl-1-hexanamine	6	48.5	48.6	-0.1
101084-50-8	2-methyl-1-heptanamine	7		53.4	
1081974-54-0	2-methyl-1-octanamine	8		58.3	
44995-93-9	2-methyl-1-octanamine	9		63.1	

^a Uncertainties are twice the standard deviation.

^b From Table S13.

^c Calculated according to the empirical equation, derived from the data collected in this table:

$$\Delta_l^g H_m^o(\text{calc}) = 4.86 \times N_C + 19.4 \text{ with } R^2 = 0.9999$$

^d Difference empiric – calc.

Table S15. Data Used for Determination of Intramolecular Hydrogen Bonding in Dialkylaminoalcohols.

CAS	Compound	$\Delta_l^g H_m^o(298\text{ K})$	Σ incr	HB _{intra} ^c
108-01-0	2-(dimethyl-amino)-ethanol	47.1±0.1 ^{18,19}	56.7	-9.6
100-37-8	2-(diethyl-amino)-ethanol	52.6±0.2 ^{18,19}	62.5	-9.9

Table S16. Parameters of the NBO-Analysis for Aminoalcohols Intramolecular Hydrogen Bonding

compound	Donor NBO (i)	Acceptor NBO (j)	$\Delta E^{(2)}_{n \rightarrow \sigma^*} /$ kcal·mol ⁻¹	E(j)-E(i) / a.u.	F (i,j) / a.u.	qCT / e
2-amino-ethanol (OH···N)	N 2	O 6 - H 7	4.35	0.81	0.053	0.00856
2-amino-ethanol (NH···O)	O 7	N 9 - H 10	0.65	0.80	0.021	0.00138
2-amino-1-propanol (OH···N)	N 4	O 8 - H 9	4.89	0.81	0.056	0.00956
2-amino-1-propanol (NH···O)	O 9	N 11 - H 13	0.95	0.80	0.025	0.00195
2-amino-1-butanol (OH···N)	N 4	O 9 - H 10	5.09	0.80	0.058	0.01051
2-amino-1-butanol (NH···O)	O 13	N 15 - H 17	1.22	0.81	0.028	0.00239
2-amino-1-pentanol (OH···N)	N 4	O 8 - H 9	5.12	0.80	0.058	0.01051
2-amino-1-pentanol (NH···O)	O 12	N 14 - H 16	1.23	0.81	0.028	0.00239
2-amino-1-hexanol (OH···N)	N 4	O 8 - H 9	5.13	0.80	0.058	0.01051
2-amino-1-hexanol (NH···O)	O 12	N 14 - H 16	1.23	0.81	0.028	0.00239
1-amino-2-propanol (OH···N)	N 12	O 10 - H 11	5.29	0.81	0.059	0.01061
1-amino-2-propanol (NH···O)	O 9	N 4 - H 6	0.51	1.08	0.021	0.00076
2-(dimethyl-amino)-1-ethanol (OH···N)	N 3	O 16 - H 17	3.64	0.77	0.049	0.00810

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