Electronic supporting information.

Top-Down and Bottom-Up evaluation of thermochemistry of α,ω-alkanediols

Riko Siewert,[1,2] Olga V. Dorofeeva,[3] Artemiy A. Samarov,[4] Arina V. Elbakari,[5] Karsten Müller,[1,2] Peter Wasserscheid, [6] Sergey P. Verevkin[1,2,*]

[1] *University of Rostock, Institute of Technical Thermodynamics, Albert-Einstein-Str.2, 18059 Rostock, Germany*
[2] *University of Rostock, Competence center °CALOR at the Department Life, Light & Matter*
[3] *Lomonosov Moscow State University, Department of Chemistry, 119991 Moscow, Russia*
[4] *Saint Petersburg State University, Department of Chemical Thermodynamics and Kinetics, Peterhof, 198504 Saint Petersburg, Russia.*
[5] *Samara State Technical University, Chemical-Technological Department, 443100 Samara, Russia*
[6] *Institute of Chemical Reaction Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany*

Materials

The samples of alkanediols used in this work were of commercial origin (see Table S1).

Table S1. Provenance and purity of the materials

Material[a]	CAS	Origin	Initial GC purity	GC purity after purification (mass fraction)
1,5-pentanediol (liq)	111-29-5	Thermo Scientific Chemicals	98%	0.9925 [a]
1,6-hexanediol (cr)	629-11-8	Sigma-Aldrich	99%	0.9998
1,7-heptanediol (liq)	629-30-1	VWR	98%	0.9994 [a]
1,8-octanediol (cr)	629-41-4	Acros	99+%	0.9997
1,9-nonanediol (cr)	3937-56-2	VWR	99%	0.9998
1,10-decanediol (cr)	112-47-0	Thermo Scientific Chemicals	99%	0.9997

[a] Samples were additionally purified using fractional distillation and used for transpiration measurements

The liquid sample of 1,7-heptanediol was purified by fractional distillation under reduced pressure. Samples of α,ω-alkanediols for the transpiration method were used as received. However, before starting the vapor pressure measurements, the samples were preconditioned in the transpiration saturator (see below for details). The crystalline sample of 1,8-octanediol used for the combustion experiments was purified by fractional sublimation under reduced pressure. The water content of the sample of 1,8-octanediol was determined by Karl Fischer titration using a Metrohm 756/831 KF Coulometer.The final purities of the samples were determined by GC. The samples were analysed with a Hewlett Packard 5890 II series gas chromatograph equipped with a flame ionisation detector and an HP-5 capillary column (length, inside diameter, and film thickness of 25 m×0.32 mm×0.25 μm). The GC temperature program started at T= 323 K, followed by heating at a rate of 0.167 K·s^{-1} to T = 573 K. No impurities (greater than 0.0006mass fraction) were detected in samples used for thermochemical measurements.

Table S2
Conformational analysis of α,ω-alkanediols at $T = 298.15$ K [a]

Conformer [b]		Symmetry	S [c]	ZPE + $(H_{298} - H_0)$ [d]	E_e [e]	H [f]	ΔH	ΔG	p_i [g]
			J·K^{-1}·mol^{-1}	hartree	hartree	kJ· mol^{-1}	kJ· mol^{-1}	kJ· mol^{-1}	%
1,2-ethanediol									
Relative population of conformers: [h] 95% of HB and 5% of F									
1	HB	C_1	301.31	0.090374	-230.039208	-603730.7	0.00	0.00	53.71
2	HB	C_1	299.24	0.090381	-230.038583	-603729.0	1.66	2.28	21.43
3	HB	C_2	304.80	0.090357	-230.037804	-603727.0	3.64	2.60	18.81
4	F	C_1	307.48	0.090231	-230.035002	-603720.0	10.67	8.83	1.52
5	HB	C_2	309.43	0.090007	-230.034478	-603719.2	11.46	9.04	1.40
6	F	C_2	307.89	0.089982	-230.034267	-603718.7	11.94	9.98	0.96
7	F	C_{2h}	299.03	0.090212	-230.035199	-603720.6	10.10	10.78	0.69
8	F	C_i	300.09	0.090313	-230.035041	-603719.9	10.78	11.14	0.60
9	F	C_1	307.67	0.089980	-230.033656	-603717.1	13.54	11.65	0.49
10	F	C_2	298.60	0.090259	-230.034726	-603719.2	11.47	12.27	0.38
1,3-propanediol									
Relative population of conformers: [h] 70% of HB and 30% of F									
1	HB	C_1	327.14	0.119987	-269.298652	-706728.6	0.00	0.00	33.10
2	HB	C_1	325.26	0.120068	-269.298404	-706727.7	0.86	1.43	18.62
3	HB	C_1	336.73	0.120002	-269.296501	-706722.9	5.69	2.83	10.57
4	F	C_2	332.27	0.119756	-269.296551	-706723.7	4.91	3.38	8.46
5	HB	C_1	336.56	0.119955	-269.296193	-706722.2	6.37	3.57	7.86
6	F	C_1	336.07	0.119745	-269.295825	-706721.8	6.79	4.13	6.26
7	F	C_1	338.33	0.119708	-269.295235	-706720.3	8.24	4.90	4.58
8	F	C_1	338.33	0.119748	-269.295132	-706720.0	8.61	5.28	3.93
9	F	C_1	337.40	0.119737	-269.295094	-706719.9	8.68	5.63	3.42
10	F	C_1	337.27	0.119724	-269.294741	-706719.0	9.58	6.56	2.35
11	F	C_2	328.23	0.119755	-269.294832	-706719.2	9.42	9.10	0.84
1,4-butanediol									
Relative population of conformers: [h] 29% of HB, 50% of F-lin and 21% of F									
1	HB [i]	C_1	352.09	0.149683	-308.557713	-809725.3	0.00	0.00	10.61
2	HB [i]	C_1	353.86	0.149638	-308.557167	-809724.0	1.32	0.79	7.72
3	HB [i]	C_1	350.87	0.149669	-308.557429	-809724.6	0.71	1.07	6.89
4	F-lin [i]	C_1	368.18	0.149139	-308.554494	-809718.3	7.02	2.22	4.33
5	F-lin [i]	C_i	363.47	0.149134	-308.554925	-809719.4	5.88	2.48	3.90
6	F-lin [i]	C_1	370.24	0.149225	-308.554226	-809717.3	7.95	2.54	3.81
7	F-lin [i]	C_1	368.43	0.149173	-308.554347	-809717.8	7.50	2.62	3.68
8	F-lin	C_1	369.01	0.149177	-308.554170	-809717.3	7.97	2.93	3.26
9	F-lin	C_1	372.21	0.149143	-308.553767	-809716.3	8.94	2.94	3.24
10	F [i]	C_1	368.64	0.149354	-308.554315	-809717.2	8.06	3.12	3.01
11	F-lin	C_1	372.42	0.149225	-308.553606	-809715.7	9.58	3.52	2.57
12	F-lin	C_1	369.96	0.149216	-308.553834	-809716.3	8.96	3.63	2.46
13	F-lin [i]	C_1	369.36	0.149227	-308.553682	-809715.9	9.39	4.24	1.92
14	F-lin	C_1	370.05	0.149123	-308.553466	-809715.6	9.68	4.32	1.85
15	F-lin	C_1	369.92	0.149251	-308.553529	-809715.4	9.85	4.53	1.71
16	F-lin	C_1	370.63	0.149147	-308.553336	-809715.2	10.08	4.55	1.69
17	F-lin [i]	C_1	367.88	0.149176	-308.553635	-809715.9	9.38	4.67	1.62
18	F-lin [i]	C_1	369.81	0.149199	-308.553438	-809715.3	9.95	4.67	1.61
19	F	C_2	362.00	0.149355	-308.554458	-809717.6	7.68	4.73	1.58
20	F-lin	C_1	369.50	0.149239	-308.553463	-809715.3	9.99	4.80	1.53
21	F-lin [i]	C_i	361.82	0.149154	-308.554161	-809717.3	7.94	5.03	1.39
22	HB [i]	C_1	355.86	0.149692	-308.555371	-809719.1	6.17	5.05	1.39
23	F-lin [i]	C_2	361.74	0.149222	-308.554223	-809717.3	7.95	5.07	1.37
24	HB [i]	C_1	353.94	0.149682	-308.555538	-809719.6	5.71	5.15	1.33
25	F-lin	C_2	363.99	0.149081	-308.553750	-809716.5	8.82	5.27	1.26
26	F	C_1	371.07	0.149365	-308.553226	-809714.3	10.94	5.28	1.26
27	F-lin [i]	C_1	368.70	0.149176	-308.553260	-809714.9	10.36	5.41	1.20

28	F	C_1	372.24	0.149301	-308.552865	-809713.6	11.73	5.72	1.06
29	F-lin	C_i	366.32	0.149288	-308.553468	-809715.2	10.11	5.86	1.00
30	F	C_1	372.76	0.149213	-308.552641	-809713.2	12.08	5.92	0.98
31	F [i]	C_2	363.63	0.149356	-308.553813	-809715.9	9.38	5.94	0.97
32	F	C_1	370.66	0.149186	-308.552826	-809713.8	11.52	5.99	0.95
33	F	C_1	372.12	0.149257	-308.552723	-809713.3	11.98	6.01	0.94
34	F-lin	C_{2h}	361.73	0.149198	-308.553830	-809716.4	8.92	6.04	0.93
35	F	C_1	371.19	0.149356	-308.552887	-809713.5	11.81	6.12	0.90
36	F-lin [i]	C_i	362.40	0.149225	-308.553592	-809715.7	9.62	6.54	0.76
37	F	C_1	369.83	0.149292	-308.552779	-809713.4	11.93	6.63	0.73
38	F	C_1	370.46	0.149295	-308.552676	-809713.1	12.20	6.73	0.70
39	F	C_1	372.61	0.149216	-308.552348	-809712.4	12.86	6.74	0.70
40	F	C_1	369.26	0.149289	-308.552779	-809713.4	11.92	6.80	0.68
41	HB [i]	C_2	354.51	0.149677	-308.554824	-809717.7	7.57	6.84	0.67
42	F	C_1	371.19	0.149285	-308.552529	-809712.7	12.56	6.87	0.66
43	F-lin	C_2	363.47	0.149257	-308.553358	-809715.0	10.32	6.92	0.65
44	F-lin	C_2	363.05	0.149190	-308.553307	-809715.0	10.27	7.01	0.63
45	F	C_1	371.04	0.149269	-308.552470	-809712.6	12.68	7.03	0.62
46	F	C_1	369.58	0.149208	-308.552573	-809713.0	12.25	7.03	0.62
47	F-lin	C_2	362.65	0.149211	-308.553305	-809714.9	10.33	7.19	0.58
48	F	C_1	371.16	0.149311	-308.552422	-809712.4	12.91	7.23	0.58
49	HB [i]	C_1	352.86	0.149647	-308.554832	-809717.8	7.47	7.24	0.57
50	F	C_1	371.80	0.149265	-308.552219	-809712.0	13.33	7.45	0.53
51	F	C_1	370.04	0.149328	-308.552440	-809712.4	12.91	7.56	0.50
52	F-lin	C_1	357.37	0.149179	-308.553730	-809716.1	9.13	7.56	0.50
53	F	C_1	367.79	0.149197	-308.552477	-809712.8	12.47	7.79	0.46
54	F	C_1	371.25	0.149314	-308.552123	-809711.6	13.71	7.99	0.42
55	F	C_2	366.32	0.149230	-308.552487	-809712.8	12.53	8.29	0.38
56	F	C_1	372.28	0.149273	-308.551775	-809710.8	14.51	8.49	0.35
57	F	C_1	369.51	0.149243	-308.552057	-809711.6	13.69	8.50	0.34
58	F	C_1	367.01	0.149219	-308.552025	-809711.6	13.72	9.27	0.25
59	F	C_1	366.35	0.149238	-308.552116	-809711.8	13.53	9.27	0.25
60	F	C_2	364.69	0.149331	-308.552324	-809712.1	13.22	9.47	0.23
61	F	C_2	366.15	0.149309	-308.551995	-809711.3	14.03	9.84	0.20
62	F	C_2	363.15	0.149269	-308.552209	-809711.9	13.36	10.06	0.18
63	F	C_1	371.80	0.149248	-308.551151	-809709.2	16.09	10.21	0.17
64	F	C_1	370.47	0.149272	-308.550927	-809708.5	16.74	11.26	0.11
65	F	C_1	368.85	0.149167	-308.550308	-809707.2	18.09	13.09	0.05
				1,5-pentanediol					
				Relative population of conformers: [h] 11% of HB, 79% of F-lin and 10% of F					
1	F-lin	C_1	401.03	0.178654	-347.812968	-912713.9	2.84	0.00	10.92
2	F-lin	C_1	403.00	0.178645	-347.812630	-912713.0	3.71	0.28	9.76
3	F-lin	C_2	396.75	0.178580	-347.813071	-912714.4	2.38	0.81	7.87
4	F-lin	C_1	402.21	0.178561	-347.812419	-912712.7	4.04	0.85	7.75
5	F-lin	C_1	399.51	0.178665	-347.812683	-912713.1	3.62	1.23	6.65
6	F-lin	C_1	400.43	0.178661	-347.812559	-912712.8	3.94	1.28	6.53
7	F-lin	C_1	402.22	0.178663	-347.812306	-912712.1	4.61	1.41	6.19
8	F-lin	C_1	402.48	0.178692	-347.812183	-912711.7	5.01	1.73	5.44
9	F-lin	C_1	402.52	0.178682	-347.812072	-912711.5	5.27	1.98	4.91
10	HB	C_1	381.60	0.179314	-347.814712	-912716.7	0.00	2.95	3.32
11	F	C_1	402.13	0.178735	-347.811716	-912710.4	6.34	3.17	3.04
12	F-lin	C_s	399.36	0.178737	-347.812011	-912711.2	5.58	3.23	2.97
13	F	C_1	399.61	0.178753	-347.811992	-912711.1	5.67	3.25	2.95
14	F-lin	C_2	398.07	0.178723	-347.812108	-912711.5	5.28	3.32	2.86
15	F	C_1	399.69	0.178787	-347.811986	-912711.0	5.77	3.33	2.85
16	F-lin	C_2	395.01	0.178592	-347.812198	-912712.0	4.71	3.66	2.50
17	F-lin	C_2	395.38	0.178659	-347.812135	-912711.7	5.04	3.89	2.28
18	F-lin	C_s	397.02	0.178625	-347.811907	-912711.2	5.56	3.91	2.26
19	HB	C_1	382.55	0.179151	-347.814024	-912715.4	1.38	4.04	2.14
20	HB	C_1	382.42	0.179277	-347.813670	-912714.1	2.64	5.34	1.27
21	HB	C_1	375.89	0.179384	-347.814351	-912715.6	1.13	5.78	1.06
22	F	C_1	399.23	0.178681	-347.810864	-912708.3	8.44	6.13	0.92
23	HB	C_1	377.93	0.179301	-347.813753	-912714.3	2.48	6.53	0.78
24	F	C_1	399.11	0.178627	-347.810670	-912707.9	8.81	6.54	0.78

25	HB	C_1	376.99	0.179281	-347.813740	-912714.3	2.46	6.79	0.71
26	HB	C_1	383.48	0.179209	-347.812583	-912711.4	5.31	7.70	0.49
27	HB	C_1	376.94	0.179463	-347.813456	-912713.0	3.69	8.03	0.43
28	HB	C_1	378.47	0.179317	-347.812550	-912711.1	5.68	9.57	0.23
29	HB	C_1	377.97	0.179218	-347.812238	-912710.5	6.24	10.28	0.17
				1,6-hexanediol					
				Relative population of conformers: [h] 2% of HB, 91% of F-lin and 7% of F					
1	F-lin	C_1	435.77	0.208102	-387.071429	-1015709.7	2.96	0.00	7.09
2	F-lin	C_1	434.12	0.208068	-387.071520	-1015710.0	2.63	0.16	6.64
3	F-lin	C_1	435.75	0.208094	-387.071305	-1015709.4	3.26	0.31	6.25
4	F-lin	C_1	434.09	0.208034	-387.071427	-1015709.8	2.78	0.33	6.21
5	F-lin	C_1	434.10	0.208034	-387.071419	-1015709.8	2.80	0.35	6.17
6	F-lin	C_1	434.06	0.208064	-387.071404	-1015709.7	2.92	0.48	5.85
7	F-lin	C_1	437.23	0.208126	-387.070959	-1015708.4	4.25	0.86	5.01
8	F-lin	C_1	436.13	0.208060	-387.070954	-1015708.5	4.09	1.03	4.68
9	F-lin	C_1	435.29	0.208112	-387.071099	-1015708.8	3.85	1.03	4.67
10	F-lin	C_i	429.09	0.208017	-387.071703	-1015710.6	2.02	1.05	4.64
11	F-lin	C_2	429.36	0.207989	-387.071475	-1015710.1	2.54	1.49	3.88
12	F-lin	C_1	434.81	0.208111	-387.070970	-1015708.4	4.18	1.52	3.85
13	F-lin	C_1	433.68	0.208071	-387.071053	-1015708.8	3.86	1.53	3.83
14	F-lin	C_1	433.30	0.208077	-387.071072	-1015708.8	3.83	1.61	3.71
15	F-lin	C_1	434.84	0.208157	-387.070953	-1015708.3	4.35	1.67	3.62
16	F-lin	C_1	434.73	0.208150	-387.070901	-1015708.2	4.47	1.82	3.40
17	F-lin	C_2	427.52	0.208046	-387.071209	-1015709.2	3.39	2.89	2.21
18	F	C_1	433.47	0.208198	-387.070661	-1015707.4	5.22	2.95	2.15
19	F	C_1	433.37	0.208229	-387.070665	-1015707.3	5.30	3.06	2.07
20	F	C_1	432.86	0.208200	-387.070662	-1015707.4	5.23	3.14	2.00
21	F-lin	C_i	430.65	0.208172	-387.070856	-1015708.0	4.64	3.21	1.94
22	F-lin	C_i	428.29	0.208111	-387.071050	-1015708.6	3.97	3.25	1.91
23	F-lin	C_2	430.69	0.208168	-387.070806	-1015707.9	4.77	3.32	1.85
24	F-lin	C_2	428.07	0.208101	-387.070998	-1015708.5	4.08	3.42	1.78
25	F-lin	C_{2h}	426.51	0.208086	-387.071090	-1015708.8	3.80	3.61	1.65
26	HB	C_1	405.05	0.209101	-387.073554	-1015712.6	0.00	6.20	0.58
27	HB	C_1	406.21	0.208987	-387.073106	-1015711.7	0.88	6.74	0.47
28	F	C_1	431.67	0.208098	-387.069160	-1015703.7	8.90	7.17	0.39
29	HB	C_1	407.73	0.208934	-387.072646	-1015710.7	1.95	7.35	0.37
30	HB	C_1	411.53	0.208762	-387.071805	-1015708.9	3.70	7.97	0.28
31	HB	C_1	410.59	0.208675	-387.071462	-1015708.2	4.37	8.92	0.19
32	HB	C_1	406.38	0.208862	-387.072117	-1015709.5	3.15	8.95	0.19
33	HB	C_1	404.46	0.208921	-387.072148	-1015709.4	3.22	9.60	0.15
34	HB	C_1	406.53	0.208851	-387.071715	-1015708.4	4.17	9.94	0.13
35	HB	C_1	408.49	0.208864	-387.071207	-1015707.1	5.54	10.72	0.09
36	HB	C_1	404.28	0.208984	-387.071668	-1015708.0	4.64	11.08	0.08
				1,7-heptanediol					
				Relative population of conformers: [h] 5% of HB, 87% of F-lin and 8% of F					
1	F-lin	C_1	466.76	0.237518	-426.330223	-1118706.4	6.23	0.00	8.10
2	F-lin	C_1	468.19	0.237548	-426.330081	-1118705.9	6.68	0.03	8.01
3	F-lin	C_1	466.74	0.237509	-426.330168	-1118706.3	6.35	0.13	7.70
4	F-lin	C_1	467.13	0.237457	-426.329999	-1118706.0	6.65	0.32	7.13
5	F-lin	C_1	466.73	0.237471	-426.330035	-1118706.0	6.60	0.38	6.95
6	F-lin	C_1	468.61	0.237517	-426.329799	-1118705.3	7.34	0.56	6.46
7	F-lin	C_1	469.96	0.237569	-426.329675	-1118704.8	7.80	0.62	6.31
8	F-lin	C_1	467.82	0.237553	-426.329770	-1118705.1	7.51	0.96	5.49
9	F-lin	C_2	461.78	0.237456	-426.330322	-1118706.8	5.80	1.06	5.28
10	F-lin	C_1	467.53	0.237558	-426.329701	-1118704.9	7.70	1.25	4.89
11	F-lin	C_1	465.85	0.237534	-426.329865	-1118705.4	7.21	1.25	4.89
12	F-lin	C_1	465.71	0.237528	-426.329872	-1118705.5	7.17	1.26	4.87
13	F-lin	C_1	467.20	0.237602	-426.329654	-1118704.7	7.94	1.58	4.28
14	HB	C_1	437.58	0.238391	-426.333468	-1118712.6	0.00	2.47	2.99
15	F-lin	C_2	463.29	0.237617	-426.329598	-1118704.5	8.13	2.94	2.48
16	F	C_1	465.95	0.237633	-426.329280	-1118703.6	9.01	3.02	2.40
17	F-lin	C_s	461.20	0.237478	-426.329647	-1118705.0	7.63	3.07	2.35
18	F	C_1	465.75	0.237634	-426.329272	-1118703.6	9.03	3.10	2.32

19	F-lin	C_s	460.61	0.237552	-426.329726	-1118705.0	7.62	3.23	2.20
20	F	C_1	464.46	0.237587	-426.329034	-1118703.1	9.53	3.99	1.62
21	F	C_1	464.46	0.237578	-426.328947	-1118702.9	9.74	4.19	1.49
22	HB	C_1	431.57	0.238405	-426.332529	-1118710.1	2.50	6.77	0.53
23	HB	C_1	435.70	0.238370	-426.331623	-1118707.8	4.79	7.82	0.35
24	HB	C_1	431.09	0.238443	-426.331687	-1118707.8	4.81	9.22	0.20
25	HB	C_1	430.75	0.238330	-426.331529	-1118707.7	4.93	9.44	0.18
26	HB	C_1	433.67	0.238305	-426.331149	-1118706.8	5.86	9.50	0.18
27	HB	C_1	431.46	0.238329	-426.331327	-1118707.2	5.46	9.76	0.16
28	HB	C_1	429.47	0.238331	-426.331316	-1118707.1	5.49	10.38	0.12
29	HB	C_1	431.57	0.238267	-426.330737	-1118705.8	6.84	11.11	0.09
				1,8-octanediol					
	Relative population of conformers: [h] 3% of HB and 77% of F-lin (F conformers were not considered)								
1	F-lin	C_1	499.30	0.266952	-465.588876	-1221702.7	4.63	0.00	8.41
2	F-lin	C_1	499.49	0.266952	-465.588822	-1221702.6	4.77	0.08	8.13
3	F-lin	C_1	499.77	0.266907	-465.588744	-1221702.5	4.86	0.09	8.11
4	F-lin	C_1	500.51	0.266996	-465.588746	-1221702.3	5.08	0.10	8.09
5	F-lin	C_1	502.43	0.267013	-465.588376	-1221701.2	6.10	0.54	6.77
6	F-lin	C_1	500.56	0.266994	-465.588512	-1221701.6	5.69	0.69	6.37
7	F-lin	C_1	500.72	0.266953	-465.588396	-1221701.4	5.89	0.84	6.00
8	F-lin	C_i	494.79	0.266889	-465.589000	-1221703.2	4.14	0.85	5.96
9	F-lin	C_1	497.31	0.266941	-465.588713	-1221702.3	5.03	0.99	5.64
10	F-lin	C_1	498.96	0.266966	-465.588512	-1221701.7	5.62	1.09	5.41
11	F-lin	C_1	499.95	0.267005	-465.588387	-1221701.3	6.05	1.23	5.12
12	F-lin	C_1	500.07	0.267035	-465.588391	-1221701.2	6.12	1.26	5.06
13	F-lin	C_1	499.81	0.267046	-465.588419	-1221701.3	6.07	1.29	4.99
14	F-lin	C_1	498.09	0.266981	-465.588502	-1221701.7	5.68	1.42	4.74
15	F-lin	C_2	493.33	0.266931	-465.588491	-1221701.8	5.58	2.74	2.79
16	F-lin	C_i	493.33	0.266928	-465.588484	-1221701.7	5.59	2.75	2.78
17	F-lin	C_i	495.85	0.267062	-465.588303	-1221700.9	6.42	2.82	2.69
18	HB	C_1	470.18	0.267838	-465.591472	-1221707.2	0.14	4.19	1.55
19	HB	C_1	461.99	0.267957	-465.591643	-1221707.3	0.00	6.50	0.61
20	HB	C_1	467.11	0.267863	-465.590344	-1221704.2	3.16	8.13	0.32
21	HB	C_2	474.61	0.267667	-465.589091	-1221701.4	5.94	8.68	0.25
22	HB	C_1	460.01	0.267880	-465.590325	-1221704.1	3.26	10.35	0.13
23	HB	C_1	459.73	0.267931	-465.590149	-1221703.5	3.85	11.02	0.10
				1,9-nonanediol					
	Relative population of conformers: [h] 9% of HB and 91% of F-lin (F conformers were not considered)								
1	F-lin	C_1	533.99	0.296381	-504.847414	-1324698.7	8.02	0.00	9.21
2	F-lin	C_1	532.24	0.296396	-504.847555	-1324699.1	7.69	0.19	8.53
3	F-lin	C_1	533.34	0.296433	-504.847414	-1324698.6	8.16	0.33	8.06
4	F-lin	C_1	533.17	0.296434	-504.847382	-1324698.5	8.24	0.47	7.62
5	F-lin	C_1	535.20	0.296454	-504.847074	-1324697.7	9.10	0.72	6.88
6	F-lin	C_1	533.52	0.296430	-504.847190	-1324698.0	8.73	0.86	6.52
7	F-lin	C_s	527.48	0.296316	-504.847602	-1324699.4	7.35	1.28	5.50
8	F-lin	C_1	532.90	0.296478	-504.847127	-1324697.7	9.03	1.33	5.38
9	F-lin	C_1	531.25	0.296411	-504.847230	-1324698.2	8.58	1.38	5.28
10	F-lin	C_1	531.10	0.296409	-504.847230	-1324698.2	8.58	1.42	5.19
11	F-lin	C_1	532.61	0.296450	-504.847087	-1324697.7	9.06	1.45	5.13
12	F-lin	C_1	532.51	0.296485	-504.847107	-1324697.7	9.10	1.52	4.99
13	HB	C_1	500.04	0.297311	-504.851398	-1324706.8	0.00	2.10	3.94
14	HB	C_1	500.37	0.297427	-504.851159	-1324705.8	0.93	2.94	2.82
15	F-lin	C_2	528.64	0.296507	-504.847009	-1324697.3	9.41	2.99	2.76
16	F-lin	C_2	525.95	0.296450	-504.847239	-1324698.1	8.66	3.04	2.71
17	F-lin	C_s	526.04	0.296359	-504.847077	-1324697.9	8.84	3.20	2.54
18	F-lin	C_s	525.58	0.296443	-504.847213	-1324698.0	8.71	3.20	2.53
19	F-lin	C_2	525.92	0.296366	-504.847088	-1324697.9	8.84	3.22	2.51
20	HB	C_1	490.50	0.297326	-504.850231	-1324703.7	3.10	8.05	0.36
21	HB	C_1	485.39	0.297664	-504.851031	-1324704.9	1.89	8.36	0.32
22	HB	C_1	493.19	0.297370	-504.849840	-1324702.5	4.25	8.39	0.31
23	HB	C_1	490.13	0.297539	-504.850239	-1324703.1	3.64	8.70	0.28
24	HB	C_1	486.47	0.297550	-504.850592	-1324704.0	2.74	8.89	0.25
25	HB	C_1	499.28	0.297265	-504.848545	-1324699.4	7.37	9.70	0.18

26	HB	C_1	490.13	0.297370	-504.849266	-1324701.0	5.75	10.81	0.12
27	HB	C_1	492.87	0.297268	-504.848636	-1324699.6	7.14	11.38	0.09
				1,10-decanediol					
	Relative population of conformers: [h] 16% of HB and 84% of F-lin (F conformers were not considered)								
1	F-lin	C1	565.14	0.325831	-544.1062206	-1427695.41	8.51	0.00	0.19
2	F-lin	C1	564.63	0.325796	-544.1060894	-1427695.16	8.77	0.41	0.16
3	F-lin	C1	566.70	0.325836	-544.1057838	-1427694.25	9.67	0.69	0.14
4	F-lin	C1	565.75	0.325924	-544.1058140	-1427694.10	9.82	1.13	0.12
5	F-lin	C1	565.32	0.325886	-544.1057742	-1427694.10	9.83	1.26	0.11
6	F-lin	Ci	559.75	0.325811	-544.1058352	-1427694.45	9.47	2.57	0.07
7	F-lin	Ci	558.66	0.325903	-544.1059564	-1427694.53	9.40	2.81	0.06
8	HB	C1	528.50	0.326985	-544.1095370	-1427701.09	2.84	5.25	0.02
9	HB	C1	520.04	0.326875	-544.1100263	-1427702.66	1.26	6.20	0.02
10	HB	C1	516.80	0.327007	-544.1104856	-1427703.52	0.40	6.30	0.01
11	HB	C1	523.29	0.326720	-544.1093150	-1427701.20	2.72	6.69	0.01
12	HB	C1	514.16	0.327099	-544.1107309	-1427703.93	0.00	6.69	0.01
13	HB	C1	525.42	0.326810	-544.1091363	-1427700.50	3.43	6.76	0.01
14	HB	C1	519.92	0.326889	-544.1097037	-1427701.78	2.15	7.12	0.01
15	HB	C1	527.28	0.326963	-544.1088561	-1427699.36	4.57	7.34	0.01
16	HB	C1	515.89	0.326851	-544.1099846	-1427702.62	1.31	7.48	0.01
17	HB	C1	519.01	0.327076	-544.1096792	-1427701.22	2.70	7.94	0.01
18	HB	C1	515.50	0.327129	-544.1100296	-1427702.01	1.92	8.21	0.01
19	HB	C1	513.86	0.327026	-544.1100756	-1427702.40	1.53	8.31	0.01
20	HB	C1	516.45	0.327039	-544.1097238	-1427701.44	2.49	8.49	0.01
21	HB	C1	519.11	0.327008	-544.1092638	-1427700.31	3.61	8.83	0.01
22	HB	C1	516.14	0.327028	-544.1092626	-1427700.26	3.67	9.77	0.00
23	HB	C1	511.22	0.327025	-544.1095464	-1427701.01	2.92	10.48	0.00
24	HB	C1	512.20	0.327237	-544.1095656	-1427700.50	3.42	10.69	0.00
25	HB	C1	520.58	0.326842	-544.1073811	-1427695.81	8.12	12.90	0.00

[a] Conformers are given in ascending Gibbs free energy order.

[b] HB are the O–H···O–H hydrogen bonded conformers, F are the conformers with free hydroxyl groups and F-lin are the conformers with free hydroxyl groups and linear carbon backbone.

[c] Entropy was calculated at B3LYP-D3(BJ)/def2-TZVPP level, the vibrational frequencies were scaled by a factor of 0.9657 (see Section 2.2 for details).

[d] Thermal correction [ZPE + $(H_{298} - H_0)$] was calculated at B3LYP-D3(BJ)/def2-TZVPP level, the vibrational frequencies were scaled by a factor of 0.9883 (see Section 2.2 for details).

[e] Electronic energy was calculated at the DLPNO-CCSD(T_1)/CBS//B3LYP-D3(BJ)/def2-TZVPP level of theory.

[f] $H = E_e + \mathrm{ZPE} + (H_{298} - H_0)$.

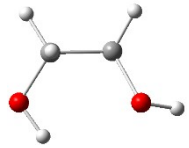
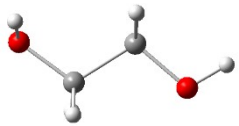
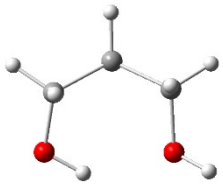
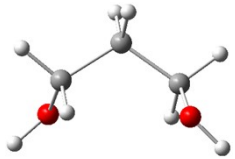
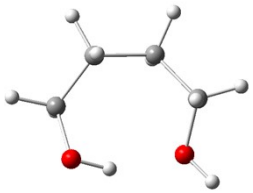
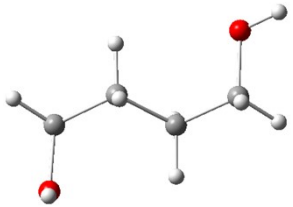
$$p_i = \frac{e^{-\Delta G(i)/RT}}{\sum_i e^{-\Delta G(i)/RT}}$$

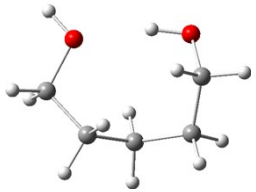
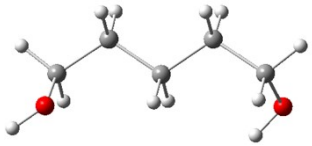
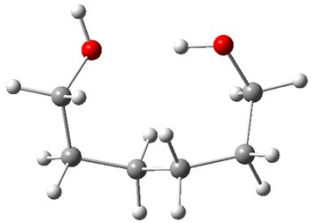
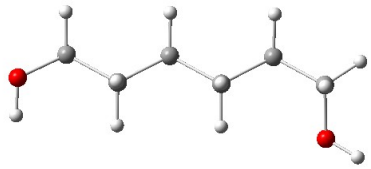
[g] Relative populations of the conformers:

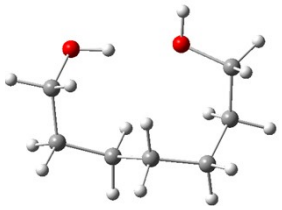
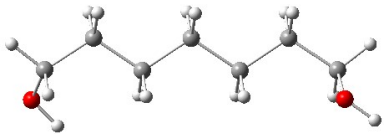
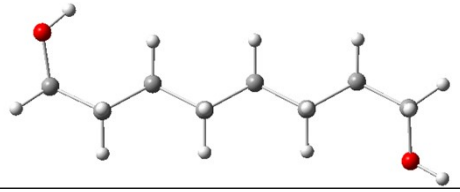
[h] Relative population of conformers is obtained for the set of conformers selected below. Only for 1,2-ethanediol and 1,4-butanediol it corresponds to all possible conformers (see text for details)

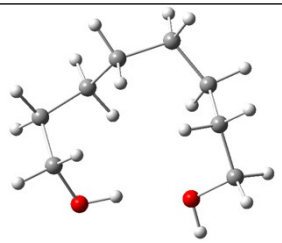
[i] Conformers of 1,4-butanediol determined from simplified population analysis using only 20 lowest-energy B3LYP/6-31G(d,p) conformers.

Table S3
Cartesian coordinates of most stable HB and F conformers of α,ω-alkanediols calculated at B3LYP-D3(BJ)/def2-TZVPP level (in Å)

HB conformer		x	y	z	F (F-lin) conformer [a]		x	y	z
1,2-ethanediol, $C_2H_6O_2$									
 symmetry C_1 r(OH···OH) = 2.372 Å	C	-0.730166	0.567511	0.271925	 symmetry C_1	C	-0.574027	-0.508520	0.003726
	H	-1.275564	1.447857	-0.069061		H	-0.489646	-1.116333	0.910169
	H	-0.695850	0.590233	1.367827		H	-0.507683	-1.178532	-0.852511
	C	0.682128	0.600135	-0.269062		C	0.567033	0.493835	-0.044630
	H	1.192610	1.507244	0.073992		H	0.469653	1.200961	0.790176
	H	0.655549	0.600583	-1.363115		H	0.507782	1.062954	-0.977877
	O	-1.444557	-0.566557	-0.189150		O	-1.840011	0.132892	-0.084642
	H	-0.896775	-1.335888	-0.001033		H	-2.005164	0.609531	0.733052
	O	1.338520	-0.572254	0.218962		O	1.783030	-0.239524	0.047185
	H	2.156555	-0.705412	-0.264283		H	2.522870	0.362582	-0.057924
1,3-propanediol, $C_3H_8O_2$									
 symmetry C_1 r(OH···OH) = 2. 024 Å	C	-1.266788	0.404302	0.291492	 symmetry C_2	C	0.000000	1.267717	0.147949
	H	-2.157388	0.967576	0.010158		H	-0.109446	2.138987	0.802867
	H	-1.178108	0.462205	1.386200		H	-0.844180	1.249801	-0.546361
	C	-0.032248	1.033903	-0.348420		C	0.000000	0.000000	0.981511
	H	-0.078127	0.892906	-1.430765		H	0.881130	-0.001134	1.627369
	H	-0.039786	2.111081	-0.158985		H	-0.881130	0.001134	1.627369
	C	1.276533	0.479343	0.183273		C	0.000000	-1.267717	0.147949
	H	2.124312	0.985106	-0.289375		H	0.844180	-1.249801	-0.546361
	H	1.337704	0.648186	1.264410		H	0.109446	-2.138987	0.802867
	O	-1.494048	-0.931856	-0.125208		O	1.238228	1.332383	-0.563506
	H	-0.644463	-1.387551	-0.089755		H	1.190164	2.041474	-1.208054
	O	1.326828	-0.927943	-0.095218		O	-1.238228	-1.332383	-0.563506
	H	2.108637	-1.306409	0.313448		H	-1.190164	-2.041474	-1.208054
1,4-butanediol, $C_4H_{10}O_2$									
 symmetry C_1 r(OH···OH) = 1.858 Å	C	1.604448	0.160821	0.313547	 symmetry C_1 ϕ(C-C-C-C) = -178.3°	C	-1.840103	0.633968	-0.199261
	H	2.635507	0.464564	0.112018		H	-1.848042	0.769399	-1.281873
	H	1.477690	0.070962	1.397393		H	-2.352899	1.495463	0.242580
	C	0.652761	1.206225	-0.242534		C	-0.408092	0.560315	0.309362
	H	1.063570	2.179622	0.038267		H	-0.420882	0.403487	1.394921
	H	0.692529	1.159309	-1.334765		H	0.074106	1.526181	0.145782
	C	-0.804232	1.146847	0.233972		C	0.410071	-0.541680	-0.358373
	H	-1.292390	2.074896	-0.078576		H	0.453808	-0.361589	-1.436158
	H	-0.835080	1.131003	1.327436		H	-0.087628	-1.503384	-0.219480
	C	-1.649268	-0.012930	-0.289407		C	1.824953	-0.646613	0.173721
	H	-1.568206	-0.059463	-1.384210		H	2.339559	-1.488507	-0.302369

	H	-2.696738	0.177840	-0.051741		H	1.803731	-0.833584	1.254922
	O	1.358685	-1.106509	-0.318556		O	-2.584441	-0.561667	0.033571
	H	1.978257	-1.755081	0.025409		H	-2.666328	-0.688527	0.982772
	O	-1.340291	-1.265542	0.293527		O	2.507360	0.576868	-0.105590
	H	-0.424536	-1.473022	0.055531		H	3.400253	0.523510	0.242356
1,5-pentanediol, $C_5H_{12}O_2$									
 symmetry C_1 r(OH···OH) = 1.966 Å	C	1.724688	0.375058	0.552957	 symmetry C_1 ϕ_1(C-C-C-C) = -179.9° ϕ_2(C-C-C-C) = -178.0°	C	2.498500	0.017937	0.527290
	H	2.771845	0.469583	0.844635		H	2.335872	-0.611027	1.411327
	H	1.125651	0.522508	1.458561		H	3.339224	0.676572	0.744767
	C	1.484022	-1.019891	-0.023286		C	1.250021	0.840678	0.239123
	H	2.219210	-1.201768	-0.810774		H	1.447126	1.489878	-0.618707
	H	1.673622	-1.756764	0.764687		H	1.069251	1.495739	1.097595
	C	0.083088	-1.224782	-0.606352		C	0.005561	-0.003699	-0.022240
	H	0.034456	-2.218324	-1.054362		H	-0.171812	-0.672348	0.823179
	H	-0.048552	-0.518666	-1.428055		H	0.168008	-0.639367	-0.899361
	C	-2.068482	0.018609	0.019781		C	-2.491235	0.015860	-0.520045
	H	-2.475361	-0.185820	-0.976490		H	-3.332111	0.677888	-0.754739
	H	-2.898983	0.038676	0.732108		H	-2.330357	-0.642434	-1.383043
	C	-1.071024	-1.056525	0.404778		C	-1.244610	0.839431	-0.261381
	H	-0.683124	-0.820086	1.397820		H	-1.086402	1.499793	-1.118983
	H	-1.623591	-1.992132	0.510814		H	-1.426056	1.483376	0.603503
	O	1.462999	1.411658	-0.379340		O	2.919918	-0.778273	-0.578304
	H	0.503704	1.527670	-0.405265		H	2.265151	-1.464056	-0.730158
	O	-1.400739	1.289514	0.022853		O	-2.774295	-0.754508	0.648409
	H	-2.010711	1.970926	-0.269054		H	-3.552302	-1.293008	0.487301
1,6-hexanediol, $C_6H_{14}O_2$									
 symmetry C_1 r(OH···OH) = 2.027 Å	C	2.133332	0.501444	-0.445667	 symmetry C_1 ϕ_1(C-C-C-C) = -179.4° ϕ_2(C-C-C-C) = -179.7° ϕ_3(C-C-C-C) = -178.8°	C	-3.085256	0.310602	-0.256878
	H	1.782683	0.465391	-1.482367		H	-3.072599	0.439849	-1.346415
	H	3.192630	0.759524	-0.479927		H	-3.226684	1.298656	0.183470
	C	1.965456	-0.867808	0.222204		C	-1.767623	-0.288281	0.211711
	H	2.572071	-0.893823	1.130412		H	-1.806523	-0.415009	1.296664
	H	2.370225	-1.630095	-0.451716		H	-1.656294	-1.290793	-0.216726
	C	0.516315	-1.189374	0.594141		C	-0.560282	0.562628	-0.174610
	H	0.475220	-2.151072	1.111033		H	-0.541930	0.697989	-1.260872
	H	0.200376	-0.444800	1.325275		H	-0.672017	1.564128	0.254113
	C	-0.450677	-1.200329	-0.594367		C	0.767688	-0.038067	0.277602
	H	-0.150718	-0.450960	-1.325865		H	0.752435	-0.173624	1.364183
	H	-0.389000	-2.161184	-1.110395		H	0.886867	-1.033178	-0.154975
	C	-1.911545	-0.926147	-0.226283		C	1.971369	0.819338	-0.104277
	H	-2.294778	-1.705702	0.438716		H	1.883107	1.808352	0.355313
	H	-2.517485	-0.959070	-1.134412		H	1.986910	0.975408	-1.186578

	C	-2.132122	0.412634	0.463308		C	3.300237	0.219849	0.313600
	H	-1.747192	0.390670	1.486502		H	3.302312	0.036349	1.395302
	H	-3.202787	0.628341	0.513694		H	4.111941	0.921171	0.090047
	O	1.483997	1.552477	0.255890		O	-4.221813	-0.448090	0.145464
	H	0.537827	1.516460	0.056666		H	-4.148515	-1.329989	-0.229368
	O	-1.459330	1.441897	-0.280647		O	3.488603	-1.002806	-0.399685
	H	-1.750958	2.298806	0.040432		H	4.309880	-1.408553	-0.113269
1,7-heptanediol, $C_7H_{16}O_2$									
 symmetry C_1 r(OH···OH) = 1.964 Å	C	-2.388793	0.525165	0.437373	 symmetry C_1 ϕ_1(C-C-C-C) = -178.4° ϕ_2(C-C-C-C) = -179.8° ϕ_3(C-C-C-C) = 180.0° ϕ_4(C-C-C-C) = 179.0°	C	-3.801103	-0.075054	0.474125
	H	-3.445972	0.746779	0.590308		H	-3.711454	-0.718729	1.358345
	H	-1.904378	0.584581	1.418601		H	-4.654761	0.583154	0.634997
	C	-2.243331	-0.881693	-0.143015		C	-2.531621	0.747514	0.299182
	H	-2.879658	-0.956459	-1.027980		H	-2.421758	1.395005	1.175204
	H	-2.630080	-1.598635	0.589273		H	-2.655230	1.404260	-0.566249
	C	-0.808907	-1.244260	-0.531386		C	-1.268995	-0.094365	0.132208
	H	-0.466333	-0.518466	-1.270614		H	-1.166277	-0.769427	0.988805
	H	-0.806117	-2.212205	-1.040324		H	-1.363936	-0.730374	-0.754181
	C	0.168667	-1.295992	0.642605		C	0.001194	0.741124	-0.003984
	H	-0.094294	-2.139556	1.287506		H	0.108825	1.377742	0.880120
	H	0.064299	-0.400159	1.254100		H	-0.105428	1.421014	-0.855692
	C	1.632892	-1.438664	0.218413		C	1.262679	-0.099456	-0.176087
	H	1.746187	-2.350480	-0.375611		H	1.156973	-0.734401	-1.062462
	H	2.249356	-1.581086	1.111227		H	1.373685	-0.774792	0.674451
	C	2.214533	-0.270118	-0.586743		C	2.528271	0.743058	-0.312059
	H	1.675163	-0.134497	-1.526237		H	2.636867	1.391872	0.561528
	H	3.241714	-0.523219	-0.862005		H	2.444821	1.399556	-1.183380
	C	2.263718	1.067664	0.131235		C	3.793296	-0.080322	-0.459056
	H	2.954673	1.737780	-0.388851		H	4.648993	0.580377	-0.637871
	H	2.628567	0.932396	1.155783		H	3.701717	-0.753080	-1.320962
	O	-1.888462	1.538049	-0.422650		O	-4.136242	-0.851749	-0.673737
	H	-0.923128	1.512330	-0.390789		H	-3.464389	-1.526974	-0.795334
	O	0.957303	1.663738	0.155950		O	3.986416	-0.830798	0.740413
	H	1.006511	2.514057	0.599715		H	4.767636	-1.379825	0.643295
1,8-octanediol, $C_8H_{18}O_2$									
	C	2.430668	-1.278973	0.163750		C	-4.459067	-0.393154	-0.289675
	H	2.732456	-1.932897	0.987359		H	-4.462645	-0.386314	-1.387062
	H	3.274140	-1.187021	-0.529201		H	-5.229917	-1.092057	0.034590
	C	2.020819	0.081423	0.691359		C	-3.097069	-0.841471	0.222862
	H	2.803670	0.453021	1.357007		H	-3.125520	-0.871780	1.315451
	H	1.135926	-0.066863	1.312255		H	-2.925467	-1.867607	-0.118136
	C	1.739102	1.098773	-0.420281		C	-1.941683	0.043432	-0.238782



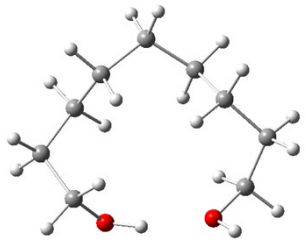
symmetry C_1
r(OH···OH) = 1.974 Å

H	2.685811	1.524465	-0.762371
H	1.317478	0.573967	-1.277087
C	0.795412	2.234585	-0.009908
H	0.708772	2.934054	-0.846284
H	1.242280	2.798975	0.814216
C	-0.605865	1.772643	0.406194
H	-0.527063	1.142493	1.294167
H	-1.187563	2.643231	0.720993
C	-1.377735	1.026832	-0.685336
H	-0.728049	0.310519	-1.190048
H	-1.686182	1.740797	-1.453523
C	-2.599883	0.267966	-0.165139
H	-3.220633	-0.045525	-1.007517
H	-3.215938	0.926657	0.456748
C	-2.251778	-0.980689	0.645074
H	-3.172652	-1.439192	1.009826
H	-1.659301	-0.714975	1.528283
O	1.300344	-1.840144	-0.518843
H	1.533140	-2.697180	-0.883579
O	-1.587643	-1.974803	-0.120147
H	-0.642335	-1.780310	-0.173601

symmetry C_1
ϕ_1(C-C-C-C) = -178.4°
ϕ_2(C-C-C-C) = -179.6°
ϕ_3(C-C-C-C) = -179.7°
ϕ_4(C-C-C-C) = -179.8°
ϕ_5(C-C-C-C) = -178.8°

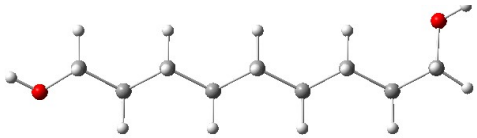
H	-1.937011	0.092138	-1.333319
H	-2.096213	1.067762	0.116405
C	-0.578445	-0.439254	0.249719
H	-0.409801	-1.461193	-0.104384
H	-0.587481	-0.495297	1.342907
C	0.578675	0.447358	-0.201315
H	0.410579	1.469461	0.155018
H	0.584304	0.505257	-1.294726
C	1.940129	-0.042936	0.282487
H	2.114627	-1.058071	-0.079119
H	1.936338	-0.101714	1.376249
C	3.092498	0.851544	-0.166936
H	2.949642	1.864062	0.222513
H	3.095892	0.931590	-1.257618
C	4.454788	0.359378	0.282362
H	4.470034	0.250801	1.374057
H	5.224298	1.089142	0.006425
O	-4.865821	0.876321	0.216280
H	-4.275942	1.549623	-0.131277
O	4.712087	-0.896410	-0.346937
H	5.555196	-1.234471	-0.037049

1,9-nonanediol, $C_9H_{20}O_2$



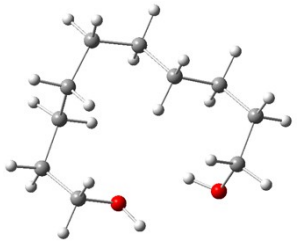
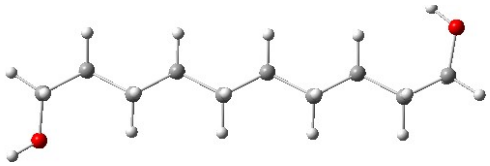
symmetry C_1
r(OH···OH) = 1.888 Å

C	-2.232752	-1.324950	0.589958
H	-3.013397	-1.970399	1.002682
H	-1.575066	-1.040174	1.409374
C	-2.851356	-0.100713	-0.072293
H	-3.515857	0.378968	0.653436
H	-3.492487	-0.437828	-0.893750
C	-1.824112	0.905364	-0.595456
H	-2.319320	1.612900	-1.265463
H	-1.098286	0.365303	-1.204412
C	-1.109457	1.685636	0.509187
H	-1.831354	2.348796	0.994243
H	-0.767453	0.998811	1.285389
C	0.081208	2.513364	0.012923
H	0.431996	3.154179	0.827081
H	-0.260388	3.186200	-0.779502
C	1.256476	1.677821	-0.505650
H	1.983942	2.340388	-0.982513
H	0.902172	1.014560	-1.297117
C	1.964739	0.859546	0.576844
H	2.549810	1.535983	1.205412



symmetry C_1
ϕ_1(C-C-C-C) = -179.9°
ϕ_2(C-C-C-C) = -180.0°
ϕ_3(C-C-C-C) = -179.9°
ϕ_4(C-C-C-C) = 179.8°
ϕ_5(C-C-C-C) = 179.9°
ϕ_6(C-C-C-C) = 179.0°

C	-4.965516	0.556888	0.149818
H	-4.983220	0.789571	1.221744
H	-4.909625	1.507281	-0.395168
C	-3.752741	-0.292746	-0.172204
H	-3.766634	-0.530211	-1.239007
H	-3.841101	-1.242823	0.360965
C	-2.438828	0.391968	0.193871
H	-2.364238	1.347833	-0.334924
H	-2.437673	0.634851	1.261569
C	-1.210523	-0.454994	-0.128183
H	-1.283737	-1.411572	0.399196
H	-1.209698	-0.697630	-1.195643
C	0.106950	0.223255	0.236103
H	0.179590	1.180145	-0.290908
H	0.105565	0.465783	1.303985
C	1.335856	-0.621979	-0.086784
H	1.336516	-0.863830	-1.154637
H	1.263861	-1.579734	0.439826
C	2.651971	0.060123	0.274581
H	2.730154	1.011644	-0.254846

	H	1.235738	0.385637	1.234763		H	2.653876	0.301111	1.343194
	C	2.867800	-0.244454	0.024832		C	3.876261	-0.792433	-0.048375
	H	3.531520	0.155023	-0.749046		H	3.827611	-1.735341	0.504705
	H	3.508078	-0.626767	0.823364		H	3.877790	-1.051095	-1.110954
	C	2.093117	-1.423019	-0.554413		C	5.192887	-0.116990	0.283394
	H	1.436786	-1.088223	-1.363633		H	5.207287	0.170665	1.342157
	H	2.797588	-2.141573	-0.988487		H	6.022167	-0.812810	0.112881
	O	-1.400056	-2.077883	-0.301781		O	-6.135610	-0.168083	-0.225148
	H	-1.932327	-2.429232	-1.020131		H	-6.909384	0.364493	-0.026990
	O	1.332264	-2.059254	0.464027		O	5.332761	1.035892	-0.547797
	H	0.430549	-2.198131	0.146313		H	6.145788	1.490655	-0.316907
1,10-decanediol, $C_{10}H_{22}O_2$									
 symmetry C_1 r(OH···OH) = 2.507 Å	C	2.193476	1.162714	-0.520315	 symmetry C_1 ϕ_1(C-C-C-C) = 178.9° ϕ_2(C-C-C-C) = 179.8° ϕ_3(C-C-C-C) = 179.8° ϕ_4(C-C-C-C) = 179.9° ϕ_5(C-C-C-C) = 179.9° ϕ_6(C-C-C-C) = 179.6° ϕ_7(C-C-C-C) = 178.4°	C	-3.205265	-0.012790	0.281631
	H	2.658688	2.118258	-0.776730		H	-3.203369	-0.121273	1.371650
	H	1.918876	0.701474	-1.473509		H	-3.328611	-1.017679	-0.126703
	C	0.924640	1.413366	0.290655		C	-1.867200	0.564485	-0.170479
	H	0.458104	0.455266	0.523728		H	-1.871179	0.672861	-1.260040
	H	1.181118	1.867185	1.254097		H	-1.750439	1.575965	0.233414
	C	-0.086430	2.293448	-0.440609		C	-0.669528	-0.284731	0.245792
	H	0.341023	3.288548	-0.591329		H	-0.787113	-1.295649	-0.157571
	H	-0.246720	1.885782	-1.441963		H	-0.664284	-0.392961	1.335382
	C	-1.434236	2.434452	0.276879		C	0.670011	0.287369	-0.209516
	H	-1.291958	3.004781	1.199404		H	0.786548	1.299053	0.193121
	H	-2.104094	3.030614	-0.349534		H	0.665316	0.394390	-1.299264
	C	-2.116007	1.105981	0.624636		C	1.867151	-0.561597	0.208461
	H	-1.512667	0.582311	1.368572		H	1.873675	-0.667465	1.297948
	H	-3.071791	1.314587	1.113911		H	1.751553	-1.573463	-0.193164
	C	-2.358480	0.194740	-0.578374		C	3.207342	0.009303	-0.247768
	H	-1.443281	0.087133	-1.160012		H	3.309478	1.022116	0.155954
	H	-3.086588	0.668370	-1.242345		H	3.205254	0.109237	-1.338835
	C	3.229412	0.280668	0.181083		C	-4.397943	0.844433	-0.133982
	H	4.084388	0.135864	-0.483333		H	-4.401984	0.972087	-1.220119
	H	3.604860	0.790314	1.074772		H	-4.304673	1.844606	0.299929
	C	2.710319	-1.088986	0.611153		C	-5.736590	0.269309	0.286816
	H	1.959136	-0.980766	1.401361		H	-6.539131	0.973273	0.039276
	H	3.530524	-1.675026	1.026704		H	-5.749599	0.112505	1.372682
	C	-2.853603	-1.206219	-0.212187		C	4.402858	-0.838585	0.179874
	H	-3.165719	-1.729234	-1.118892		H	4.284136	-1.854583	-0.210475
	H	-3.733617	-1.139226	0.434596		H	4.427442	-0.919383	1.269979
	C	-1.818007	-2.066074	0.493139		C	5.743399	-0.299650	-0.301065
	H	-1.521935	-1.615546	1.446250		H	6.546433	-0.974291	-0.004725
	H	-2.246904	-3.049261	0.709373		H	5.751927	-0.240392	-1.396857

	O	2.185905	-1.861034	-0.464547		O	-5.932819	-0.968644	-0.397614
	H	1.329082	-1.499001	-0.717736		H	-6.759866	-1.358971	-0.106466
	O	-0.675931	-2.206688	-0.357763		O	6.084098	0.962751	0.267347
	H	-0.066820	-2.845183	0.024733		H	5.462847	1.621877	-0.051569

[a] F conformers for 1,2-ethanediol and 1,3-propanediol and F-lin for all other conformers.

Table S4

Cartesian coordinates of all conformers of 1,4-butanediols calculated at B3LYP-D3(BJ)/def2-TZVPP level (in Å)

Atom	x	y	z	Atom	x	y	z	Atom	x	y	z	Atom	x	y	z
	1				**2**				**3**				**4**		
C	1.604448	0.160821	0.313547	C	1.440909	-0.095732	0.540295	C	-1.593227	0.094862	-0.346760	C	-1.840103	0.633968	-0.199261
H	2.635507	0.464564	0.112018	H	0.927587	-0.541667	1.398954	H	-2.645685	0.352384	-0.197944	H	-1.848042	0.769399	-1.281873
H	1.477690	0.070962	1.397393	H	2.464899	0.116948	0.850863	H	-1.428316	-0.022635	-1.417605	H	-2.352899	1.495463	0.242580
C	0.652761	1.206225	-0.242534	C	0.753432	1.210337	0.140957	C	-0.704589	1.197959	0.214350	C	-0.408092	0.560315	0.309362
H	1.063570	2.179622	0.038267	H	1.404718	1.757661	-0.544252	H	-1.139554	2.149058	-0.106903	H	-0.420882	0.403487	1.394921
H	0.692529	1.159309	-1.334765	H	0.652447	1.827522	1.040003	H	-0.781246	1.190105	1.308290	H	0.074106	1.526181	0.145782
C	-0.804232	1.146847	0.233972	C	-0.617063	1.051406	-0.528549	C	0.770750	1.175787	-0.201272	C	0.410071	-0.541680	-0.358373
H	-1.292390	2.074896	-0.078576	H	-0.496273	0.620824	-1.524791	H	1.230079	2.103591	0.152735	H	0.453808	-0.361589	-1.436158
H	-0.835080	1.131003	1.327436	H	-1.051754	2.042971	-0.673507	H	0.845409	1.186936	-1.292414	H	-0.087628	-1.503384	-0.219480
C	-1.649268	-0.012930	-0.289407	C	-1.624831	0.200974	0.225170	C	1.614668	0.014183	0.322583	C	1.824953	-0.646613	0.173721
H	-1.568206	-0.059463	-1.384210	H	-2.632484	0.390205	-0.156946	H	1.471154	-0.082760	1.408741	H	2.339559	-1.488507	-0.302369
H	-2.696738	0.177840	-0.051741	H	-1.614409	0.446251	1.293163	H	2.668574	0.244166	0.160838	H	1.803731	-0.833584	1.254922
O	1.358685	-1.106509	-0.318556	O	1.525193	-1.032188	-0.521417	O	-1.340856	-1.201791	0.214605	O	-2.584441	-0.561667	0.033571
H	1.978257	-1.755081	0.025409	H	0.643152	-1.412075	-0.615774	H	-1.554202	-1.180663	1.151864	H	-2.666328	-0.688527	0.982772
O	-1.340291	-1.265542	0.293527	O	-1.293652	-1.182932	0.032464	O	1.383498	-1.218112	-0.332788	O	2.507360	0.576868	-0.105590
H	-0.424536	-1.473022	0.055531	H	-1.864889	-1.729585	0.576669	H	0.467026	-1.477707	-0.155537	H	3.400253	0.523510	0.242356
	5				**6**				**7**				**8**		
C	1.829134	0.639076	-0.185637	C	-2.038372	0.362939	0.310377	C	1.934851	-0.375558	0.313206	C	1.840121	0.620396	0.215977
H	1.825166	0.784480	-1.273042	H	-2.036127	0.263204	1.402672	H	2.211626	-1.245881	-0.284552	H	1.863930	0.697634	1.309777
H	2.338671	1.497454	0.266156	H	-2.798507	1.104687	0.041221	H	2.522363	-0.412778	1.237846	H	2.345308	1.501471	-0.195149
C	0.405462	0.558164	0.326768	C	-0.675642	0.827281	-0.167137	C	0.448861	-0.407042	0.641627	C	0.401634	0.580037	-0.263956
H	-0.083914	1.517280	0.149924	H	-0.701055	0.907658	-1.257397	H	0.187542	0.482242	1.221522	H	-0.054926	1.544667	-0.023900
H	0.432688	0.408131	1.410106	H	-0.503651	1.835742	0.220269	H	0.257205	-1.266083	1.293392	H	0.403829	0.484881	-1.354308
C	-0.405463	-0.558161	-0.326776	C	0.462798	-0.095314	0.262372	C	-0.442884	-0.485186	-0.594751	C	-0.411210	-0.554717	0.355131
H	0.083915	-1.517276	-0.149935	H	0.256397	-1.107340	-0.094851	H	-0.251076	-1.420717	-1.128630	H	-0.454794	-0.424490	1.440213
H	-0.432692	-0.408126	-1.410113	H	0.511268	-0.146314	1.353488	H	-0.191026	0.325822	-1.279760	H	0.095872	-1.502778	0.164522
C	-1.829133	-0.639077	0.185634	C	1.812861	0.363553	-0.266798	C	-1.922925	-0.413753	-0.273020	C	-1.830815	-0.648000	-0.184898
H	-1.825160	-0.784492	1.273037	H	2.046549	1.362920	0.104012	H	-2.195427	-1.214319	0.426346	H	-2.348903	-1.490117	0.273450
H	-2.338670	-1.497453	-0.266164	H	1.785278	0.422145	-1.362180	H	-2.508726	-0.553423	-1.188211	H	-1.809756	-0.825725	-1.267108
O	2.504428	-0.574085	0.151846	O	-2.327311	-0.892165	-0.305205	O	2.312974	0.752251	-0.472492	O	2.491697	-0.573709	-0.215875
H	3.394835	-0.545749	-0.205112	H	-3.169784	-1.214978	0.022240	H	2.067462	1.550595	0.003756	H	3.387317	-0.584380	0.129087
O	-2.504428	0.574085	-0.151835	O	2.891088	-0.460471	0.164960	O	-2.197654	0.864144	0.303670	O	-2.630480	0.495485	0.115268
H	-3.394834	0.545746	0.205126	H	2.729542	-1.357391	-0.140403	H	-3.129923	0.912620	0.526497	H	-2.315986	1.238339	-0.405255
	9				**10**				**11**				**12**		
C	-1.805146	0.348310	-0.269741	C	1.421543	0.153223	-0.706732	C	1.877429	-0.515336	0.009282	C	2.048232	0.354454	0.321253
H	-2.021172	1.359087	0.099452	H	0.857040	-0.482037	-1.397141	H	1.855689	-1.139135	0.911189	H	2.047453	0.236867	1.411994
H	-1.783055	0.393255	-1.365484	H	2.095361	0.775971	-1.305141	H	1.868690	-1.188216	-0.849010	H	2.806005	1.097330	0.073060
C	-0.460613	-0.117257	0.251049	C	0.477755	1.044122	0.079511	C	0.655648	0.391970	-0.026175	C	0.680041	0.830023	-0.151003

H	-0.259863	-1.119736	-0.126995	H	1.070249	1.732956	0.685642	H	0.698610	1.081328	0.824609	H	0.714704	0.969647	-1.234769
H	-0.514787	-0.191527	1.340579	H	-0.085038	1.646396	-0.636314	H	0.704950	1.005298	-0.929417	H	0.491295	1.813495	0.291578
C	0.672817	0.823448	-0.149301	C	-0.489125	0.283664	0.990510	C	-0.652941	-0.392929	0.013718	C	-0.453321	-0.124004	0.216887
H	0.493519	1.822191	0.259861	H	-1.101399	1.006893	1.539366	H	-0.700398	-1.004810	0.918092	H	-0.478268	-0.278249	1.299361
H	0.707138	0.929192	-1.237256	H	0.076658	-0.275454	1.738284	H	-0.703734	-1.081178	-0.833649	H	-0.292562	-1.102479	-0.242948
C	2.035632	0.357198	0.326635	C	-1.404858	-0.691379	0.263259	C	-1.872072	0.507183	-0.023053	C	-1.810137	0.382002	-0.230738
H	2.020017	0.213478	1.413904	H	-2.061010	-1.190468	0.984810	H	-1.861389	1.110221	-0.938997	H	-1.810899	0.529897	-1.317332
H	2.788896	1.119801	0.098625	H	-0.822170	-1.468660	-0.230006	H	-1.850996	1.197216	0.829506	H	-2.018417	1.351786	0.237562
O	-2.801304	-0.569700	0.175380	O	2.165240	-0.646922	0.214785	O	3.105816	0.198018	-0.081079	O	2.477715	-0.847989	-0.310029
H	-3.654422	-0.295370	-0.168492	H	2.745279	-1.231574	-0.278013	H	3.186358	0.770747	0.686237	H	1.916340	-1.570091	-0.017185
O	2.350402	-0.866563	-0.335530	O	-2.173360	-0.082714	-0.774665	O	-3.034701	-0.315420	0.024817	O	-2.791381	-0.580245	0.147764
H	3.174801	-1.210456	0.015145	H	-2.741903	0.585284	-0.381735	H	-3.815085	0.242418	-0.011095	H	-3.655210	-0.277187	-0.141595
		13				**14**				**15**				**16**	
C	2.043269	0.353064	-0.323553	C	1.922938	0.388111	0.334210	C	-1.818840	0.392268	-0.225275	C	-2.043454	0.352298	-0.330890
H	2.037480	0.254645	-1.409989	H	2.493431	0.430104	1.268903	H	-2.028681	1.353229	0.246300	H	-2.802901	1.104979	-0.090859
H	2.810753	1.090561	-0.064405	H	2.158801	1.289639	-0.244905	H	-1.823528	0.554730	-1.309903	H	-2.034101	0.230727	-1.415014
C	0.679749	0.823354	0.166788	C	0.437080	0.349934	0.639640	C	-0.455145	-0.118917	0.218102	C	-0.677268	0.819437	0.154762
H	0.699866	0.891656	1.260713	H	0.203613	1.188389	1.303647	H	-0.472341	-0.264943	1.301913	H	-0.703276	0.915818	1.246695
H	0.515336	1.842131	-0.198330	H	0.236058	-0.568739	1.198429	H	-0.287949	-1.101819	-0.235920	H	-0.503466	1.827912	-0.234648
C	-0.467241	-0.080393	-0.277736	C	-0.442913	0.417162	-0.606812	C	0.679535	0.826521	-0.169783	C	0.461984	-0.106954	-0.259966
H	-0.253790	-1.107506	0.030849	H	-0.211081	-0.420645	-1.265093	H	0.489607	1.817755	0.254451	H	0.517868	-0.159339	-1.350311
H	-0.533051	-0.086675	-1.368774	H	-0.211652	1.334096	-1.159365	H	0.709505	0.946345	-1.255968	H	0.264124	-1.119597	0.093209
C	-1.809281	0.352545	0.292479	C	-1.934091	0.413944	-0.298110	C	2.050424	0.363675	0.307215	C	1.804100	0.350546	0.274636
H	-2.046202	1.369423	-0.024487	H	-2.504447	0.541762	-1.217915	H	2.059303	0.282406	1.400853	H	1.774420	0.387830	1.370995
H	-1.766124	0.357142	1.389334	H	-2.183896	1.255179	0.361934	H	2.807332	1.096300	0.027836	H	2.025481	1.363474	-0.084834
O	2.402420	-0.935786	0.168449	O	2.260558	-0.784208	-0.404507	O	-2.889551	-0.461462	0.162496	O	-2.421143	-0.920626	0.185489
H	2.520062	-0.878552	1.120613	H	3.192181	-0.753572	-0.633460	H	-2.790112	-1.304674	-0.287593	H	-2.497263	-0.853961	1.141320
O	-2.894759	-0.447087	-0.163797	O	-2.398059	-0.811427	0.262309	O	2.471240	-0.861221	-0.287433	O	2.800054	-0.567425	-0.169275
H	-2.724600	-1.361272	0.079395	H	-1.971088	-0.946033	1.111845	H	1.947512	-1.579155	0.075977	H	3.655642	-0.285397	0.162475
		17				**18**				**19**				**20**	
C	1.849810	0.616809	-0.224791	C	2.042387	0.349773	0.337374	C	-1.405801	-0.335849	-0.643887	C	-2.047048	0.350201	0.332315
H	1.876838	0.699546	-1.312196	H	2.031762	0.224285	1.421193	H	-0.821957	-1.251197	-0.789681	H	-2.803357	1.098970	0.097998
H	2.361875	1.494556	0.184515	H	2.803536	1.101924	0.101590	H	-2.085726	-0.237953	-1.497168	H	-2.040330	0.219824	1.421855
C	0.405534	0.579800	0.259265	C	0.677613	0.821053	-0.148065	C	-0.487239	0.870094	-0.590499	C	-0.680088	0.826260	-0.142840
H	-0.045871	1.551766	0.035574	H	0.707160	0.936786	-1.237699	H	-1.099547	1.773293	-0.542193	H	-0.486202	1.806288	0.305012
H	0.398500	0.476393	1.351583	H	0.497214	1.821689	0.258145	H	0.072334	0.907974	-1.526383	H	-0.718756	0.973526	-1.225314
C	-0.415206	-0.541778	-0.371907	C	-0.463461	-0.116285	0.238814	C	0.487239	0.870094	0.590498	C	0.457351	-0.130485	0.208310
H	0.096089	-1.493615	-0.210522	H	-0.501016	-0.205117	1.330641	H	-0.072334	0.907974	1.526382	H	0.295293	-1.106389	-0.256477
H	-0.469474	-0.389097	-1.453216	H	-0.270946	-1.116812	-0.149853	H	1.099547	1.773293	0.542192	H	0.478266	-0.290943	1.292799
C	-1.828835	-0.650356	0.180844	C	-1.812737	0.366763	-0.271461	C	1.405801	-0.335848	0.643887	C	1.816017	0.384248	-0.246270
H	-1.796304	-0.847337	1.259922	H	-1.795798	0.446151	-1.359605	H	0.821957	-1.251197	0.789681	H	2.019849	1.359866	0.211975
H	-2.348192	-1.486455	-0.286799	H	-2.029440	1.368020	0.122672	H	2.085726	-0.237952	1.497168	H	1.817269	0.528364	-1.327333
O	2.574423	-0.571908	0.080001	O	2.418053	-0.922161	-0.182772	O	-2.143674	-0.404366	0.578697	O	-2.486047	-0.842105	-0.310688

H	2.659184	-0.643762	1.034688	H	2.506229	-0.850465	-1.137253	H	-2.731015	-1.162659	0.545794	H	-1.918118	-1.568486	-0.042200
O	-2.636107	0.493893	-0.090855	O	-2.877994	-0.529823	0.024332	O	2.143674	-0.404366	-0.578697	O	2.876428	-0.527761	0.016378
H	-2.306986	1.235280	0.422810	H	-2.931988	-0.638407	0.977721	H	2.731015	-1.162659	-0.545793	H	2.955644	-0.643436	0.967081
		21				**22**				**23**				**24**	
C	-1.835934	0.642971	0.186110	C	1.649015	0.078307	0.234214	C	1.936220	-0.396827	0.253787	C	-1.576704	0.245299	0.294414
H	-1.826103	0.820547	1.262833	H	1.666266	0.364205	1.294129	H	2.211371	-1.193362	-0.439589	H	-2.604573	0.495557	0.020937
H	-2.351866	1.489384	-0.280437	H	2.666857	0.198327	-0.146196	H	2.548415	-0.520063	1.153963	H	-1.462535	0.455236	1.358889
C	-0.412557	0.542861	-0.342166	C	0.711036	1.001214	-0.535903	C	0.458882	-0.488501	0.609597	C	-0.591871	1.067699	-0.530104
H	-0.441907	0.353425	-1.421707	H	0.570681	0.590893	-1.538443	H	0.192772	0.345924	1.264799	H	-1.009097	2.068840	-0.667316
H	0.077922	1.511236	-0.219136	H	1.206191	1.966329	-0.667107	H	0.297046	-1.399901	1.194215	H	-0.527862	0.625292	-1.527412
C	0.412557	-0.542862	0.342166	C	-0.654209	1.254484	0.120128	C	-0.458882	-0.488501	-0.609597	C	0.813902	1.201842	0.069683
H	-0.077922	-1.511236	0.219136	H	-1.278772	1.820212	-0.574649	H	-0.297046	-1.399901	-1.194215	H	0.776127	1.870612	0.936015
H	0.441906	-0.353425	1.421707	H	-0.522419	1.880247	1.007145	H	-0.192772	0.345924	-1.264799	H	1.460191	1.681260	-0.668867
C	1.835934	-0.642971	-0.186110	C	-1.405784	0.009448	0.559490	C	-1.936220	-0.396827	-0.253787	C	1.456824	-0.109750	0.519583
H	1.826103	-0.820547	-1.262833	H	-2.415970	0.280348	0.878783	H	-2.211371	-1.193362	0.439589	H	0.958596	-0.482491	1.421020
H	2.351866	-1.489384	0.280437	H	-0.895529	-0.465603	1.402242	H	-2.548415	-0.520063	-1.153963	H	2.500364	0.070898	0.780996
O	-2.588276	-0.556927	0.012649	O	1.312886	-1.301423	0.130147	O	2.274426	0.816277	-0.416880	O	-1.378097	-1.173707	0.153586
H	-2.690834	-0.718849	-0.929220	H	0.449991	-1.378808	-0.296702	H	2.117126	1.549156	0.184849	H	-1.865886	-1.471342	-0.618169
O	2.588276	0.556927	-0.012649	O	-1.466669	-0.906357	-0.545782	O	-2.274426	0.816277	0.416880	O	1.453283	-1.109810	-0.487729
H	2.690835	0.718848	0.929220	H	-2.017381	-1.654626	-0.301698	H	-2.117124	1.549156	-0.184849	H	0.560279	-1.476261	-0.484406
		25				**26**				**27**				**28**	
C	1.920276	0.399673	0.329785	C	1.728371	0.057805	0.547534	C	1.932452	-0.434610	-0.269717	C	1.429103	-0.079056	0.487880
H	2.166503	1.279102	-0.279439	H	2.662241	0.545985	0.847056	H	2.498046	-0.619856	-1.182648	H	1.620586	0.677335	1.260777
H	2.484661	0.472330	1.266378	H	1.267238	-0.356371	1.450798	H	2.203284	-1.218924	0.448199	H	0.956736	-0.930293	0.977151
C	0.433725	0.377697	0.628217	C	0.810678	1.081725	-0.099906	C	0.439714	-0.484661	-0.566462	C	0.520817	0.496440	-0.589963
H	0.203993	-0.501357	1.231333	H	1.343415	1.538675	-0.936413	H	0.213868	-1.453679	-1.023548	H	1.062159	1.293172	-1.110915
H	0.197564	1.254904	1.239138	H	0.626046	1.877558	0.627837	H	0.197053	0.277806	-1.307750	H	0.307292	-0.278622	-1.326157
C	-0.433725	0.377697	-0.628217	C	-0.519530	0.517296	-0.604936	C	-0.438023	-0.296692	0.667809	C	-0.789872	1.071955	-0.048066
H	-0.203993	-0.501358	-1.231333	H	-0.316946	-0.269687	-1.335489	H	-0.216573	0.666111	1.142778	H	-1.321360	1.577413	-0.856958
H	-0.197564	1.254904	-1.239138	H	-1.069906	1.303948	-1.125040	H	-0.209516	-1.068900	1.410766	H	-0.580787	1.829586	0.713215
C	-1.920276	0.399673	-0.329785	C	-1.414219	-0.038828	0.493720	C	-1.930994	-0.352018	0.367336	C	-1.725113	0.039678	0.559228
H	-2.484661	0.472330	-1.266378	H	-1.624541	0.732219	1.237159	H	-2.503142	-0.293401	1.300236	H	-2.625024	0.540859	0.933020
H	-2.166503	1.279102	0.279439	H	-0.920654	-0.867658	1.012522	H	-2.181210	-1.300412	-0.110631	H	-1.247901	-0.459510	1.409760
O	2.263063	-0.798316	-0.366802	O	1.985960	-0.979128	-0.398914	O	2.375127	0.839035	0.196439	O	2.653991	-0.584714	-0.032936
H	3.200487	-0.782672	-0.572054	H	2.570311	-1.627975	-0.000545	H	2.049271	0.973326	1.089326	H	3.094496	0.120014	-0.515740
O	-2.263063	-0.798316	0.366802	O	-2.688086	-0.452021	0.006324	O	-2.359587	0.652275	-0.546867	O	-2.062411	-0.908591	-0.451121
H	-3.200487	-0.782672	0.572054	H	-2.551996	-1.135500	-0.655636	H	-2.194288	1.515330	-0.157107	H	-2.608449	-1.597621	-0.066168
		29				**30**				**31**				**32**	
C	-1.877279	0.517986	0.035739	C	1.824990	0.212491	-0.070515	C	1.433949	-0.635191	-0.368925	C	-1.265657	-0.388499	0.228111
H	-1.863139	1.234375	-0.786548	H	2.178059	0.640207	0.876564	H	0.883474	-0.708390	-1.306072	H	-1.196309	-0.521258	1.314530
H	-1.860016	1.094416	0.968623	H	2.615015	0.354530	-0.816500	H	2.071976	-1.522926	-0.300425	H	-0.780938	-1.246792	-0.239937
C	-0.656197	-0.388007	-0.040456	C	0.570184	0.936379	-0.522720	C	0.476086	-0.598965	0.815199	C	-0.576184	0.903173	-0.173178

H	-0.704284	-0.958544	-0.971229	H	0.204989	0.484079	-1.446248	H	1.056943	-0.594988	1.743313	H	-1.177082	1.728944	0.214992
H	-0.700528	-1.116459	0.776642	H	0.867355	1.959016	-0.769411	H	-0.099803	-1.527270	0.812868	H	-0.596845	0.991521	-1.262942
C	0.656197	0.388006	0.040456	C	-0.564402	0.981238	0.505747	C	-0.476086	0.598967	0.815198	C	0.860105	1.052596	0.333255
H	0.704285	0.958544	0.971228	H	-1.242075	1.801215	0.256037	H	0.099803	1.527273	0.812864	H	0.896977	0.904187	1.416176
H	0.700529	1.116457	-0.776643	H	-0.158959	1.201027	1.498243	H	-1.056943	0.594993	1.743311	H	1.185511	2.079695	0.150206
C	1.877279	-0.517987	-0.035738	C	-1.392957	-0.289939	0.593238	C	-1.433949	0.635190	-0.368927	C	1.884525	0.136335	-0.311250
H	1.860015	-1.094419	-0.968620	H	-2.118081	-0.196338	1.410282	H	-0.883474	0.708386	-1.306073	H	2.892357	0.467908	-0.037623
H	1.863140	-1.234373	0.786551	H	-0.747319	-1.145033	0.795360	H	-2.071977	1.522925	-0.300429	H	1.797325	0.192330	-1.403352
O	-3.105632	-0.187007	-0.099881	O	1.549517	-1.181777	0.091653	O	2.227415	0.544833	-0.489510	O	-2.632787	-0.286082	-0.179558
H	-3.195429	-0.794514	0.639052	H	2.353957	-1.625145	0.370670	H	2.786504	0.619102	0.288756	H	-3.068985	-1.122996	-0.004912
O	3.105633	0.187006	0.099878	O	-2.079667	-0.460113	-0.650597	O	-2.227415	-0.544834	-0.489508	O	1.672069	-1.203508	0.138465
H	3.195412	0.794536	-0.639038	H	-2.338636	-1.379453	-0.737932	H	-2.786504	-0.619102	0.288758	H	2.316997	-1.778447	-0.280019
		33				**34**				**35**				**36**	
C	-1.723462	0.019909	0.560978	C	-1.872460	0.503402	0.000001	C	-1.451887	0.016486	0.485504	C	1.842666	0.630317	0.212940
H	-2.640979	0.496463	0.924049	H	-1.857096	1.150843	0.885173	H	-0.979905	-0.750110	1.108787	H	1.850737	0.745395	1.303519
H	-1.247846	-0.474055	1.416051	H	-1.857094	1.150847	-0.885168	H	-1.691029	0.861603	1.133429	H	2.353676	1.494685	-0.210639
C	-0.803069	1.079009	-0.022271	C	-0.652045	-0.395684	0.000000	C	-0.513300	0.460243	-0.628664	C	0.406337	0.575879	-0.293008
H	-0.606756	1.820605	0.758059	H	-0.701712	-1.046130	0.876954	H	-0.293906	-0.395172	-1.273295	H	-0.068056	1.529236	-0.038927
H	-1.340728	1.596913	-0.819093	H	-0.701712	-1.046128	-0.876955	H	-1.038171	1.196031	-1.241047	H	0.422207	0.500774	-1.384385
C	0.516474	0.543958	-0.581113	C	0.652045	0.395684	0.000001	C	0.802866	1.056632	-0.124936	C	-0.406337	-0.575879	0.293007
H	1.075622	1.367577	-1.029793	H	0.701712	1.046129	0.876956	H	0.600322	1.880099	0.567708	H	-0.422206	-0.500774	1.384384
H	0.316376	-0.176600	-1.374075	H	0.701712	1.046130	-0.876954	H	1.342055	1.498778	-0.968753	H	0.068056	-1.529236	0.038926
C	1.403052	-0.108108	0.462694	C	1.872460	-0.503401	0.000001	C	1.724522	0.061184	0.573590	C	-1.842666	-0.630317	-0.212940
H	0.928760	-1.013823	0.855276	H	1.857093	-1.150846	-0.885169	H	1.245175	-0.359018	1.457172	H	-2.353676	-1.494685	0.210639
H	1.559044	0.580213	1.303944	H	1.857096	-1.150843	0.885172	H	2.631942	0.573556	0.911627	H	-1.850738	-0.745394	-1.303519
O	-2.022211	-0.930567	-0.459745	O	-3.034120	-0.322014	-0.000003	O	-2.704571	-0.449552	-0.007445	O	2.621000	-0.497690	-0.176743
H	-2.595663	-1.609756	-0.097888	H	-3.814779	0.236542	0.000007	H	-2.548355	-1.230492	-0.545440	H	2.322885	-1.266582	0.314987
O	2.647299	-0.430398	-0.156500	O	3.034120	0.322013	-0.000003	O	2.056016	-1.061735	-0.239708	O	-2.621000	0.497690	0.176744
H	3.193489	-0.908429	0.471697	H	3.814779	-0.236542	0.000016	H	2.547109	-0.752251	-1.005927	H	-2.322884	1.266583	-0.314985
		37				**38**				**39**				**40**	
C	-1.434904	0.701635	-0.207554	C	1.723291	0.001569	0.574074	C	-1.292768	-0.365978	-0.297035	C	-1.431840	-0.593686	-0.424440
H	-0.882915	1.000583	-1.099487	H	2.643327	0.466982	0.945532	H	-1.293204	-0.376477	-1.387809	H	-2.092460	-1.460117	-0.435480
H	-2.069555	1.548837	0.075280	H	1.248634	-0.490843	1.422750	H	-0.786969	-1.273307	0.035991	H	-0.866110	-0.609378	-1.362361
C	-0.483696	0.367270	0.936063	C	0.808764	1.072893	-0.011749	C	-0.568182	0.878310	0.205657	C	-0.491848	-0.684386	0.770556
H	-1.073995	0.126375	1.825809	H	0.614741	1.815530	0.769090	H	-1.166423	1.744363	-0.086356	H	0.076806	-1.612452	0.686521
H	0.077677	1.270688	1.195627	H	1.349382	1.602251	-0.802830	H	-0.549564	0.869597	1.301652	H	-1.092529	-0.752807	1.680019
C	0.479414	-0.786974	0.647991	C	-0.511636	0.550370	-0.579066	C	0.859221	1.053523	-0.323080	C	0.482544	0.488973	0.909425
H	-0.095177	-1.683989	0.406025	H	-0.316460	-0.165390	-1.378576	H	1.179681	2.080892	-0.132362	H	1.079688	0.349985	1.812866
H	1.054681	-1.004241	1.550391	H	-1.068370	1.379064	-1.021255	H	0.874519	0.920808	-1.408537	H	-0.068832	1.423482	1.051271
C	1.454082	-0.529106	-0.494783	C	-1.400365	-0.111948	0.456710	C	1.905051	0.141503	0.291657	C	1.427276	0.667942	-0.266239
H	0.916615	-0.389349	-1.438283	H	-1.545036	0.562601	1.311029	H	1.870577	0.224539	1.385311	H	2.089230	1.519764	-0.075494
H	2.102107	-1.395902	-0.621511	H	-0.933450	-1.029457	0.828416	H	2.900942	0.459123	-0.036749	H	0.866190	0.886584	-1.183191
O	-2.229824	-0.406004	-0.620807	O	2.025605	-1.046399	-0.342228	O	-2.669327	-0.373529	0.084321	O	-2.298305	0.539982	-0.383159

H	-2.782378	-0.680330	0.116398	H	2.470130	-0.669067	-1.106475	H	-2.720920	-0.483421	1.037274	H	-1.772997	1.336593	-0.488748
O	2.333087	0.568815	-0.251643	O	-2.650112	-0.407261	-0.164259	O	1.660719	-1.206180	-0.113237	O	2.182997	-0.530949	-0.424110
H	1.837454	1.387881	-0.320946	H	-3.187170	-0.919690	0.444391	H	2.340286	-1.772604	0.259718	H	2.786685	-0.426968	-1.163066
		41				**42**				**43**				**44**	
C	-1.742053	0.157919	0.098074	C	1.547815	-0.418671	-0.299787	C	1.876747	-0.519491	-0.007254	C	-1.933271	0.399306	0.321225
H	-2.637860	0.276725	-0.511480	H	1.484417	-0.420475	-1.395530	H	1.870074	-1.160916	-0.889353	H	-2.500339	0.472152	1.248982
H	-2.008076	0.426534	1.127265	O	2.905010	-0.393997	0.128397	H	1.850803	-1.175626	0.871719	H	-2.176132	1.282790	-0.282604
C	-0.652566	1.098452	-0.407675	C	0.730403	0.738160	0.262170	C	0.656370	0.390331	-0.014240	C	-0.439741	0.373568	0.624287
H	-1.080260	2.104607	-0.399490	H	0.769267	0.699450	1.353880	H	0.709164	1.037696	-0.893042	H	-0.235482	-0.512094	1.232226
H	-0.439170	0.867556	-1.456231	H	1.212575	1.675655	-0.032161	H	0.694469	1.046949	0.862280	H	-0.200104	1.250048	1.236015
C	0.652567	1.098452	0.407675	C	-0.721755	0.763840	-0.218166	C	-0.656370	-0.390331	-0.014239	C	0.439740	0.373568	-0.624287
H	0.439170	0.867555	1.456231	H	-0.758169	0.785026	-1.310485	H	-0.694468	-1.046949	0.862281	H	0.200104	1.250048	-1.236015
H	1.080260	2.104607	0.399492	H	-1.204185	1.680150	0.127035	H	-0.709164	-1.037697	-0.893040	H	0.235482	-0.512094	-1.232226
C	1.742053	0.157919	-0.098074	H	3.302927	0.431751	-0.160884	C	-1.876747	0.519491	-0.007254	C	1.933271	0.399306	-0.321225
H	2.637861	0.276725	0.511479	H	1.158763	-1.375315	0.047646	H	-1.870074	1.160915	-0.889353	H	2.176132	1.282790	0.282604
H	2.008075	0.426534	-1.127266	C	-1.549054	-0.409647	0.274956	H	-1.850803	1.175627	0.871719	H	2.500339	0.472152	-1.248982
O	-1.410310	-1.225402	0.021690	H	-1.166923	-1.351560	-0.133036	O	3.106419	0.194097	-0.067324	O	-2.401401	-0.785468	-0.313837
H	-0.721370	-1.410435	0.669637	H	-1.486593	-0.470656	1.368733	H	3.181570	0.745804	0.715944	H	-2.010076	-0.846394	-1.188731
O	1.410311	-1.225402	-0.021691	O	-2.895881	-0.199484	-0.142612	O	-3.106419	-0.194097	-0.067323	O	2.401401	-0.785468	0.313837
H	0.721363	-1.410434	-0.669631	H	-3.429562	-0.948267	0.133490	H	-3.181572	-0.745801	0.715947	H	2.010077	-0.846393	1.188731
		45				**46**				**47**				**48**	
C	1.428339	-0.024005	0.478043	C	1.268376	-0.402775	0.244701	C	0.417201	1.914833	0.399270	C	1.430850	-0.084359	0.480407
H	0.954281	-0.850218	1.020128	H	0.767692	-1.267991	-0.180099	H	1.067610	1.916978	1.283072	H	1.610910	0.664091	1.263557
H	1.636844	0.770296	1.205475	O	2.618960	-0.469162	-0.209300	O	1.181007	2.114436	-0.785158	H	0.967695	-0.948180	0.955488
C	0.509879	0.506340	-0.607398	C	0.581352	0.888158	-0.186541	C	-0.417201	0.639597	0.373297	C	0.517025	0.494522	-0.591750
H	0.327987	-0.288476	-1.336021	H	1.180113	1.729863	0.178731	H	-1.074310	0.643309	1.249676	H	1.054972	1.292362	-1.114219
H	1.045178	1.287808	-1.149673	H	0.599056	0.949374	-1.278175	H	-1.057410	0.674889	-0.512476	H	0.304259	-0.281575	-1.328040
C	-0.814501	1.065558	-0.083308	C	-0.852687	1.061836	0.322340	C	0.417201	-0.639597	0.373297	C	-0.791789	1.063671	-0.040006
H	-1.353201	1.532743	-0.909961	H	-1.169443	2.089949	0.129885	H	1.074310	-0.643309	1.249676	H	-1.325192	1.581500	-0.843515
H	-0.616221	1.854235	0.649737	H	-0.888112	0.923649	1.406703	H	1.057410	-0.674889	-0.512476	H	-0.580255	1.823016	0.720058
C	-1.735746	0.035331	0.563494	H	3.107129	0.266215	0.170901	H	1.848252	1.426420	-0.846122	C	-1.724860	0.024459	0.574220
H	-2.650410	0.523674	0.898933	H	1.218791	-0.504790	1.335565	H	-0.234734	2.785085	0.471715	H	-2.622799	0.520009	0.960006
H	-1.264147	-0.407321	1.448363	C	-1.885036	0.146625	-0.311422	C	-0.417201	-1.914833	0.399270	H	-1.247760	-0.475391	1.416862
O	2.631195	-0.467551	-0.145101	H	-2.889789	0.488764	-0.039124	H	0.234734	-2.785085	0.471715	O	2.662125	-0.566215	-0.046644
H	3.222292	-0.815943	0.526476	H	-1.799586	0.191939	-1.404101	H	-1.067610	-1.916978	1.283072	H	3.109196	0.158522	-0.492293
O	-2.160563	-0.983904	-0.335660	O	-1.679440	-1.188439	0.151760	O	-1.181007	-2.114436	-0.785158	O	-2.075573	-1.019536	-0.328730
H	-1.395481	-1.494510	-0.612355	H	-2.314044	-1.769225	-0.274437	H	-1.848252	-1.426420	-0.846122	H	-2.550800	-0.638098	-1.072144
		49				**50**				**51**				**52**	
C	1.608852	0.150308	0.281114	C	1.552847	-0.408025	-0.312626	C	-1.430493	-0.032877	0.494231	C	2.034512	0.355342	0.333215
H	1.505697	0.380986	1.351148	H	1.505914	-0.405386	-1.402727	H	-0.953719	-0.845761	1.042090	H	2.789213	1.116218	0.104801
H	2.641350	0.373719	0.006883	O	2.936465	-0.303172	0.008338	H	-1.643707	0.761733	1.220330	H	2.019158	0.212486	1.420985
C	0.662851	1.034975	-0.529017	C	0.730258	0.747445	0.244307	C	-0.515562	0.499139	-0.601394	C	0.673042	0.824377	-0.143319

H	0.587531	0.611609	-1.533444	H	0.763613	0.718163	1.339469	H	-1.048167	1.282130	-1.150074	H	0.485810	1.814510	0.282904
H	1.116116	2.021741	-0.648682	H	1.214903	1.678076	-0.056620	H	-0.328510	-0.297789	-1.325910	H	0.711448	0.949930	-1.228809
C	-0.735788	1.227991	0.078074	C	-0.726024	0.760680	-0.224497	C	0.807079	1.070951	-0.084583	C	-0.461995	-0.127716	0.227237
H	-1.376670	1.729552	-0.654056	H	-0.767502	0.782546	-1.316456	H	0.606348	1.854890	0.652897	H	-0.496542	-0.241761	1.317320
H	-0.671460	1.904624	0.935309	H	-1.211577	1.674440	0.123228	H	1.339051	1.544765	-0.911813	H	-0.267550	-1.116146	-0.189057
C	-1.420695	-0.043257	0.564317	H	3.032622	-0.322357	0.964369	C	1.737788	0.043415	0.553761	C	-1.814020	0.365459	-0.265345
H	-2.447316	0.175506	0.872204	H	1.155689	-1.370927	0.027320	H	1.275422	-0.404237	1.440305	H	-1.805837	0.457899	-1.352284
H	-0.899928	-0.451496	1.429788	C	-1.545879	-0.416416	0.272779	H	2.651193	0.537291	0.884470	H	-2.024567	1.362318	0.143526
O	1.429333	-1.240777	0.057955	H	-1.169701	-1.355816	-0.146117	O	-2.636730	-0.589451	-0.016171	O	2.345926	-0.870137	-0.327361
H	0.509443	-1.409516	-0.186285	H	-1.468166	-0.484150	1.365661	H	-3.105466	0.090517	-0.507919	H	3.192258	-1.191994	-0.008993
O	-1.409539	-1.104083	-0.398553	O	-2.898651	-0.203730	-0.123230	O	2.161825	-0.969789	-0.352686	O	-2.879910	-0.531460	0.029516
H	-1.814439	-0.797944	-1.215003	H	-3.425515	-0.961475	0.141230	H	1.413921	-1.533378	-0.565604	H	-2.920758	-0.655456	0.981639
		53				**54**				**55**				**56**	
C	1.872952	0.122605	-0.339390	C	1.557526	-0.403859	-0.310485	C	1.547888	-0.409100	0.284442	C	-1.423481	-0.032054	0.491363
H	2.892849	0.448733	-0.106836	H	1.519061	-0.413659	-1.400792	H	1.484895	-0.440818	1.379480	H	-0.950090	-0.860722	1.031032
O	1.710108	-1.255152	-0.003368	O	2.937480	-0.286943	0.020283	H	1.161503	-1.360133	-0.098348	H	-1.609368	0.758795	1.219579
C	0.869849	1.048917	0.337446	C	0.725216	0.754781	0.226152	C	0.726002	0.754629	-0.239442	C	-0.518418	0.486223	-0.618998
H	0.921420	0.896962	1.422009	H	0.754388	0.742552	1.321686	H	1.212449	1.676926	0.083293	H	-1.066242	1.254153	-1.168280
H	1.202740	2.076192	0.163901	H	1.204364	1.684068	-0.087455	H	0.764473	0.748682	-1.331858	H	-0.325635	-0.318072	-1.338402
C	-0.577185	0.920395	-0.141246	C	-0.730316	0.742674	-0.248154	C	-0.726002	0.754629	0.239442	C	0.809818	1.066395	-0.125540
H	-0.622148	1.073232	-1.222802	H	-0.769771	0.721333	-1.340226	H	-1.212449	1.676927	-0.083293	H	0.610788	1.878407	0.581231
H	-1.174584	1.716706	0.308932	H	-1.209920	1.676665	0.061422	H	-0.764473	0.748682	1.331858	H	1.340863	1.508058	-0.971068
H	1.875607	-1.360815	0.937353	H	3.029898	-0.326397	0.976011	C	-1.547888	-0.409100	-0.284442	C	1.741217	0.065452	0.552115
H	1.755100	0.169884	-1.423123	H	1.162244	-1.364383	0.037159	H	-1.161503	-1.360133	0.098348	H	1.283391	-0.341828	1.459956
C	-1.250080	-0.398919	0.193961	C	-1.549583	-0.421259	0.296857	H	-1.484896	-0.440817	-1.379480	H	2.658235	0.570465	0.854670
H	-0.783943	-1.220714	-0.351958	H	-1.163990	-1.373150	-0.066522	O	2.896487	-0.217742	-0.137894	O	-2.708964	-0.421326	0.018722
H	-1.140288	-0.607676	1.266391	H	-1.483754	-0.440231	1.392633	H	3.428085	-0.955900	0.169074	H	-2.601217	-1.119619	-0.632751
O	-2.631450	-0.272077	-0.149963	O	-2.907229	-0.385434	-0.126947	O	-2.896487	-0.217742	0.137894	O	2.158328	-0.988996	-0.311365
H	-3.049238	-1.132661	-0.071853	H	-3.301583	0.438186	0.173177	H	-3.428086	-0.955900	-0.169075	H	1.409550	-1.563154	-0.488474
		57				**58**				**59**				**60**	
C	-1.898427	0.131031	-0.313777	C	1.259610	-0.409541	0.220868	C	-1.388068	-0.425687	0.531321	C	-1.550139	-0.418324	0.290961
H	-2.906008	0.443420	-0.016992	H	1.183488	-0.558451	1.306295	H	-2.051790	-0.494359	1.400982	H	-1.163508	-1.367788	-0.077710
H	-1.839536	0.214307	-1.400280	H	0.772675	-1.255626	-0.256028	O	-2.145993	-0.480125	-0.677270	H	-1.490513	-0.446136	1.386414
C	-0.867570	1.046916	0.334556	C	0.579535	0.898504	-0.168383	C	-0.536922	0.836713	0.632818	C	-0.726182	0.748178	-0.241583
H	-1.196113	2.075999	0.162641	H	0.606166	0.998991	-1.256610	H	-1.204605	1.703220	0.579556	H	-1.203924	1.681069	0.073763
H	-0.891952	0.903565	1.421202	H	1.177021	1.724625	0.232844	H	-0.076629	0.870243	1.625535	H	-0.762787	0.734733	-1.333998
C	0.568490	0.896365	-0.175894	C	-0.858876	1.055212	0.331711	C	0.543120	0.958107	-0.448629	C	0.726182	0.748178	0.241583
H	1.165199	1.740898	0.176009	H	-1.182127	2.085088	0.154898	H	0.779465	2.012102	-0.615351	H	0.762787	0.734733	1.333998
H	0.568453	0.949805	-1.270322	H	-0.895097	0.912146	1.418113	H	0.155313	0.569111	-1.392098	H	1.203924	1.681069	-0.073763
C	1.279294	-0.378866	0.266003	C	-1.883840	0.137497	-0.324359	H	-2.764109	0.255886	-0.683417	C	1.550139	-0.418325	-0.290961
H	0.785702	-1.262025	-0.142788	H	-1.795086	0.194475	-1.410355	H	-0.752928	-1.307337	0.517754	H	1.490513	-0.446136	-1.386414
H	1.246755	-0.459238	1.354384	H	-2.894868	0.468285	-0.061229	C	1.849917	0.262910	-0.113543	H	1.163508	-1.367788	0.077710
O	-1.710162	-1.254917	-0.034365	O	2.620748	-0.454360	-0.197982	H	2.578576	0.451909	-0.909957	O	-2.905029	-0.377049	-0.141715

H	-1.822573	-1.395987	0.909653	H	3.093076	0.276367	0.210406	H	2.256988	0.676314	0.818214	H	-3.305930	0.435395	0.179253
O	2.666307	-0.363714	-0.069947	O	-1.718524	-1.242619	-0.006279	O	1.623042	-1.139723	0.028511	O	2.905029	-0.377049	0.141715
H	2.750178	-0.434369	-1.024332	H	-1.861619	-1.360091	0.936728	H	2.455045	-1.570562	0.237051	H	3.305930	0.435395	-0.179253
		61				**62**				**63**				**64**	
C	-1.555112	-0.409220	-0.311409	C	0.234821	1.554536	-0.350029	C	1.966072	0.107449	-0.199606	C	1.354289	-0.227228	0.427128
H	-1.506721	-0.419621	-1.401631	H	-0.141307	2.573296	-0.260243	H	2.908208	0.347338	0.294061	H	0.836303	-1.182521	0.486654
H	-1.161953	-1.369042	0.040578	O	1.651263	1.679826	-0.427479	O	1.730397	-1.272394	0.076429	O	2.595492	-0.501380	-0.213644
C	-0.729657	0.751150	0.231875	C	-0.234821	0.729046	0.842939	C	0.871276	1.041554	0.303196	C	0.519305	0.806196	-0.322840
H	-1.211509	1.679195	-0.081472	H	0.113680	1.214236	1.756684	H	0.804727	0.959591	1.391681	H	1.081936	1.744547	-0.342235
H	-0.763040	0.736632	1.327120	H	-1.328603	0.764685	0.877980	H	1.201290	2.061980	0.091110	H	0.418089	0.491663	-1.366185
C	0.729657	0.751151	-0.231875	C	0.234821	-0.729046	0.842939	C	-0.509433	0.812163	-0.326006	C	-0.863331	1.051655	0.296679
H	1.211509	1.679195	0.081472	H	-0.113680	-1.214236	1.756684	H	-0.403850	0.482501	-1.364321	H	-1.185463	2.073601	0.079376
H	0.763040	0.736633	-1.327120	H	1.328603	-0.764685	0.877980	H	-1.066891	1.749616	-0.362189	H	-0.802517	0.971975	1.385700
C	1.555112	-0.409220	0.311409	H	2.031502	0.820236	-0.624108	H	1.084295	-1.607279	-0.549562	H	3.110940	0.309147	-0.248153
H	1.161953	-1.369042	-0.040578	H	-0.163121	1.148276	-1.287942	H	2.112362	0.257701	-1.275551	H	1.513135	0.110355	1.458550
H	1.506721	-0.419622	1.401631	C	-0.234821	-1.554536	-0.350029	C	-1.361013	-0.196175	0.426294	C	-1.961052	0.121971	-0.208766
O	-2.938533	-0.294329	0.005188	H	0.163121	-1.148276	-1.287942	H	-0.845872	-1.157869	0.510508	H	-2.905110	0.376065	0.274190
H	-3.039542	-0.324116	0.960450	H	0.141307	-2.573296	-0.260243	H	-1.535574	0.168365	1.445790	H	-2.096588	0.263974	-1.287165
O	2.938533	-0.294329	-0.005188	O	-1.651263	-1.679826	-0.427479	O	-2.593485	-0.339747	-0.277047	O	-1.739313	-1.256139	0.083413
H	3.039542	-0.324113	-0.960451	H	-2.031502	-0.820236	-0.624108	H	-3.155398	-0.954768	0.200154	H	-1.115426	-1.614221	-0.552097
		65													
C	1.260895	-0.422525	-0.183169												
H	1.126842	-0.680009	-1.233960												
O	2.666964	-0.396049	0.029857												
C	0.597081	0.914962	0.124352												
H	0.657474	1.105289	1.202219												
H	1.195596	1.688541	-0.361914												
C	-0.859019	1.052368	-0.332018												
H	-0.929866	0.894041	-1.411455												
H	-1.172325	2.083886	-0.148197												
H	2.837083	-0.159783	0.946000												
H	0.815021	-1.230777	0.412319												
C	-1.869654	0.135215	0.350287												
H	-1.719156	0.148530	1.437223												
H	-2.877302	0.504234	0.159873												
O	-1.872069	-1.202467	-0.142004												
H	-1.068350	-1.645944	0.138370												

Table S5

Enthalpies of formations of most stable HB and F-lin conformers of α,ω–alkanediols calculated at the DLPNO-CCSD(T_1)/CBS//B3LYP-D3(BJ)/def2-TZVPP level using isodesmic-type reactions (at T = 298.15 K, in kJ·mol^{-1}) [a]

	Reaction	HB conformer			F-lin conformer	
		$\Delta_r H^o_m$	$\Delta_f H^o_m$	Δ_{HB} [b]	$\Delta_f H^o_m$	$\Delta_{F\text{-}lin}$ [c]
	1,2-ethanediol ($C_2H_6O_2$), $\Delta_f H^o_m$(g, exp) = -390.2 ± 0.6 kJ·mol^{-1}					
1	$C_2H_6O_2 + 4\ CH_4 \rightarrow 3\ C_2H_6 + 2\ H_2O$	-47.8	-389.8		-379.2	
2	$C_2H_6O_2 + H_2 \rightarrow 2\ CH_3OH$	-13.2	-388.6		-378.0	
3	$C_2H_6O_2 + C_2H_6 \rightarrow 2\ CH_3CH_2OH$	5.3	-391.4		-380.7	
4	$C_2H_6O_2 + n\text{-}C_4H_{10} \rightarrow 2\ CH_3CH_2CH_2OH$	6.8	-391.3		-380.6	
5	$C_2H_6O_2 + n\text{-}C_4H_{10} \rightarrow 2\ CH_3CH(OH)CH_3$	-29.8	-390.1		-379.4	
6	$C_2H_6O_2 + CH_4 \rightarrow CH_2(OH)_2 + C_2H_6$	-12.9	-389.9		-379.3	
7	$C_2H_6O_2 + C_2H_6 \rightarrow HOCH_2CH(OH)CH_3 + CH_4$	-29.6	-389.3		-378.7	
8	$C_2H_6O_2 + C_2H_6 \rightarrow HOCH_2CH_2CH_2OH + CH_4$	-12.5	-389.3		-378.6	
		weighted average	**-390.0 ± 2.3** [d]	-0.2	-379.3 ± 2.3 [d]	-10.9
	1,3-propanediol ($C_3H_8O_2$), $\Delta_f H^o_m$ (g, exp) = -411.3 ± 1.6 kJ·mol^{-1}					
1	$C_3H_8O_2 + 5\ CH_4 \rightarrow 4\ C_2H_6 + 2\ H_2O$	-35.2	-412.1		-407.1	
2	$C_3H_8O_2 + 3\ CH_4 \rightarrow 2\ C_2H_6 + 2\ CH_3OH$	64.2	-410.8		-405.9	
3	$C_3H_8O_2 + CH_4 \rightarrow 2\ CH_3CH_2OH$	17.8	-413.6		-408.7	
4	$C_3H_8O_2 + C_3H_8 \rightarrow 2\ CH_3CH_2CH_2OH$	8.1	-413.5		-408.6	
5	$C_3H_8O_2 + C_3H_8 \rightarrow 2\ CH_3CH(OH)CH_3$	-28.5	-412.3		-407.4	
6	$C_3H_8O_2 + C_2H_6 \rightarrow CH_2(OH)_2 + n\text{-}C_4H_{10}$	-22.6	-412.6		-407.7	
7	$C_3H_8O_2 + C_2H_6 \rightarrow HOCH_2CH_2OH + C_3H_8$	1.6	-412.9		-408.0	
8	$C_3H_8O_2 \rightarrow HOCH_2CH(OH)CH_3$	-17.0	-411.6		-406.7	
		weighted average	**-412.4 ± 2.3** [d]	1.1	-407.5 ± 2.3 [d]	-3.8
	1,4-butanediol ($C_4H_{10}O_2$), $\Delta_f H^o_m$(g, exp) = -425.7 ± 1.8 kJ·mol^{-1}					
1	$C_4H_{10}O_2 + 6\ CH_4 \rightarrow 5\ C_2H_6 + 2\ H_2O$	-23.5	-433.1		-426.0	
2	$C_4H_{10}O_2 + 4\ CH_4 \rightarrow 3\ C_2H_6 + 2\ CH_3OH$	76.0	-431.8		-424.8	
3	$C_4H_{10}O_2 + 2\ CH_4 \rightarrow C_2H_6 + 2\ CH_3CH_2OH$	29.5	-434.6		-427.6	
4	$C_4H_{10}O_2 + C_2H_6 \rightarrow 2\ CH_3CH_2CH_2OH$	8.8	-435.0		-428.0	
5	$C_4H_{10}O_2 + C_2H_6 \rightarrow 2\ CH_3CH(OH)CH_3$	-27.7	-433.8		-426.8	
6	$C_4H_{10}O_2 + CH_4 \rightarrow HOCH_2CH_2OH + C_3H_8$	13.3	-434.0		-426.9	
7	$C_4H_{10}O_2 + CH_4 \rightarrow HOCH_2CH(OH)CH_3 + C_2H_6$	-5.3	-432.6		-425.6	
8	$C_4H_{10}O_2 + CH_4 \rightarrow HOCH_2CH_2CH_2OH + C_2H_6$	11.7	-432.5		-425.5	
		weighted average	-433.4 ± 2.6 [d]	7.7	**-426.4 ± 2.6** [d]	0.7
	1,5-pentanediol ($C_5H_{12}O_2$), $\Delta_f H^o_m$(g, exp) = -443.6 ± 2.6 kJ·mol^{-1}					
1	$C_5H_{12}O_2 + 7\ CH_4 \rightarrow 6\ C_2H_6 + 2\ H_2O$	-17.3	-448.8		-446.0	
2	$C_5H_{12}O_2 + 4\ CH_4 \rightarrow 2\ C_2H_6 + C_3H_8 + 2\ CH_3OH$	71.3	-448.1		-445.2	
3	$C_5H_{12}O_2 + 2\ CH_4 \rightarrow C_3H_8 + 2\ CH_3CH_2OH$	24.8	-450.9		-448.0	
4	$C_5H_{12}O_2 + CH_4 \rightarrow 2\ CH_3CH_2CH_2OH$	15.1	-450.8		-447.9	
5	$C_5H_{12}O_2 + CH_4 \rightarrow 2\ CH_3CH(OH)CH_3$	-21.5	-449.5		-446.7	
6	$C_5H_{12}O_2 + CH_4 \rightarrow HOCH_2CH_2OH + n\text{-}C_4H_{10}$	8.3	-449.7		-446.8	
7	$C_5H_{12}O_2 + CH_4 \rightarrow HOCH_2CH(OH)CH_3 + C_3H_8$	-10.0	-448.9		-446.0	
8	$C_5H_{12}O_2 + CH_4 \rightarrow HOCH_2CH_2CH_2OH + C_3H_8$	7.0	-448.8		-446.6	
		weighted average	-449.4 ± 2.4 [d]	5.8	**-446.6 ± 2.4** [d]	3.0
	1,6-hexanediol ($C_6H_{14}O_2$), $\Delta_f H^o_m$(g, exp) = -467.7 ± 2.5 kJ·mol^{-1}					

1	$C_6H_{14}O_2 + 8\ CH_4 \rightarrow 7\ C_2H_6 + 2\ H_2O$	-6.6	-469.0		-466.1	
2	$C_6H_{14}O_2 + 4\ CH_4 \rightarrow C_2H_6 + 2\ C_3H_8 + 2\ CH_3OH$	71.0	-468.8		-465.8	
3	$C_6H_{14}O_2 + 2\ CH_4 \rightarrow n\text{-}C_4H_{10} + 2\ CH_3CH_2OH$	24.3	-471.0		-468.1	
4	$C_6H_{14}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH_2CH_2OH + C_2H_6$	25.8	-471.0		-468.0	
5	$C_6H_{14}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH(OH)CH_3 + C_2H_6$	-10.8	-469.7		-466.8	
6	$C_6H_{14}O_2 + CH_4 \rightarrow HOCH_2CH_2OH + n\text{-}C_5H_{12}$	7.9	-469.7		-466.7	
7	$C_6H_{14}O_2 + CH_4 \rightarrow HOCH_2CH(OH)CH_3 + n\text{-}C_4H_{10}$	-10.5	-469.0		-466.0	
8	$C_6H_{14}O_2 + CH_4 \rightarrow HOCH_2CH_2CH_2OH + n\text{-}C_4H_{10}$	6.5	-468.9		-466.0	
		weighted average	-469.7 ± 2.1 [d]	2.0	**-466.7 ± 2.1** [d]	-1.0
	1,7-heptanediol ($C_7H1_6O_2$), $\Delta_f H^o_m$(g, exp) = -487.9 ± 1.6 kJ·mol^{-1}					
1	$C_7H1_6O_2 + 9\ CH_4 \rightarrow 8\ C_2H_6 + 2\ H_2O$	8.2	-493.3		-487.1	
2	$C_7H1_6O_2 + 4\ CH_4 \rightarrow 3\ C_3H_8 + 2\ CH_3OH$	74.8	-493.6		-487.4	
3	$C_7H1_6O_2 + 2\ CH_4 \rightarrow n\text{-}C_5H_{12} + 2\ CH_3CH_2OH$	28.1	-495.1		-488.9	
4	$C_7H1_6O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH_2CH_2OH + C_3H_8$	29.6	-495.8		-489.6	
5	$C_7H1_6O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH(OH)CH_3 + C_3H_8$	-6.9	-494.6		-488.3	
6	$C_7H1_6O_2 + CH_4 \rightarrow HOCH_2CH_2OH + n$-C6H14	11.5	-494.0		-487.7	
7	$C_7H1_6O_2 + CH_4 \rightarrow HOCH_2CH(OH)CH_3 + n\text{-}C_5H_{12}$	-6.8	-493.1		-486.9	
8	$C_7H1_6O_2 + CH_4 \rightarrow HOCH_2CH_2CH_2OH + n\text{-}C_5H_{12}$	10.2	-493.1		-486.8	
		weighted average	-494.1 ± 2.4 [d]	6.2	**-487.9 ± 2.4** [d]	0.0
	1,8-octanediol ($C_8H_{18}O_2$), $\Delta_f H^o_m$(g, exp) = -509.9 ± 0.9 kJ·mol^{-1}					
1	$C_8H_{18}O_2 + 10\ CH_4 \rightarrow 9\ C_2H_6 + 2\ H_2O$	17.6	-512.2		-507.7	
2	$C_8H_{18}O_2 + 4\ CH_4 \rightarrow 2\ C_3H_8 + n\text{-}C_4H_{10} + 2\ CH_3OH$	73.0	-512.4		-507.9	
3	$C_8H_{18}O_2 + 2\ CH_4 \rightarrow n\text{-}C_6H_{14} + 2\ CH_3CH_2OH$	26.2	-514.0		-509.5	
4	$C_8H_{18}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH_2CH_2OH + n\text{-}C_4H_{10}$	27.8	-514.6		-510.1	
5	$C_8H_{18}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH(OH)CH_3 + n\text{-}C_4H_{10}$	-8.7	-513.4		-508.9	
6	$C_8H_{18}O_2 + CH_4 \rightarrow HOCH_2CH_2OH + n\text{-}C_7H_{16}$	9.8	-512.7		-508.2	
7	$C_8H_{18}O_2 + CH_4 \rightarrow HOCH_2CH(OH)CH_3 + n\text{-}C_6H_{14}$	-8.6	-512.0		-507.5	
8	$C_8H_{18}O_2 + CH_4 \rightarrow HOCH_2CH_2CH_2OH + n$-C6H14	8.4	-511.9		-507.4	
		weighted average	-512.9 ± 2.4 [d]	3.0	**-508.5 ± 2.4** [d]	-1.4
	1,9-nonanediol ($C_9H_{20}O_2$), $\Delta_f H^o_m$(g, exp) = -531.0 ± 0.8 kJ·mol^{-1}					
1	$C_9H_{20}O_2 + 11\ CH_4 \rightarrow 10\ C_2H_6 + 2\ H_2O$	32.0	-536.1		-528.1	
2	$C_9H_{20}O_2 + 4\ CH_4 \rightarrow C_3H_8 + 2\ n\text{-}C_4H_{10} + 2\ CH_3OH$	76.2	-536.2		-528.2	
3	$C_9H_{20}O_2 + 2\ CH_4 \rightarrow n\text{-}C_7H_{16} + 2\ CH_3CH_2OH$	29.4	-537.7		-529.7	
4	$C_9H_{20}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH_2CH_2OH + n\text{-}C_5H_{12}$	31.1	-538.3		-530.3	
5	$C_9H_{20}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH(OH)CH_3 + n\text{-}C_5H_{12}$	-5.5	-537.1		-529.1	
6	$C_9H_{20}O_2 + CH_4 \rightarrow HOCH_2CH_2OH + n\text{-}C_8H_{18}$	13.0	-536.5		-528.4	
7	$C_9H_{20}O_2 + CH_4 \rightarrow HOCH_2CH(OH)CH_3 + n\text{-}C_7H_{16}$	-5.4	-535.7		-527.7	
8	$C_9H_{20}O_2 + CH_4 \rightarrow HOCH_2CH_2CH_2OH + n\text{-}C_7H_{16}$	11.6	-535.6		-527.6	
		weighted average	-536.7 ± 2.3 [d]	5.7	**-528.7 ± 2.3** [d]	-2.3
	1,10-decanediol ($C_{10}H_{22}O_2$), $\Delta_f H^o_m$(g, exp) = -551.8 ± 0.9 kJ·mol^{-1}					
1	$C_{10}H_{22}O_2 + 12\ CH_4 \rightarrow 11\ C_2H_6 + 2\ H_2O$	41.1	-554.7		-549.0	
2	$C_{10}H_{22}O_2 + 4\ CH_4 \rightarrow 3\ n\text{-}C_4H_{10} + 2\ CH_3OH$	74.1	-554.8		-549.1	
3	$C_{10}H_{22}O_2 + 2\ CH_4 \rightarrow n\text{-}C_8H_{18} + 2\ CH_3CH_2OH$	27.4	-556.3		-550.6	
4	$C_{10}H_{22}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH_2CH_2OH + n\text{-}C_6H_{14}$	29.0	-556.9		-551.3	
5	$C_{10}H_{22}O_2 + 2\ CH_4 \rightarrow 2\ CH_3CH(OH)CH_3 + n\text{-}C_6H_{14}$	-7.5	-555.7		-550.0	
6	$C_{10}H_{22}O_2 + CH_4 \rightarrow HOCH_2CH_2OH + n\text{-}C_9H_{20}$	10.9	-554.5		-548.8	
7	$C_{10}H_{22}O_2 + CH_4 \rightarrow HOCH_2CH(OH)CH_3 + n\text{-}C_8H_{18}$	-7.5	-554.2		-548.6	
8	$C_{10}H_{22}O_2 + CH_4 \rightarrow HOCH_2CH_2CH_2OH + n\text{-}C_8H_{18}$	9.6	-554.2		-548.5	
		weighted average	-555.2 ± 2.4 [d]	3.4	**-549.5 ± 2.4** [d]	-2.3

[a] Recommended values are given in bold.

[b] Difference between the experimental enthalpy of formation and that calculated for HB conformer.
[c] Difference between the experimental enthalpy of formation and that calculated for F-lin conformer.
[d] The uncertainty was defined as $s_d \times t$, where s_d is the standard deviation from the weighted average value and t is Student's coefficient for the 95% confidence level.

Transpiration method: Vapor pressure measurements

Absolute vapor pressures were measured using the transpiration method [1]. 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) maintained by Julabo FP51-SL refrigerated circulator, and the transported material was collected in a cold trap. The amount of condensed substance was usually determined by GC using a suitable n-alkane as an internal standard. 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:

$$p_i = m_i \cdot R \cdot T_a / V \cdot M_i \; ; \qquad V = (n_{N2} + n_i) \cdot R \cdot T_a / P_a \qquad \text{(S1)}$$

where V is the volume of the gas phase consisting of the n_{N2} 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_{N2} 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_{N2} was read from the digital flow 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). To ensure that preconditioning was completed at the selected temperature, three samples were taken sequentially during sample rinsing and analyzed by 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.

The procedure for calculating the expanded uncertainties (0.95 level of confidence) of the vaporization enthalpies from the transpiration method includes uncertainties from the experimental transpiration conditions, uncertainties in the vapor pressure and uncertainties in the temperature adjustment to T = 298.15 K, as described elsewhere [2,3].

The uncertainties of the $\Delta_l^g H_m^o$(298.15 K)-values derived from the vapor pressures reported in the literature include uncertainties from the fitting equation and uncertainties from temperature adjustment to the reference temperature. Uncertainties in the temperature adjustment of vaporization enthalpies to T= 298.15 K are estimated to account with 20% to the total adjustment.

Absolute vapor pressures

The experimental absolute vapor pressures measured in this work are given in Table S6.

Table S6. Absolute vapor pressures *p*, and standard molar vaporization enthalpies and entropies determined using the transpiration method

T/ K[a]	*m*/ mg[b]	*V*(N_2)[c] / dm^3	T_a/ K[d]	Flow/ $dm^3 \cdot h^{-1}$	*p*/ Pa[e]	*u(p)*/ Pa[f]	$\Delta_l^g H_m^o$/ $kJ \cdot mol^{-1}$	$\Delta_l^g S_m^o$/ $J \cdot K^{-1} \cdot mol^{-1}$
1,5-pentanediol (liq)								
$\Delta_l^g H_m^o$(298.15 K) = (87.1±0.5) $kJ \cdot mol^{-1}$								
$\Delta_l^g S_m^o$(298.15 K) = (182.8±1.0) $J \cdot K^{-1} \cdot mol^{-1}$								
$\Delta_l^g G_m^o$(298.15 K) = (32.6±0.1) $kJ \cdot mol^{-1}$								
$\ln(p/p_{ref}) = \frac{373.1}{R} - \frac{115281.3}{RT} - \frac{94.6}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa								
303.4	0.65	43.22	296.1	3.39	0.36	0.01	86.6	181.3
308.2	0.84	33.22	296.1	3.39	0.61	0.02	86.1	179.7
313.1	1.79	42.04	296.1	3.39	1.03	0.03	85.7	178.1
318.3	0.14	1.921	296.1	3.39	1.72	0.05	85.2	176.4
323.2	1.39	11.50	296.1	3.39	2.90	0.08	84.7	175.3
328.2	1.67	8.673	296.1	3.39	4.63	0.12	84.2	173.7
333.2	1.55	5.057	296.1	3.39	7.39	0.21	83.8	172.3
336.2	1.36	3.390	296.1	3.39	9.70	0.27	83.5	171.5
339.2	1.37	2.627	296.1	3.39	12.60	0.34	83.2	170.7
342.2	1.33	1.978	296.1	3.39	16.24	0.43	82.9	169.8
345.2	1.48	1.695	296.1	3.39	21.01	0.55	82.6	169.0
348.2	1.39	1.243	296.1	3.39	26.84	0.70	82.3	168.2
351.2	1.27	0.904	296.1	3.39	33.86	0.87	82.1	167.3
1,6-hexanediol (cr)								
$\Delta_{cr}^g H_m^o$(298.15 K) = (111.9±0.7) $kJ \cdot mol^{-1}$								
$\Delta_{cr}^g S_m^o$(298.15 K) = (255.5±2.0) $J \cdot K^{-1} \cdot mol^{-1}$								
$\Delta_{cr}^g G_m^o$(298.15 K) = (35.7±0.1) $kJ \cdot mol^{-1}$								
$\ln(p/p_{ref}) = \frac{381.4}{R} - \frac{120884.1}{RT} - \frac{30.1}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa								
290.4	0.12	155.6	296.0	3.43	0.0164	0.01	112.1	256.3
295.4	0.26	148.5	296.0	3.43	0.0360	0.01	112.0	255.8
297.3	0.23	101.2	296.0	3.43	0.0481	0.01	111.9	255.6
300.3	0.43	120.1	296.0	3.43	0.0754	0.01	111.8	255.3
303.7	0.54	91.20	296.0	3.43	0.1233	0.01	111.7	254.9
306.5	0.34	38.32	296.0	2.94	0.1864	0.01	111.7	254.7
308.2	0.61	52.31	296.0	3.43	0.2421	0.01	111.6	254.7
311.4	0.51	28.52	296.0	2.94	0.3751	0.01	111.5	254.3
314.2	0.63	24.11	296.0	2.94	0.5420	0.02	111.4	253.9
1,7-heptanediol (liq)								
$\Delta_l^g H_m^o$(298.15 K) = (94.4±0.4) $kJ \cdot mol^{-1}$								

$\Delta_l^g S_m^o$(298.15 K) = (191.7±2.0) J·K^{-1}·mol^{-1}

$\Delta_l^g G_m^o$(298.15 K) = (37.2±0.1) kJ·mol^{-1}

$\ln(p/p_{ref}) = \frac{407.0}{R} - \frac{129995.9}{RT} - \frac{119.5}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa

336.2	0.56	5.222	298.9	2.90	2.03	0.06	89.8	177.4
339.2	0.70	4.835	298.9	2.90	2.71	0.07	89.5	176.4
342.2	0.91	4.738	298.9	2.90	3.63	0.10	89.1	175.4
345.2	0.84	3.385	300.2	2.90	4.67	0.12	88.8	174.2
348.1	0.95	2.998	300.2	2.90	6.00	0.18	88.4	173.2
351.2	1.48	3.483	299.7	2.82	8.03	0.23	88.0	172.3
354.2	1.02	1.883	299.7	2.82	10.21	0.28	87.7	171.2
357.2	1.14	1.647	298.9	2.82	13.00	0.35	87.3	170.1
360.2	1.19	1.365	298.9	2.82	16.45	0.44	87.0	169.0
363.2	1.27	1.112	298.2	2.90	21.47	0.56	86.6	168.2
366.2	1.24	0.870	298.7	2.90	26.69	0.69	86.2	167.1
369.2	1.37	0.749	299.3	2.90	34.50	0.89	85.9	166.4
373.2	1.53	0.629	300.0	2.90	45.82	1.17	85.4	165.0

1,8-octanediol (liq)

$\Delta_l^g H_m^o$(298.15 K) = (99.2±1.0) kJ·mol^{-1}

$\Delta_l^g S_m^o$(298.15 K) = (200.7±1.3) J·K^{-1}·mol^{-1}

$\Delta_l^g G_m^o$(298.15 K) = (39.4±0.1) kJ·mol^{-1}

$\ln(p/p_{ref}) = \frac{428.0}{R} - \frac{138447.3}{RT} - \frac{131.6}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa

343.2	0.71	5.789	297.7	4.09	2.08	0.06	93.3	182.2
347.2	0.82	4.563	297.7	4.09	3.06	0.08	92.8	180.8
352.2	0.84	2.928	297.5	4.09	4.84	0.13	92.1	178.9
357.2	0.85	1.968	297.7	2.88	7.29	0.21	91.4	176.8
357.3	1.02	2.384	297.5	4.09	7.23	0.21	91.4	176.7
360.2	0.94	1.680	297.2	2.88	9.50	0.26	91.0	175.8
363.2	0.98	1.344	297.2	2.88	12.26	0.33	90.7	174.8
366.2	0.98	1.056	297.7	2.88	15.76	0.42	90.3	173.7
369.2	1.02	0.864	297.7	2.88	19.99	0.52	89.9	172.6
373.2	1.15	0.720	297.5	2.88	27.03	0.70	89.3	171.1
376.2	1.47	0.720	297.5	2.88	34.54	0.89	88.9	170.2
379.3	1.56	0.605	297.5	2.88	43.54	1.11	88.5	169.1

1,8-octanediol (cr)

$\Delta_{cr}^g H_m^o$(298.15 K) = (132.9±1.4) kJ·mol^{-1}

$\Delta_{cr}^g S_m^o$(298.15 K) = (300.9±4.6) J·K^{-1}·mol^{-1}

$\Delta_{cr}^g G_m^o$(298.15 K) = (43.2±0.1) kJ·mol^{-1}

$\ln(p/p_{ref}) = \frac{434.3}{R} - \frac{144110.8}{RT} - \frac{37.7}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa

304.4	0.08	165.5	299.2	5.14	0.00813	0.01	132.6	300.1
308.3	0.12	130.1	299.2	5.14	0.01582	0.01	132.5	299.6
313.2	0.24	114.1	299.2	5.14	0.03646	0.01	132.3	299.2
317.2	0.27	68.14	298.2	5.14	0.06741	0.01	132.2	298.5
320.2	0.24	39.00	299.2	5.14	0.10665	0.01	132.0	298.1
322.7	0.36	37.54	299.5	5.14	0.16421	0.01	131.9	298.2
328.2	0.41	18.86	299.5	5.14	0.36658	0.01	131.7	297.4
331.2	0.29	9.00	298.2	5.14	0.54814	0.02	131.6	296.8

1,9-nonanediol (liq)

$\Delta_l^g H_m^o$(298.15 K) = (103.0±1.0) kJ·mol^{-1}

$\Delta_l^g S_m^o$(298.15 K) = (205.8±2.6) J·K^{-1}·mol^{-1}

$\Delta_l^g G_m^o$(298.15 K) = (41.6±0.1) kJ·mol^{-1}

$\ln(p/p_{ref}) = \frac{445.5}{R} - \frac{145899.9}{RT} - \frac{144.0}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa

343.2	1.34	20.92	297.2	4.47	0.99	0.03	96.5	185.3
348.2	0.57	5.395	297.7	3.30	1.63	0.05	95.8	183.4
348.2	0.67	6.328	297.2	4.47	1.64	0.05	95.8	183.5
353.2	1.06	6.179	297.2	4.47	2.64	0.07	95.0	181.5
354.2	0.98	5.328	297.2	3.33	2.85	0.08	94.9	180.9
357.2	0.90	3.552	297.2	3.33	3.89	0.10	94.5	180.1
357.2	0.92	3.774	297.2	3.33	3.76	0.10	94.5	179.8
358.2	0.79	2.978	297.2	4.47	4.08	0.11	94.3	179.3
360.2	0.73	2.387	299.7	3.33	4.77	0.12	94.0	178.4
363.2	0.75	1.832	296.9	3.33	6.30	0.18	93.6	177.3
363.2	0.88	2.159	297.2	4.47	6.31	0.18	93.6	177.4
366.2	0.83	1.554	296.9	3.33	8.19	0.23	93.2	176.2
366.2	0.73	1.388	297.2	3.33	8.13	0.23	93.2	176.2
368.2	0.88	1.425	297.2	3.80	9.50	0.26	92.9	175.3
369.2	0.89	1.332	296.6	3.33	10.25	0.28	92.7	174.9
373.2	1.00	1.055	296.2	3.33	14.51	0.39	92.2	173.5
373.2	1.13	1.189	296.7	3.40	14.61	0.39	92.2	173.6
376.2	1.08	0.906	297.2	3.40	18.44	0.49	91.7	172.4
379.2	1.07	0.736	297.2	3.40	22.51	0.59	91.3	171.0

1,9-nonanediol (cr)

$\Delta_{cr}^g H_m^o$(298.15 K) = (137.6±2.2) kJ·mol^{-1}

$\Delta_{cr}^g S_m^o$(298.15 K) = (312.6±6.6) J·K^{-1}·mol^{-1}

$\Delta_{cr}^g G_m^o$(298.15 K) = (44.4±0.1) kJ·mol^{-1}

$\ln(p/p_{ref}) = \frac{449.9}{R} - \frac{149961.1}{RT} - \frac{41.5}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa

298.2	0.05	424.972	299.7	6.51	0.00170	0.01	137.6	312.7
301.2	0.06	314.119	299.7	6.51	0.00283	0.01	137.5	312.0
303.2	0.10	359.350	299.7	6.51	0.00420	0.01	137.4	311.9
308.2	0.17	249.006	297.2	5.58	0.01039	0.01	137.2	311.5
311.2	0.05	40.648	297.2	5.58	0.01743	0.01	137.0	311.1
313.2	0.08	54.071	299.7	6.51	0.02374	0.01	137.0	310.6
318.7	0.11	30.323	299.7	5.58	0.05818	0.01	136.7	309.7

1,10-decanediol (cr)

$\Delta_{cr}^g H_m^o$(298.15 K) = (147.2±1.2) kJ·mol^{-1}

$\Delta_{cr}^g S_m^o$(298.15 K) = (327.7±3.2) J·K^{-1}·mol^{-1}

$\Delta_{cr}^g G_m^o$(298.15 K) = (49.5±0.1) kJ·mol^{-1}

$\ln(p/p_{ref}) = \frac{468.4}{R} - \frac{160591.6}{RT} - \frac{44.9}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa

315.5	0.11	300.207	296.0	4.90	0.0055	0.005	146.4	325.2
321.2	0.10	96.936	296.0	4.90	0.0145	0.005	146.2	324.2
323.3	0.18	115.489	296.0	4.90	0.0216	0.006	146.1	324.3
328.1	0.39	119.576	296.0	4.90	0.0467	0.006	145.9	323.4
330.5	0.33	67.920	296.0	4.90	0.0686	0.007	145.8	323.1
333.0	0.64	87.700	296.0	4.90	0.1039	0.008	145.6	322.9
335.7	0.34	30.813	296.0	4.90	0.1555	0.009	145.5	322.4

335.7	0.34	30.813	296.0	4.90	0.1555	0.009	145.5	322.4
338.0	0.12	7.111	296.0	4.90	0.2285	0.011	145.4	322.3
338.2	0.34	20.597	296.0	4.90	0.2353	0.011	145.4	322.3
339.6	0.37	18.267	296.0	4.90	0.2847	0.012	145.3	321.9
341.1	0.30	11.933	296.0	4.90	0.3532	0.014	145.3	321.6
343.7	0.58	15.856	296.0	4.90	0.5196	0.018	145.2	321.2

[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 dm^3) 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 $u(p_i/\text{Pa}) = 0.025 + 0.025(p_i/\text{Pa})$ for pressures from 5 to 3000 Pa. The standard uncertainties for T, V, p, m, are standard uncertainties with 0.683 confidence level. Uncertainty of the vaporization/sublimation enthalpy $U(\Delta^{g}_{l,cr}H^{o}_{m})$ is the expanded uncertainty (0.95 level of confidence) calculated according to procedure described elsewhere [2,3]. Uncertainties include uncertainties from the experimental conditions and the fitting equation, vapor pressures, and uncertainties from adjustment of vaporization enthalpies to the reference temperature T = 298.15 K.

The vapor pressure-temperature dependencies were fitted by the following equation [1]:

$$R\cdot\ln\left(p_i/p_{ref}\right) = a + \frac{b}{T} + \Delta^{g}_{l,cr}C^{o}_{p,m}\cdot ln\left(\frac{T}{T_0}\right) \quad \text{(S2)},$$

where R = 8.314462 J·K^{-1}·mol^{-1} is the molar gas constant, the reference pressure $p_{ref} = 1\ Pa$, a and b are adjustable parameters, the arbitrary temperature T_0 applied in Eq. (S2) was chosen to be T_0 = 298.15 K and $\Delta^{g}_{l}C^{o}_{p,m} = C^{o}_{p,m}(g) - C^{o}_{p,m}(liq)$ is the difference between the molar heat capacities of the gaseous $C^{o}_{p,m}(g)$ and the liquid phase $C^{o}_{p,m}(liq)$, respectively. For the solid compounds $\Delta^{g}_{cr}C^{o}_{p,m} = C^{o}_{p,m}(g) - C^{o}_{p,m}(cr)$ were used. The $\Delta^{g}_{l}C^{o}_{p,m}$- and $\Delta^{g}_{cr}C^{o}_{p,m}$-values used in Eq. (S2) are given in Table S7.

Table S7

Compilation of the standard molar heat capacities, $C^{o}_{p,m}$, and the heat capacity differences, $\Delta^{g}_{l}C^{o}_{p,m}$, evaluated in our previous work [4] for α,ω-alkanediols in our previous work (in J·K^{-1}·mol^{-1} at T = 298.15 K)

Diol	$C^{o}_{p,m}(g)$ [a]	$C^{o}_{p,m}(liq)$ [b]	$C^{o}_{p,m}(cr)$ [b]	$\Delta^{g}_{l}C^{o}_{p,m}$ [c]	$\Delta^{l}_{cr}C^{o}_{p,m}$ [c]	$\Delta^{g}_{cr}C^{o}_{p,m}$ [c]
1	2	3	4	5	6	7
1,2-ethanediol	78.0	149.7		**-62.5**		
1,3-propanediol	96.5	175.8		**-72.6**		
1,4-butanediol	115.1	203.3		**-83.3**		
1,5-pentanediol	137.1	232.5		**-94.6**		
1,6-hexanediol	157.7	265.1	190.7	**-105.5**	**-77.5**	**-30.1**
1,7-heptanediol	177.4	296.0	211.7	**-119.5**	**-84.3**	**-33.6**
1,8-octanediol	197.5	326.8	236.5	**-131.6**	**-91.0**	**-37.7**
1,9-nonanediol	217.7	357.7	258.7	**-144.0**	**-97.8**	**-41.5**
1,10-decanediol	238.0	388.5 [d]	279.6	**-155.2**	**-104.5**	**-44.9**
1,11-undecanediol	257.9	419.4 [d]	298.4		**-111.3**	**-48.1**
1,12-dodecanediol	278.1	450.2 [d]	330.7		**-118.0**	**-53.5**
1,13-tridecanediol	298.2	481.1 [d]	365.8		**-124.8**	**-59.3**

1,14-tetradecanediol	318.4	511.9 [d]	380.4	**-131.5**	**-61.8**
1,15-pentadecanediol	338.5	542.8 [d]	404.5	**-138.3**	**-65.8**
1,16-hexadecanediol	358.6	573.6 [d]	426.4	**-145.0**	**-69.4**

[a] DFT and empirical calculated results.
[b] Experimental and empirical data.
[c] The data in bold recommended in Ref. [4] for thermochemical calculations.
[d] From Ref. [4].

Adjustment of phase-change enthalpies to the reference temperature T = 298.18 K

The standard molar enthalpies of vaporization/sublimation at temperatures *T* were derived from the temperature dependence of the vapor pressures, approximated by Eq. (S2) using the following equation:

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

where *b* is one of the adjustable parameters of Eq. (S2).

Empirical correlations developed for alkanediols in our recent work [4]:

$C_{p,m}^{o}$(g)/ J·K^{-1}·mol^{-1} = 20.14 × N_C + 36.4 with R^2 = 0.9997 for C2 to C10 (S4)

$C_{p,m}^{o}$(liq)/ J·K^{-1}·mol^{-1} = 30.85× N_C +80.0 with R^2 = 0.9985 (S5),

$C_{p,m}^{o}$(cr)/ J·K^{-1}·mol^{-1} = 24.1 × N_C + 43.0 with R^2 = 0.9952 for C6 to C16 (S6)

$\Delta_l^g C_{p,m}^{o}$/ J·K^{-1}·mol^{-1} = −0.3885×$C_{p,m}^{o}$(liq) – 4.3 with R^2 = 0.9996 (S7)

$\Delta_{cr}^{g} C_{p,m}^{o}$/ J·K^{-1}·mol^{-1} = − 0.1668×$C_{p,m}^{o}$(cr) + 1.7 with R^2 = 0.9216, (S8),

$\Delta_{cr}^{l} C_{p,m}^{o}$/ J·K^{-1}·mol^{-1} = − 0.2188×$C_{p,m}^{o}$(liq) – 19.5 with R^2 = 0,9999 (S9)

The standard molar vaporization entropies at temperatures *T* were also derived from the temperature dependences of the vapor pressures (approximated by Eq. S2) as follows:

$$\Delta_{l,cr}^{g} S_m^o(T) = \Delta_{l,cr}^{g} H_m^o / T + R \times ln\left(p_i / p^o\right) \quad \text{(S10)}$$

with p^o = 0.1 MPa.

The BP method

The very limited data on vapor pressures that are generally available for the long-chained α,ω-alkanediols has prompted us to involve experimental boiling temperatures at different pressures compiled by databases [5–7].The accuracy of this data is questionable as it comes from the distillation of a compound after its synthesis and not from special physico-chemical studies. However, the numerous data on boiling temperatures at standard pressure as well as at reduced pressures provide at least a reliable level of the experimental vapor pressures and trend of the dependence of the vapor pressure with temperature [8]. This type of data is especially important and helps to reconcile the results in a case where the conventional methods show significant disagreement. In this work we treated the available vapor pressure for 1,5-pentanediol data found in [5–7] and calculated the vaporization enthalpies using Eqs. S2, S3 and S10 with the $\Delta_l^g C_{p,m}^{o}$(298.15 K)-values recommended in Table S7, column 5.

Table S8

The vapor pressures p, and standard vaporization enthalpies and entropies obtained by the approximation of boiling points at different pressures available in the literature[5–7]

T/ K[a]	p/ Pa	$\Delta_l^g H_{m/a}^o$ kJ·mol^{-1}	$\Delta_l^g S_{m/}^o$ J·K^{-1}·mol^{-1}
1,5-pentanediol (liq)			
$\Delta_l^g H_m^o$(298.15 K) = (85.5±2.8) kJ·mol^{-1}			
$\Delta_l^g S_m^o$(298.15 K) = (179.0±5.2) J·K^{-1}·mol^{-1}			
$\Delta_l^g G_m^o$(298.15 K) = (32.2±0.2) kJ·mol^{-1}			
$\ln(p/p_{ref}) = \frac{369.3}{R} - \frac{113745.8}{RT} - \frac{94.6}{R} ln\frac{T}{298.15}$; p_{ref} = 1 Pa			
352	33	80.5	162.4
357	53	80.0	161.4
360	67	79.7	160.6
366	107	79.1	159.3
376	200	78.2	156.2
378	267	78.0	157.0
378	200	78.0	154.6
391	533	76.8	152.8
393	667	76.6	153.2
401	1067	75.8	151.3
402	1067	75.7	150.6
406	1533	75.3	150.8
407	1600	75.2	150.5
407	1733	75.2	151.2
407	1600	75.2	150.5
407	1533	75.2	150.1
408	1867	75.1	151.1
410	1600	75.0	148.4
410	2000	75.0	150.3
411	1600	74.9	147.8
412	2000	74.8	149.0
415	2400	74.5	148.5
417	2666	74.3	148.0
426	3866	73.4	145.4
428	3866	73.3	144.1
428	4133	73.3	144.7
435	5333	72.6	142.5
513	101325	65.2	127.2

515	101325	65.0	126.4
516	101325	65.0	126.2

[a] Uncertainties in this table are expressed as the expanded uncertainty (0.95 level of confidence. k = 2). Uncertainties of the vaporization enthalpies include uncertainties from the fitting equation S2 and uncertainties from temperature adjustment to T = 298.15 K. Uncertainties in the temperature adjustment of vaporization enthalpies to the reference temperature T = 298.15 K are estimated to account with 20 % to the total adjustment.

Table S9

Chain-length dependence of the vaporization enthalpies $\Delta_l^g H_m^o$(298.15 K) of α,ω-alkanediols[a]

Compound	N_C [b]	$\Delta_l^g H_m^o(298.15\ K)_{exp}$ [c] kJ·mol^{-1}	$\Delta_l^g H_m^o(298.15\ K)_{calc}$ [d] kJ·mol^{-1}	Δ [e] kJ·mol^{-1}
1,2-ethanediol	2	65.7±0.2	(74.6)	-8.9
1,3-propanediol	3	71.5±0.3	(78.6)	-7.1
1,4-butanediol	4	79.0±0.7	(82.6)	-3.6
1,5-pentanediol	5	86.6±0.6	86.7	-0.1
1,6-hexanediol	6	90.7±0.4	90.7	0.0
1,7-heptanediol	7	94.8±0.4	94.7	0.1
1,8-octanenediol	8	98.7±0.3	98.7	0.0
1,9-nonanediol	9	102.7±0.3	102.7	0.0
1,10-decanediol	10	106.7±0.3	106.7	0.0
1,11-	11		110.7	
1,12-	12		114.7	
1,13-	13		118.7	
1,14-	14		122.7	
1,15-	15		126.8	
1,16-	16		130.8	

[a] The uncertainties in this table are given as two times the standard deviation.

[b] Number of the carbon atoms in alkyl chain.

[c] Experimental values from Table 3.

[d] Calculated using the following equation:

$\Delta_l^g H_m^o(298.15\ K)_{calc}$/ kJ·mol^{-1} = 4.01 × N_C+ 66.6 with R^2 = 0.9999, (for C ≥ 5),

which was developed from the correlation of the data given in columns 2 and 3 of this table, with the assessed expanded uncertainty of ±0.5 kJ·mol^{-1} (0.95 level of confidence, k = 2). Data in parentheses were not involved in the correlation.

[e] Difference between experimental and calculated values.

Table S10

Correlation of vaporization enthalpies $\Delta_l^g H_m^o$(298.15 K) of α,ω-alkanediols with the their T_b (normal boiling temperatures)[a]

Compound	T_b [b] K	$\Delta_l^g H_m^o(298.15\ K)_{exp}$ [c] kJ·mol^{-1}	$\Delta_l^g H_m^o(298.15\ K)_{calc}$ [d] kJ·mol^{-1}	Δ [e] kJ·mol^{-1}
1,2-ethanediol	472.0	65.7±0.2	(74.5)	-8.8
1,3-propanediol	485.9	71.5±0.3	(78.9)	-7.4
1,4-butanediol	499.7	79.0±0.7	(83.1)	-4.1
1,5-pentanediol	511.6	86.6±0.6	86.9	-0.3
1,6-hexanediol	523.7	90.7±0.4	90.7	0.0
1,7-heptanediol	535.2	94.8±0.4	94.2	0.6

1,8-octanenediol	549.5	98.7±0.3	98.7	0.0
1,9-nonanediol	562.3	102.7±0.3	102.7	0.0
1,10-decanediol	575.6	106.7±0.3	106.8	-0.1
1,11-	588.6		110.9	
1,12-	602.0		115.0	
1,13-	614.5		118.9	
1,14-	627.3		122.9	
1,15-	640.1		126.9	
1,16-	653.6		131.1	

[a] The uncertainties in this table are given as two times the standard deviation.
[b] Normal boiling temperatures are from Ref. [5–7].
[c] Experimental values given in Table 3.
[d] Calculated using the following equation:
$\Delta_l^g H^o_m(298.15\ K)_{calc}$/ kJ·mol^{-1} = 0.3177 × T_b– 72.6 with R^2 = 0.9885, (for C ≥ 5),
which was developed from the correlation of the data given in columns 2 and 3 of this table, with the assessed expanded uncertainty of ±0.5 kJ·mol^{-1} (0.95 level of confidence, k = 2). Data in parentheses were not involved in the correlation.
[e] Difference between experimental and calculated values.

Table S11

Correlation of vaporization enthalpies, $\Delta_l^g H^o_m(298.15\ K)$, of α,ω-alkanediols with their Kovats indices (J_x) [a]

Diol	J_x [b]	$\Delta_l^g H^o_m(298\ K)_{exp}$ [c] kJ·mol^{-1}	$\Delta_l^g H^o_m(298\ K)_{calc}$ [d] kJ·mol^{-1}	Δ [e] kJ·mol^{-1}
1,2-ethanediol	705	65.7±0.2	(74.6)	-8.9
1,3-propanediol	814	71.5±0.3	(78.9)	-7.4
1,4-butanediol	922	79.0±0.7	(83.2)	-4.2
1,5-pentanediol	1016	86.6±0.6	86.9	-0.3
1,6-hexanediol	1111	90.7±0.4	90.7	0.0
1,7-heptanediol	1201	94.8±0.4	94.3	0.5
1,8-octanenediol	1313	98.7±0.3	98.7	0.0
1,9-nonanediol	1414	102.7±0.3	102.7	0.0
1,10-decanediol	1518	106.7±0.3	106.9	-0.2
1,11-	1620		110.9	
1,12-	1725		115.1	
1,13-	1823		119.0	
1,14-	1924		123.0	
1,15-	2024		127.0	
1,16-	2130		131.2	

[a] The uncertainties in this table are given as two times the standard deviation.
[b] Kovats indices, J_x, on the standard non-polar column DB-1 [9].
[c] Experimental values from Table 3.
[d] Calculated using the following equation:
$\Delta_l^g H^o_m(298.15\ K)_{calc}$/ kJ·mol^{-1} = 0.0397 × J_x+ 46.6 with R^2 = 0.9807, (for C ≥ 5),
which was developed from the correlation of the data given in columns 2 and 3 of this table, with the assessed expanded uncertainty of ±0.5 kJ·mol^{-1} (0.95 level of confidence, k = 2). Data in parentheses were not involved in the correlation.
[e] Difference between experimental and calculated values.

Table S12

Experimental enthalpies of fusion ($^{\Delta^{l}_{cr}H^{o}_{m}}$) at melting points ($T_{fus}$) of α,ω-alkanediols available from the literature[a]

	T_{fus}	$\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$	Ref
Compound	K	kJ·mol^{-1}	
1,2-	260.6	10.0±0.5	[10]
	260.8	11.6±1.0	[11]
	256.6	9.5±0.4	[12]
	259.3	**9.9±0.3**	average[b]
1,3-	245.5	7.1±0.6	[12]
	(249.0)	(11.4±1.0)	[13]
1,4-	293.6	18.7±0.5	[14]
	289.9	12.0±0.6	[12]
	294.2	16.0±0.8	[15]
	292.6	**(15.9±0.4)**	average[b]
1,5-	(248.0)	(15.7±1.0)	[16]
	254.4	**9.7±0.4**	[12]
1,6	320.6	25.5±0.8	[17]
	314.6	22.2±1.2	[12]
	315.0	22.6±0.1	[18]
	316.0	25.5±0.5	[19]
	314.7	26.4±0.4	[20]
	317.0	22.9±0.8	[15]
	316.3	**22.9±0.2**	average[b]
1,7	(295.0)	(21.3±0.6)	[12]
	290.5	**26.3±0.6**	[20]
1,8-	332.7	36.1±0.4	[12]
	331.6	36.3±0.3	[20]
	332.2	**36.2±0.2**	average[b]
1,9	319.5	36.4±0.4	[12]
	318.7	36.7±0.7	[20]
	319.1	**36.5±0.4**	average[b]

1,10	(345.4)	(41.7±0.6)	[12]
	345.7	45.8±0.4	[21]
	345.6	44.2±0.5	[22]
	345.8	45.0±0.2	[20]
	(347.8)	(37.8±0.8)	[15]
	345.7	**45.1±0.2**	average[b]
1,11	334.1	45.9±0.5	[20]
1,12	352.0	51.2±1.3	[23]
	352.9	54.2±0.7	[20]
	352.5	**53.5±0.6**	average[b]
1,13[c]	351.0	46.7±2.0	[24]
	350.3	54.8±0.8	[20]
	350.7	**53.7±0.7**	average[b]
1,14	360.4	61.9±3.7	[24]
	359.2	63.5±0.3	[20]
	359.8	**63.4±0.4**	average[b]
1,15 [d]	361.4	58.7±0.5	[24]
	361.2	(65.3±1.6)	[20]
	364.0	57.4±0.3	[15]
	362.7	**58.0±0.5**	average[b]
1,16 [e]	365.4	64.2±1.0	[24]
	366.0	72.8±0.5	[20]
	366.5	63.3±1.0	[15]
	366.0	**69.8±0.4**	average[b]

[a] Uncertainties are presented as expanded uncertainties (0.95 level of confidence with k=2).
[b] Weighted average value (experimental uncertainty was taken as the weighing factor).

[c] From [24] a solid–solid phase transition at T_{trs} = 343.0 K with $\Delta_{trs}H_m$= 28.9 kJ·mol^{-1}was observed. The value of $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ includes $\Delta_{trs}H_m$. Also Badea *et. al.* [20] observed the solid–solid phase transition at T_{trs} = (339.3 ± 0.5) K. However, since the T_{trs} was too close to T_{fus}, a precise determination of $\Delta_{trs}H_m$, therefore the value of $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ includes $\Delta_{trs}H_m$.

[d] From [20] a solid–solid phase transition at T_{trs} = (349.0 ± 0.6) K with $\Delta_{trs}H_m$= (38.3 ± 1.2) kJ·mol^{-1}was observed. The value of $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ includes $\Delta_{trs}H_m$. From [15] T_{trs} = 348.7 K with $\Delta_{trs}H_m$ = 33.2 kJ·mol^{-1} and T_{fus} = 364.0 K with $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ = 24.2 kJ·mol^{-1}. From [24] T_{trs} = 349.4 K with $\Delta_{trs}H_m$ = 35.1 kJ·mol^{-1} and T_{fus} = 361.4 K with $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ = 23.6 kJ·mol^{-1}, therefore the value of $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ in this table includes $\Delta_{trs}H_m$.

[e] The solid–solid phase transition at T_{trs} = (364.1 ± 0.2) K [20] or at T_{trs} = 363.0 K [24] was observed, but the transition temperature in both cases was too close to melting point for $\Delta_{trs}H_m$ to be determined, therefore the value of $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ in this table includes $\Delta_{trs}H_m$. However, from [15] T_{trs} = 366.5 K with $\Delta_{trs}H_m$ = 36.2 kJ·mol^{-1} and T_{fus} = 367.1 K with $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ = 27.1 kJ·mol^{-1}. The value of $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$ from [15] given in this table includes $\Delta_{trs}H_m$.

Table S13

Correlation of enthalpies of fusion, $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$, with their fusion temperatures, T_{fus}, for the *odd* members of the α,ω-alkanediol family

Diol	T_{fus} [a]	$\Delta_{cr}^{l}H_{m}^{o}(T_{fus})$ [a]	$\Delta_{cr}^{l}H_{m}^{o}(T_{fus})$ [b]	Δ [c]
	K	kJ·mol^{-1}	kJ·mol^{-1}	kJ·mol^{-1}
1,3-	245.5	7.1	6.2	0.9
1,5-	254.4	9.7	10.1	-0.4
1,7-	290.5	26.3	26.1	0.2
1,9-	319.1	36.5	38.7	-2.2
1,11-	334.1	45.9	45.3	0.6
1,13-	350.7	53.7	52.7	1.0
1,15-	362.7	58.0	58.0	0.0

[a] Evaluated experimental data from Table S12.

[b] Calculated according to the approximation of the data given in this table:

$\Delta_{cr}^{l}H_{m}^{o}$(298.15 K)/(kJ·mol^{-1}) = 0.4416×J_x − 102.2 with R^2 = 0.9967.

[c] Difference between column 2 and 3 in this table.

Table S14

Correlation of enthalpies of fusion, $\Delta_{cr}^{l}H_{m}^{o}(T_{fus})$, with their fusion temperatures, T_{fus}, for the *even* members of the α,ω-alkanediols family

	T_{fus}	$\Delta_{cr}^{l}H_{m}^{o}(T_{fus})$ [b]	$\Delta_{cr}^{l}H_{m}^{o}(T_{fus})$ [b]	Δ [b]
	K	kJ·mol^{-1}	kJ·mol^{-1}	kJ·mol^{-1}
1,6-	316.3	22.9	21.2	1.7
1,8-	332.2	36.2	36.1	0.1
1,10-	345.7	45.1	48.7	-3.6
1,12-	352.5	53.5	55.1	-1.6
1,14-	359.8	63.4	62.0	1.4
1,16-	366.0	69.8	67.8	2.0

[a] Evaluated experimental data from Table S12.

[b] Calculated according to the approximation of the data given in this table:

$\Delta_{cr}^{l}H_{m}^{o}$(298.15 K)/(kJ·mol^{-1}) = 0.9365×J_x − 275.0 with R^2 = 0.9835.

[c] Difference between column 2 and 3 in this table.

Table S15

Calculation of sublimation enthalpies $\Delta_{cr}^{g}H_{m}^{o}$(298.15 K) from enthalpies of vaporization, $\Delta_{l}^{g}H_{m}^{o}$(298.15 K), and enthalpies of fusion, $\Delta_{cr}^{l}H_{m}^{o}$(298.15 K), in kJ·mol^{-1}

Diol	$\Delta_{l}^{g}H_{m}^{o}$(298.15 K) [a]	$\Delta_{cr}^{l}H_{m}^{o}$(298.15 K) [b]	$\Delta_{cr}^{g}H_{m}^{o}$(298.15 K) [c]
1,6-	90.7±0.4	21.5±0.5	112.2±0.7
1,8-	98.7±0.3	33.1±1.0	131.8±1.1
1,9-	102.7±0.3	34.5±0.7	137.2±0.8
1,10-	106.7±0.3	40.1±1.5	146.8±1.5

[a] From Table 3.

[b] From Table 6.

[c] Sum of column 2 and 3 in this table.

Table S16

Correlation of experimental enthalpies of sublimation, $\Delta^{g}_{cr}H^{o}_{m}$(298.15 K), and enthalpies of fusion, $\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$, in kJ·mol^{-1}

	$\Delta^{l}_{cr}H^{o}_{m}(T_{fus})$[a]	$\Delta^{g}_{cr}H^{o}_{m}(298.15\ K)_{exp}$[b]	$\Delta^{g}_{cr}H^{o}_{m}(298.15\ K)_{calc}$[c]	Δ[d]
6	22.9	112.1	113.1	-1.0
7	26.3	121.3	118.8	2.5
8	36.2	132.1	135.4	-3.3
9	36.5	137.3	135.9	1.4
10	45.1	147.0	150.2	-3.2
11	45.9	152.8	151.6	1.2
12	53.5	162.2	164.2	-2.0
13	53.7	166.1	164.6	1.5
14	63.4	178.3	180.8	-2.5
15	58.0	176.1	171.8	4.3
16	69.8	191.2	191.5	-0.3

[a] Experimental values from Table S12.
[b] Experimental values from Table 5.
[c] Calculated according to equation:

$$\Delta^{g}_{cr}H^{o}_{m}(298.15\ K)_{exp}/\ kJ{\cdot}mol^{-1} = 1.67 \times \Delta^{l}_{cr}H^{o}_{m}(T_{fus})+74.9 \qquad \text{with } R^2 = 0.9899,$$

developed from the data given in this table.

Combustion calorimetry: enthalpy of formation determination

The standard molar energy of combustion was measured with a self-made high-precision isoperibolic calorimeter with a static bomb and a stirred water bath. About 0.3-0.5 g of the solid sample was encapsulated in a polyethylene bulb (Fa. NeoLab, Heidelberg, Germany) and weighed with a microbalance with a resolution of 10^{-6} g. The bulb was compressed with special tweezers and sealed by heating the neck near a glowing wire. The bulb with the sample was placed in the crucible and burnt in oxygen at a pressure of 3.04 MPa.

The bomb was not purged with oxygen beforehand. Test experiments with and without purging with O_2 showed results that were also consistent within the experimental uncertainty. The detailed procedure has already been described [25,26].The combustion products were examined for carbon monoxide (Dräger tube) and unburned carbon, but neither was detected. The energy equivalent of the calorimeter ε_{calor} was determined with a standard reference sample of benzoic acid (sample SRM 39j, N.I.S.T.). Correction for nitric acid formation was based on titration with 0.1 mol·dm^{-3} NaOH (aq). Conventional procedures [27] were used for reduction of the data to standard conditions. Auxiliary data required for the reduction are collected in Table S17.

Table S17

Auxiliary quantities: formula, density ρ(293 K), massic heat capacity c_p(298.15 K), and expansion coefficients $(\delta V/\delta T)_p$ of the materials used in the present study [a]

Compounds	Formula	*Water* content[b]	ρ(293 K)	c_p(298.15 K)	$(\delta V/\delta T)_p$[c]
		ppm	g·cm^{-3}	J·K^{-1} g^{-1}	10^{-3}·cm^3·K^{-1}·g^{-1}
1,8-octanediol (cr)	$C_8H_{18}O_2$	63.3	0.94[d]	1.62[e]	0.1
polyethylene [c]	$CH_{1.93}$		0.92	2.53	0.1
cotton [c]	$CH_{1.774}O_{0.887}$		1.50	1.67	0.1

[a] Data for the densities, ρ(293 K), and the specific heat capacities,c_p(298.15 K), of auxiliary materials are from our previous work [28]. Thespecific energy of combustion $\Delta_c u^o$(cotton) = -16945.2 J·g^{-1}; $u(\Delta_c u^o)$ = 4.2 J·g^{-1}. The specific

energy of combustion $\Delta_c u^o$(polyethylene) = -46354.5 J·g^{-1}; $u(\Delta_c u^o)$ = 3.6 J·g^{-1}. The standard uncertainties are reported for the specific energies of combustion.

[b] The results of combustion experiments were corrected for this residual amount of water.

[c] Estimated.

[d] Calculated at 293 K using Advanced Chemistry Development (ACD/Labs) Software V11.02 (© 1994-2024 ACD/Labs) with uncertainty ±0.06 g/cm^3

[e] Calculated from the standard molar heat capacity at 298.15 K (see Table S7).

Table S18

Results of typical combustion experiment for 1,8-octanediol at T = 298.15 K ($p°$ = 0.1 MPa)[a]

m (substance) /g	0.369658
m'(cotton) /g	0.003015
m"(polyethylene) /g	0.291645
ΔT_c /K	1.78370
$(\varepsilon_{calor})\cdot(-\Delta T_c)$ /J	-26411.4
$(\varepsilon_{cont})\cdot(-\Delta T_c)$ /J	-34.0
$\Delta U_{decomp\ HNO3}$/J	51.36
ΔU_{corr}/J	7.89
$-m'\cdot\Delta_c u'$ /J	51.09
$-m"\cdot\Delta_c u"$ /J	13519.1
$\Delta_c u^o$(cr) /(J·g^{-1})	-34669.9

[a] The definition of the symbols is in accordance with the Hubbard et al. [27]

The standard specific energies of combustion, $\Delta_c u^o$(cr), of 1,8-octanediol are listed in Table S19.

Table S19. Summary of all results of the combustion experiments with 1,8-octanediol at T = 298.15 K ($p°$ = 0.1 MPa) [a]

Combustion experiment	$\Delta_c u^o$
1	-34669.1
2	-34675.2
3	-34675.3
4	-34668.3
5	-34668.3
$\langle\Delta_c u^o\rangle$(cr) /(J·g^{-1}) [a]	-34671.2 ± 1.6
$\Delta_c H^o_m$(cr)/(kJ·mol^{-1})[b]	-5078.6 ± 0.9
$\Delta_f H^o_m$(cr)/(kJ·mol^{-1})[b]	-642.0 ± 1.4

[a] Uncertainty of combustion energy is expressed as standard deviation of the mean.

[b] Uncertainties are expressed as the twice standard deviation of the mean.

The total uncertainties of $\Delta_c H^o_m$ and $\Delta_f H^o_m$-values have been calculated according to the guidelines presented by Hubbard *et al.*[27] and Olofsson [29]. The uncertainty of combustion energy, $\Delta_c u^o$(cr), is expressed as standard deviation of the mean. According to the thermochemical practice, the uncertainties assigned to the $\Delta_f H^o_m$(cr)-value is twice the overall standard deviations and include the

uncertainties of the calibration, the combustion energies of the auxiliary materials, and the uncertainties of the enthalpies of formation of the reaction products H_2O and CO_2.

Table S20
Enthalpies of formation of the auxiliary molecules involved in reactions R1 and R2

Compound	$\Delta_f H^o_m$(liq, 298.18 K)/ kJ·mol^{-1}
2,2-dimethyl-1,3-dioxolane (CAS 2916-31-6)	-430.5±0.3 [30]
2,2-dimethyl-1,3-dioxane (CAS 695-30-7)	-468.9±2.1 [31]
acetone	-248.1±0.7 [32]
H_2O	-285.83±0.04[33]

Table S21
Calculation of the experimental liquid-phase enthalpies of formation of α,ω-alkanediols, in kJ·mol^{-1}

Diol	$\Delta_f H^o_m$(cr, 298.18 K) [a]	$\Delta^l_{cr} H^o_m$(298.15 K)[b]	$\Delta_f H^o_m$(liq, 298.18 K)[c]
1,6-hexanediol	-579.8±2.5	21.5±0,5	-558.3±2.6
1,8-octanediol	-642.0±1.4	33.1±1.0	-608.9±1.7
1,9-nonanediol	-668.3±1.7[d]	34.5±0.7	-633.8±1.5[e]
1,10-decanediol	-698.8±1.0	40.1±1.5	-658.7±1.8

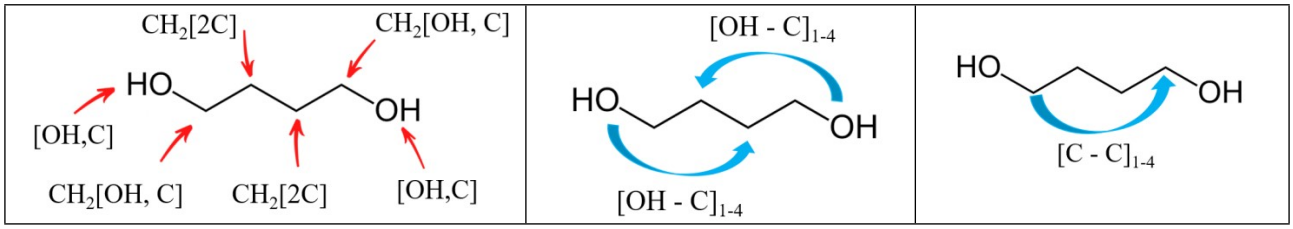
[a] Experimental values from Table 8.
[b] Experimental values from Table S12.
[c] Sum of columns 2 and 3 from this table.
[d] Difference between column 4 and 3.
[e] From Table S22.

Table S22
Chain length dependence of the liquid-phase enthalpies of formation, $\Delta_f H^o_m$(liq), for α,ω-alkanediols (at T = 298.15 K and $p°$ = 0.1 MPa, in kJ·mol^{-1})[a]

Diol	N_C	$\Delta_f H^o_m(\text{liq})_{exp}$ [b]	$\Delta_f H^o_m(\text{liq})_{calc}$ [c]	Δ [d]
1,5-pentanediol	5	-530.2±2.5	-531.5	1.3
1,6-hexanediol	6	-558.3±2.6	-557.1	-1.2
1,7-heptanediol	7		-582.7	
1,8-octanenediol	8	-608.9±1.7	-608.2	-0.7
1,9-nonanediol	9		-633.8	
1,10-decanenediol	10	-658.7±1.8	-659.4	0.7

[a] Uncertainties correspond to expanded uncertainties of the mean (0.95 level of confidence).
[b] From Table S21.
[c] Calculated according to equation:
$\Delta_f H^o_m$(liq, 298.15 K)/(kJ·mol^{-1}) = -403.6 – 25.58×N_C with R^2 = 0.9996 (for C ≥ 5)
derived from the data in this table.
[d] Difference between column 3 and 4.

Table S23.
Group-contributions used for the additive calculations of thermochemical properties of alkanediols, in kJ·mol^{-1}, at T = 298.15 K ($p°$ = 0.1 MPa)



Example for 1,4-butanediol: 2×[OH,C] + 2×CH_2[OH, C] + 2×CH_2[C] + 2×[OH - C]$_{1-4}$+ [C - C]$_{1-4}$

Symbol [a]	Contribution to $\Delta_f H^o_m$(liq)[b]	Contribution to $\Delta^g_l H^o_m$/298.15 K[b]	Contribution to $\Delta_f H^o_m$(g)[b]
[OH,C]	-190.4	31.80	-158.60
CH_2[OH, C]	-32.25	6.90	-29.03
CH_2[2 C]	-28.93	4.52	-23.80
[OH - C]$_{1-4}$	-2.25	-2.10	-1.00
[C - C]$_{1-4}$	3.11	-0.26	2.10

[a] The explanation can be found in the figure above.
[b] The group-contributions were developed in our previous work [34] using experimental data for alkanes and alkanols. The contributions for [OH - C]$_{1-4}$ and [C - C]$_{1-4}$ were adjusted for the experimental data of diols in this work.

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