

Treating entropy and conformational changes in implicit solvent simulations of small molecules: Supporting Information

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TABLE 1: The small molecule test set used here, with names and experimental hydration free energy values (in kcal/mol), as well as references to the source of the experimental values. Numbering up to 600 corresponds to the numbering used in the Rizzo test set¹ and is not necessarily consecutive. Numbering after 600 is unique to this set, which contains only neutral molecules. Values are transfer free energies from 1M gas to 1M in solvent. In the column with names of compounds, spaces have been replaced by underscores, following the formatting of Rizzo *et al.*

Number	Name	Hydration free energy	Reference
1	methane	1.99	1
2	ethane	1.83	1
3	propane	1.96	1
4	n-butane	2.07	1
5	2-methylpropane	2.32	1
6	n-pentane	2.32	1
7	2-methylbutane	2.38	1
8	2,2-dimethylpropane	2.51	1
9	n-hexane	2.48	1
10	2-methylpentane	2.51	1
11	3-methylpentane	2.51	1
12	2,2-dimethylbutane	2.51	1
13	2,3-dimethylbutane	2.34	1
14	n-heptane	2.67	1
15	2-methylhexane	2.93	1
16	3-methylhexane	2.71	1
17	2,2-dimethylpentane	2.88	1
18	2,3-dimethylpentane	2.52	1
19	2,4-dimethylpentane	2.83	1
20	3,3-dimethylpentane	2.56	1
21	n-octane	2.88	1
22	3-methylheptane	2.97	1
23	2,2,4-trimethylpentane	2.89	1
24	2,3,4-trimethylpentane	2.56	1
25	n-nonane	3.13	1
26	2,2,5-trimethylhexane	2.93	1
27	n-decane	3.16	1
28	cyclopropane	0.75	1
29	cyclopentane	1.20	1
30	methylcyclopentane	1.59	1
31	n-propylcyclopentane	2.13	1
32	n-pentylcyclopentane	2.55	1
33	cyclohexane	1.23	1
34	methylcyclohexane	1.70	1
35	cis-1,2-dimethylcyclohexane	1.58	1
36	trans-1,4-dimethylcyclohexane	2.11	1
37	ethene	1.28	1
38	propene	1.32	1
39	but-1-ene	1.38	1

40	pent-1-ene	1.68	1
41	(Z)-pent-2-ene	1.31	1
42	3-methyl-but-1-ene	1.83	1
43	2-methyl-but-2-ene	1.31	1
44	hex-1-ene	1.58	1
45	2-methylpent-1-ene	1.47	1
46	hept-1-ene	1.66	1
47	(E)-hept-2-ene	1.68	1
48	oct-1-ene	1.92	1
49	non-1-ene	2.06	1
50	buta-1,3-diene	0.61	1
51	2-methylbuta-1,3-diene	0.68	1
52	2,3-dimethylbuta-1,3-diene	0.40	1
53	penta-1,4-diene	0.93	1
54	hexa-1,5-diene	1.01	1
55	cyclopentene	0.56	1
56	cyclohexene	0.37	1
57	1-methylcyclohexene	0.67	1
58	cyclohepta-1,3,5-triene	-0.99	1
59	propyne	-0.48	1
60	but-1-yne	-0.16	1
61	pent-1-yne	0.01	1
62	hex-1-yne	0.29	1
63	hept-1-yne	0.60	1
64	oct-1-yne	0.71	1
65	tetrafluoromethane	3.12	1
66	chloromethane	-0.55	1
67	dichloromethane	-1.31	1
68	trichloromethane	-1.08	1
69	tetrachloromethane	0.08	1
70	chloroethane	-0.63	1
71	1,1-dichloroethane	-0.84	1
72	1,2-dichloroethane	-1.79	1
73	1,1,1-trichloroethane	-0.19	1
74	1,1,2-trichloroethane	-1.99	1
75	1,1,2,2-tetrachloroethane	-2.47	1
76	1,1,1,2-tetrachloroethane	-1.28	1
77	pentachloroethane	-1.39	1
78	1-chloropropane	-0.33	1
79	2-chloropropane	-0.25	1
80	1,2-dichloropropane	-1.27	1
81	1,3-dichloropropane	-1.89	1
82	1-chlorobutane	-0.16	1
83	2-chlorobutane	0.00	1
84	2-chloro-2-methylpropane	1.09	1
85	1,4-dichlorobutane	-2.32	1
86	1-chloropentane	-0.07	1
87	1-chlorohexane	0.00	1
88	1-chloroheptane	0.29	1
89	1,1-dichloroethene	0.25	1
90	(Z)-1,2-dichloroethene	-1.17	1
91	(E)-1,2-dichloroethene	-0.78	1
92	trichloroethene	-0.44	1
93	tetrachloroethene	0.10	1
94	3-chloroprop-1-ene	-0.57	1
95	bromomethane	-0.82	1
96	dibromomethane	-1.96	1
97	tribromomethane	-2.13	1
98	bromoethane	-0.74	1
99	1,2-dibromoethane	-2.33	1

100	1-bromopropane	-0.56	1
101	2-bromopropane	-0.48	1
102	1-bromobutane	-0.40	1
103	1-bromo-2-methylpropane	-0.03	1
104	2-bromo-2-methylpropane	0.84	1
105	1-bromopentane	-0.10	1
106	1-bromohexane	0.18	1
107	1-bromoheptane	0.34	1
108	1-bromooctane	0.52	1
109	iodomethane	-0.89	1
110	iodoethane	-0.74	1
111	1-iodopropane	-0.53	1
112	1-iodobutane	-0.25	1
113	1-iodopentane	-0.14	1
114	1-iodohexane	0.08	1
115	1-iodoheptane	0.27	1
116	halothane	-0.11	1
117	teflurane	0.50	1
118	diethyl_ether	-1.59	1
119	di-n-propyl_ether	-1.16	1
120	diisopropyl_ether	-0.53	1
121	di-n-butyl_ether	-0.83	1
122	methoxyflurane	-1.12	1
123	isoflurane	0.10	1
124	tetrahydrofuran	-3.47	1
125	2-methyltetrahydrofuran	-3.30	1
126	2,5-dimethyltetrahydrofuran	-2.92	1
127	tetrahydropyran	-3.12	1
128	1,4-dioxane	-5.06	1
129	isobutyraldehyde	-2.86	1
130	formaldehyde	-2.75	1
131	acetaldehyde	-3.50	1
132	propionaldehyde	-3.43	1
133	butyraldehyde	-3.18	1
134	pentanal	-3.03	1
135	hexanal	-2.81	1
136	heptanal	-2.67	1
137	octanal	-2.29	1
138	nonanal	-2.07	1
139	(E)-but-2-enal	-4.22	1
140	(E)-hex-2-enal	-3.68	1
141	(E)-oct-2-enal	-3.43	1
142	propanone	-3.80	1
143	butanone	-3.71	1
144	pentan-2-one	-3.52	1
145	pentan-3-one	-3.41	1
146	3-methylbutan-2-one	-3.24	1
147	hexan-2-one	-3.28	1
148	4-methylpentan-2-one	-3.05	1
149	heptan-2-one	-3.04	1
150	heptan-4-one	-2.92	1
151	octan-2-one	-2.88	1
152	nonan-2-one	-2.49	1
153	nonan-5-one	-2.64	1
154	decan-2-one	-2.34	1
155	undecan-2-one	-2.15	1
156	cyclopentanone	-4.70	1
157	cyclohexanone	-4.91	1
158	methyl_formate	-2.78	1
159	ethyl_formate	-2.56	1

160	n-propyl_formate	-2.48	1
161	isopropyl_formate	-2.02	1
162	isobutyl_formate	-2.22	1
163	isoamyl_formate	-2.13	1
164	methyl_acetate	-3.13	1
165	ethyl_acetate	-2.94	1
166	n-propyl_acetate	-2.79	1
167	isopropyl_acetate	-2.64	1
168	n-butyl_acetate	-2.64	1
169	isobutyl_acetate	-2.36	1
170	n-pentyl_acetate	-2.51	1
171	isoamyl_acetate	-2.21	1
172	n-hexyl_acetate	-2.26	1
173	methyl_propanoate	-2.93	1
174	ethyl_propanoate	-2.68	1
175	n-propyl_propanoate	-2.44	1
176	n-pentyl_propanoate	-2.11	1
177	methyl_butanoate	-2.83	1
178	ethyl_butanoate	-2.49	1
179	n-propyl_butyrate	-2.28	1
180	methyl_pentanoate	-2.56	1
181	ethyl_pentanoate	-2.49	1
182	methyl_hexanoate	-2.49	1
183	ethyl_hexanoate	-2.23	1
184	isobutyl_isobutanoate	-1.69	1
186	propanenitrile	-3.84	1
187	butanenitrile	-3.64	1
188	pentanenitrile	-3.52	1
189	ammonia	-4.29	1
190	methylamine	-4.55	1
191	ethylamine	-4.50	1
192	n-propylamine	-4.39	1
193	n-butylamine	-4.24	1
194	n-pentylamine	-4.09	1
195	n-hexylamine	-3.95	1
196	n-heptylamine	-3.79	1
197	n-octylamine	-3.65	1
198	cyclohexylamine	-4.59	1
199	dimethylamine	-4.29	1
200	diethylamine	-4.07	1
201	di-n-propylamine	-3.65	1
202	diisopropylamine	-3.22	1
203	di-n-butylamine	-3.24	1
204	trimethylamine	-3.20	1
205	triethylamine	-3.22	1
206	nitromethane	-4.02	1
207	nitroethane	-3.71	1
208	1-nitropropane	-3.34	1
209	2-nitropropane	-3.13	1
210	1-nitrobutane	-3.09	1
211	1-nitropentane	-2.82	1
212	n-butylacetamide	-9.31	1
213	N,N-dimethylformamide	-7.81	1
214	acetic_acid	-6.69	1
215	propanoic_acid	-6.46	1
216	butanoic_acid	-6.35	1
217	pentanoic_acid	-6.16	1
218	3-methylbutanoic_acid	-6.09	1
219	hexanoic_acid	-6.21	1
221	methanol	-5.10	1

222	ethanol	-5.00	1
223	propan-1-ol	-4.85	1
224	propan-2-ol	-4.74	1
225	butan-1-ol	-4.72	1
226	2-methylpropan-1-ol	-4.50	1
227	butan-2-ol	-4.62	1
228	2-methylpropan-2-ol	-4.47	1
229	pentan-1-ol	-4.57	1
230	pentan-2-ol	-4.39	1
231	pentan-3-ol	-4.35	1
232	2-methylbutan-1-ol	-4.42	1
233	3-methylbutan-1-ol	-4.42	1
234	2-methylbutan-2-ol	-4.43	1
235	hexan-1-ol	-4.40	1
236	hexan-3-ol	-4.06	1
237	2-methylpentan-2-ol	-3.92	1
238	4-methylpentan-2-ol	-3.73	1
239	2-methylpentan-3-ol	-3.88	1
240	heptan-1-ol	-4.21	1
241	octan-1-ol	-4.09	1
242	nonan-1-ol	-3.88	1
243	decan-1-ol	-3.64	1
244	cyclopentanol	-5.49	1
245	cyclohexanol	-5.46	1
246	cycloheptanol	-5.48	1
247	prop-2-en-1-ol	-5.03	1
248	2-methoxyethanol	-6.76	1
249	2-ethoxyethanol	-6.69	1
250	2-propoxyethanol	-6.40	1
251	2-butoxyethanol	-6.25	1
252	2,2,2-trifluoroethanol	-4.31	1
253	hexafluoropropene	-3.76	1
254	ethanethiol	-1.14	1
255	n-propanethiol	-1.06	1
256	n-butanethiol	-0.99	1
257	diethyl_sulfide	-1.46	1
258	di-n-propyl_sulfide	-1.28	1
259	di-isopropyl_sulfide	-1.21	1
260	diethyl_disulfide	-1.64	1
262	triethyl_phosphate	-7.54	1
263	N-methylpiperidine	-3.88	1
264	N-acetylpyrrolidine	-9.80	1
265	morpholine	-7.17	1
266	N-methylmorpholine	-6.32	1
267	benzene	-0.86	1
268	toluene	-0.89	1
269	ethylbenzene	-0.79	1
270	o-xylene	-0.90	1
271	m-xylene	-0.83	1
272	p-xylene	-0.80	1
273	n-propylbenzene	-0.53	1
274	isopropylbenzene	-0.30	1
275	1,2,3-trimethylbenzene	-1.21	1
276	1,2,4-trimethylbenzene	-0.86	1
277	1,3,5-trimethylbenzene	-0.90	1
278	2-ethyltoluene	-1.04	1
279	4-ethyltoluene	-0.95	1
280	n-butylbenzene	-0.40	1
281	isobutylbenzene	0.16	1
282	sec-butylbenzene	-0.45	1

283	tert-butylbenzene	-0.44	1
284	4-isopropyltoluene	-0.68	1
285	n-pentylbenzene	-0.23	1
286	n-hexylbenzene	-0.04	1
287	styrene	-1.24	1
288	alpha-methylstyrene	-1.24	1
289	biphenyl	-2.66	1
290	naphthalene	-2.40	1
291	1-methylnaphthalene	-2.44	1
292	1,3-dimethylnaphthalene	-2.47	1
293	1,4-dimethylnaphthalene	-2.82	1
294	2,3-dimethylnaphthalene	-2.78	1
295	2,6-dimethylnaphthalene	-2.63	1
296	1-ethylnaphthalene	-2.40	1
297	indane	-1.46	1
298	acenaphthene	-3.15	1
299	fluorene	-3.35	1
300	fluorobenzene	-0.80	1
301	benzotrifluoride	-0.25	1
302	chlorobenzene	-1.12	1
303	1,2-dichlorobenzene	-1.36	1
304	1,3-dichlorobenzene	-0.98	1
305	1,4-dichlorobenzene	-1.01	1
306	1,2,3-trichlorobenzene	-1.24	1
307	1,2,4-trichlorobenzene	-1.12	1
308	1,3,5-trichlorobenzene	-0.78	1
309	1,2,3,4-tetrachlorobenzene	-1.34	1
310	1,2,3,5-tetrachlorobenzene	-1.62	1
311	1,2,4,5-tetrachlorobenzene	-1.34	1
312	2-chlorotoluene	-1.14	1
313	bromobenzene	-1.46	1
314	4-bromotoluene	-1.39	1
315	iodobenzene	-1.74	1
316	anisole	-2.45	1
317	ethyl_phenyl_ether	-2.22	1
318	benzaldehyde	-4.02	1
319	4-methylbenzaldehyde	-4.27	1
320	acetophenone	-4.58	1
321	4-methylacetophenone	-4.70	1
322	methyl_benzoate	-3.92	1
323	ethyl_benzoate	-3.64	1
324	benzonitrile	-4.21	1
325	o-toluidine	-5.53	1
326	p-toluidine	-5.57	1
327	2,6-dimethylaniline	-5.21	1
328	2-chloroaniline	-4.91	1
329	3-chloroaniline	-5.82	1
330	4-chloroaniline	-5.90	1
331	2-methoxyaniline	-6.12	1
332	3-methoxyaniline	-7.29	1
333	4-methoxyaniline	-7.48	1
334	2-nitroaniline	-7.37	1
335	3-nitroaniline	-8.84	1
336	4-nitroaniline	-10.27	1
337	1-naphthylamine	-7.28	1
338	2-naphthylamine	-7.47	1
339	N-methylaniline	-4.69	1
340	N,N-dimethylaniline	-3.45	1
341	nitrobenzene	-4.12	1
342	2-nitrotoluene	-3.58	1

343	3-nitrotoluene	-3.45	1
344	benzamide	-11.00	1
345	phenol	-6.61	1
346	o-cresol	-5.87	1
347	p-cresol	-6.13	1
348	2,3-dimethylphenol	-6.16	1
349	2,4-dimethylphenol	-6.01	1
350	2,5-dimethylphenol	-5.91	1
351	2,6-dimethylphenol	-5.26	1
352	3,4-dimethylphenol	-6.50	1
353	3,5-dimethylphenol	-6.27	1
354	3-ethylphenol	-6.25	1
355	4-ethylphenol	-6.13	1
356	4-n-propylphenol	-5.90	1
357	4-tert-butylphenol	-5.91	1
358	2-fluorophenol	-5.29	1
359	4-fluorophenol	-6.19	1
360	2-chlorophenol	-4.55	1
361	3-chlorophenol	-6.62	1
362	4-chlorophenol	-7.03	1
363	4-chloro-3-methylphenol	-6.79	1
364	4-bromophenol	-7.13	1
365	2-iodophenol	-6.20	1
366	2-methoxyphenol	-5.57	1
367	3-methoxyphenol	-7.66	1
368	3-hydroxybenzaldehyde	-9.50	1
369	4-hydroxybenzaldehyde	-8.83	1
370	3-cyanophenol	-9.65	1
371	4-cyanophenol	-10.17	1
372	2-nitrophenol	-4.58	1
373	3-nitrophenol	-9.62	1
374	4-nitrophenol	-10.64	1
375	1-naphthol	-7.67	1
376	2-naphthol	-8.11	1
377	benzyl_alcohol	-6.62	1
378	2-phenylethanol	-6.79	1
379	3-phenylpropanol	-6.92	1
380	thiophenol	-2.55	1
381	phenyl_methyl_sulfide	-2.73	1
382	pyridine	-4.69	1
383	2-methylpyridine	-4.63	1
384	3-methylpyridine	-4.77	1
385	4-methylpyridine	-4.93	1
386	2,3-dimethylpyridine	-4.82	1
387	2,4-dimethylpyridine	-4.86	1
388	2,5-dimethylpyridine	-4.72	1
389	2,6-dimethylpyridine	-4.59	1
390	3,4-dimethylpyridine	-5.22	1
391	3,5-dimethylpyridine	-4.84	1
392	2-ethylpyridine	-4.33	1
393	3-ethylpyridine	-4.59	1
394	4-ethylpyridine	-4.73	1
395	2-chloropyridine	-4.39	1
396	3-chloropyridine	-4.01	1
397	3-cyanopyridine	-6.75	1
398	4-cyanopyridine	-6.02	1
399	3-formylpyridine	-7.10	1
400	4-formylpyridine	-7.00	1
401	3-acetylpyridine	-8.26	1
402	4-acetylpyridine	-7.62	1

403	quinoline	-5.72	1
404	2-methylpyrazine	-5.51	1
405	2-ethylpyrazine	-5.45	1
406	2-isobutylpyrazine	-5.04	1
407	thiophene	-1.42	1
408	2-methylthiophene	-1.38	1
409	dimethyl_ether	-1.91	1
410	methyl_ethyl_ether	-2.10	1
411	methyl-tert-butyl_ether	-2.21	1
412	3,3-dimethylbutan-2-one	-3.11	1
413	2,4-dimethylpentan-3-one	-2.74	1
414	methyl_cyclopropyl_ketone	-4.61	1
415	methyl_cyclohexyl_ketone	-3.90	1
416	methyl.trimethylacetate	-2.40	1
417	methyl_cyclopropanecarboxylate	-4.10	1
418	methyl_cyclohexanecarboxylate	-3.30	1
419	dimethyl_sulfide	-1.61	1
420	methyl_ethyl_sulfide	-1.50	1
422	4-methoxyacetophenone	-4.40	1
424	anthracene	-3.95	1
425	phenanthrene	-3.88	1
426	pyrene	-4.52	1
500	2-methylpropene	1.16	1
502	1,2-ethanediol	-9.30	1
503	m-cresol	-5.49	1
504	methyl-propyl-ether	-1.66	1
505	methyl-isopropyl-ether	-2.01	1
506	1,2-dimethoxyethane	-4.84	1
507	methyl-octanoate	-2.04	1
509	azetidine	-5.56	1
510	pyrrolidine	-5.48	1
511	piperazine	-7.40	1
512	N-methylpiperazine	-7.77	1
513	piperidine	-5.11	1
514	aniline	-5.49	1
515	ethanamide	-9.71	1
516	N-methylacetamide	-10.00	1
517	2-methoxyethanamine	-6.55	1
518	hydrazine	-9.30	1
519	methanethiol	-1.24	1
520	hydrogen_sulfide	-0.70	1
521	dimethyl-disulfide	-1.83	1
522	fluoromethane	-0.22	1
523	1,1-difluoroethane	-0.11	1
524	chloroethylene	-0.59	1
525	p-dibromobenzene	-2.30	1
526	diiodomethane	-2.49	1
527	2-iodopropane	-0.46	1
528	bromotrifluoromethane	1.79	1
529	chlorofluoromethane	-0.77	1
530	chlorodifluoromethane	-0.50	1
531	1-bromo-2-chloroethane	-1.95	1
532	1-chloro-2,2,2-trifluoroethane	0.06	1
533	1,1,2-trichloro-1,2,2-trifluoroethane	1.77	1
534	1,1,1-trifluoropropan-2-ol	-4.16	1
535	1H-imidazole	-9.63	1
536	1H-pyrrole	-4.78	1
537	1-methyl-pyrrole	-2.89	1
538	1-methyl-imidazole	-8.41	1
600	2-methylbut-2-ene	1.31	2

601	3-methylbut-1-ene	1.82	2
602	acetonitrile	-3.88	2
610	3-methyl-1h-indole	-5.88	3
611	4-methyl-1h-imidazole	-10.27	3
701	diethyl_succinate	-5.71	4
702	1,2-diacetoxyethane	-6.34	4
704	methyl_t-butyl_ether	-2.21	4
705	1,1-diethoxyethane	-3.28	4
706	diethyl_malonate	-6.00	4
707	1,1-diacetoxyethane	-4.97	4
708	methyl_trifluoroacetate	-1.10	5
711	N,N'-dimethyl_piperazine	-7.58	4
712	methyl_chloroacetate	-4.00	6
714	methyl_p-nitrobenzoate	-6.88	7
716	dimethoxymethane	-2.93	8
717	bis(2-chloroethyl)_ether	-4.23	4
718	m-bis(trifluoromethyl)_benzene	1.07	4
719	benzyl_chloride	-1.93	4
720	2,2,2-trifluoroethanol	-4.31	9
721	benzyl_bromide	-2.38	4
722	1,1,1-trifluoro-2,2,2-trimethoxyethane	-0.80	5
723	1,1,1-trimethoxyethane	-4.42	10
724	2-methoxy-1,1,1-trimethoxyethane	-5.73	6
725	2-chloro-1,1,1-trimethoxyethane	-4.59	6
726	1,2-diethoxyethane	-3.54	8
728	trimethoxy_methane	-4.42	9
729	methyl_p-methoxybenzoate	-5.33	7
730	phenyl_trifluoroethyl_ether	-1.29	11
731	N-methyl-N-(2,2,2-trifluoroethyl)-aniline	-1.92	12
732	trimethoxymethylbenzene	-4.04	6
733	N,N-dimethylbenzamide	-9.29	7
734	N,N-dimethyl_p-nitrobenzamide	-11.95	7
735	triacetyl_glycerol	-8.84	4
736	phenyl_formate	-3.82	13
738	N,N-dimethyl-p-methylbenzamide	-9.76	7
739	N,N-dimethyl-p-methoxybenzamide	-11.01	7
740	diethoxymethoxybenzene	-5.23	14
743	dimethyl_sulfoxide	-8.71	15
744	methanesulfonyl_chloride	-4.87	16
745	dimethyl_sulfone	-10.08	17,18,19
746	methyl_methanesulfonate	-4.87	16
747	dimethyl_sulfate	-5.10	20
749	methyl_cyanoacetate	-6.72	6
750	3,3,3-trimethoxypropionitrile	-6.40	6
751	cyanobenzene	-4.10	21
752	trimethyl_phosphate	-8.70	22

Compound	$T\Delta S$ (kcal/mol)	Num. rot. bonds
4-nitroaniline	0.50	1
2-ethoxyethanol	0.86	3
dimethoxymethane	0.65	2
3-phenylpropanol	0.59	3
2-nitrophenol	1.38	1
1,1-diethoxyethane	0.59	4
trimethyl phosphate	0.60	3
methyl formate	0.50	1
2-nitroaniline	0.96	1
1,2-ethanediol	0.63	1
1,2-diacetoxyethane	0.70	5
2-methoxyethanol	0.83	2
2-phenylethanol	0.71	2
triacetyl glycerol	2.33	5
2-propoxyethanol	0.95	4
2-butoxyethanol	0.88	5
N-methylpiperidine	1.29	0

TABLE 2: Molecules with $T\Delta S$ of hydration larger than 0.5 kcal/mol. The solute entropic component of hydration, $T\Delta S$, is shown, along with the number of rotatable bonds.

TABLE 3: Comparison of results with experimental hydration free energies (Expt. column) using the full free energy scheme (ΔG) and different single conformation schemes using IGB=5.

Molecule name	Expt. (kcal/mol)	ΔG (kcal/mol)	Best solv. (kcal/mol)	Best vac. (kcal/mol)	Range (kcal/mol)
2-methylpentan-2-ol	-3.92	-2.67±0.00	-2.76±0.14	-2.38±0.08	-3.70±0.04 to -1.70±0.05
nitroethane	-3.71	-9.78±0.01	-9.95±0.04	-9.49±0.13	-11.58±0.12 to -8.31±0.10
tetrahydrofuran	-3.47	-1.32±0.00	-1.33±0.05	-1.35±0.04	-1.97±0.05 to -0.80±0.02
N-methylmorpholine	-6.32	-2.21±0.01	-2.36±0.13	-2.05±0.15	-3.63±0.14 to -1.09±0.09
3,3-dimethylbutan-2-one	-3.11	-4.16±0.00	-4.30±0.05	-4.08±0.07	-5.01±0.03 to -3.41±0.04
acetaldehyde	-3.50	-6.08±0.00	-6.18±0.03	-5.99±0.04	-6.92±0.03 to -5.29±0.05
N-acetylpyrrolidine	-9.80	-7.27±0.00	-7.37±0.12	-7.03±0.10	-8.63±0.06 to -6.21±0.03
ethyl pentanoate	-2.49	-4.46±0.00	-4.61±0.04	-4.35±0.10	-5.79±0.23 to -3.44±0.05
di-n-butyl ether	-0.83	0.47±0.00	0.41±0.09	0.65±0.07	-0.40±0.04 to 1.23±0.04
acetic acid	-6.69	-7.69±0.15	-10.89±2.01	-7.27±0.10	-12.53±1.81 to -6.20±0.10
dimethylamine	-4.29	-3.21±0.00	-3.16±0.07	-2.90±0.08	-4.71±0.06 to -2.25±0.06
1,4-dioxane	-5.06	-3.55±0.00	-3.57±0.02	-3.45±0.04	-4.45±0.02 to -2.62±0.07
di-n-propylamine	-3.65	-0.40±0.02	-0.56±0.14	-0.31±0.11	-1.94±0.07 to 0.71±0.07
1,1-difluoroethane	-0.11	-2.03±0.00	-2.07±0.04	-2.02±0.04	-2.58±0.02 to -1.54±0.01
2-methoxyphenol	-5.57	-6.09±0.01	-6.53±0.18	-5.95±0.14	-12.13±0.05 to -4.79±0.06
methyl-octanoate	-2.04	-4.46±0.00	-4.49±0.11	-4.32±0.14	-5.71±0.04 to -3.56±0.04
1-bromo-2-chloroethane	-1.95	-2.06±0.01	-2.66±0.07	-1.43±0.02	-3.34±0.03 to -1.18±0.01
hex-1-ene	1.58	1.35±0.00	1.34±0.01	1.36±0.01	1.18±0.00 to 1.48±0.00
m-xylene	-0.83	-1.16±0.00	-1.17±0.02	-1.12±0.02	-1.34±0.01 to -0.97±0.01
ammonia	-4.29	-7.24±0.00	-7.49±0.02	-6.95±0.03	-9.48±0.05 to -5.71±0.06
1,2,4,5-tetrachlorobenzene	-1.34	0.47±0.00	0.46±0.01	0.46±0.01	0.34±0.01 to 0.62±0.01
decan-1-ol	-3.64	-2.66±0.00	-2.78±0.08	-2.69±0.07	-3.41±0.03 to -1.78±0.09
1,1,1-trifluoropropan-2-ol	-4.16	-5.53±0.00	-5.78±0.15	-4.97±0.15	-8.80±0.06 to -3.92±0.07
pent-1-ene	1.68	1.18±0.00	1.17±0.01	1.18±0.02	1.01±0.01 to 1.31±0.01
ethyl benzoate	-3.64	-6.74±0.01	-6.71±0.09	-6.77±0.13	-7.88±0.04 to -5.80±0.03
1-chlorohexane	0.00	0.47±0.00	0.50±0.01	0.53±0.02	0.16±0.03 to 0.73±0.01
2,3,4-trimethylpentane	2.56	2.46±0.00	2.48±0.00	2.47±0.01	2.39±0.00 to 2.52±0.00
4-cyanophenol	-10.17	-9.89±0.00	-9.72±0.06	-9.74±0.05	-10.95±0.02 to -9.15±0.03
nonan-2-one	-2.49	-3.92±0.01	-3.89±0.08	-3.87±0.06	-4.69±0.03 to -3.11±0.04
fluorene	-3.35	-4.22±0.00	-4.24±0.03	-4.24±0.03	-4.58±0.02 to -3.93±0.01
4-bromotoluene	-1.39	-1.54±0.00	-1.58±0.03	-1.50±0.03	-1.78±0.02 to -1.31±0.01
ethanethiol	-1.14	-1.44±0.00	-1.46±0.02	-1.42±0.04	-1.84±0.01 to -1.11±0.01

2-methylbutan-2-ol	-4.43	-2.96±0.01	-3.06±0.11	-2.79±0.09	-3.91±0.04 to -2.03±0.06
1-chloropropane	-0.33	-0.01±0.00	-0.05±0.02	0.04±0.03	-0.28±0.01 to 0.24±0.01
1,4-dichlorobutane	-2.32	-1.64±0.00	-1.73±0.10	-1.49±0.15	-2.65±0.05 to -0.97±0.02
1,2,3-trimethylbenzene	-1.21	-0.90±0.00	-0.93±0.01	-0.88±0.01	-1.14±0.01 to -0.67±0.01
n-pentyl acetate	-2.51	-4.78±0.00	-4.79±0.03	-4.76±0.10	-5.95±0.08 to -3.81±0.03
dimethyl sulfone	-10.08	-12.30±0.01	-12.69±0.13	-11.98±0.18	-14.79±0.04 to -10.60±0.06
1,1,2,2-tetrachloroethane	-2.47	-1.81±0.01	-2.16±0.02	-1.28±0.02	-2.83±0.02 to -1.03±0.01
methyl p-nitrobenzoate	-6.88	-14.76±0.01	-14.97±0.09	-14.34±0.08	-17.46±0.14 to -13.27±0.12
1,2-dichloropropane	-1.27	-1.41±0.01	-1.67±0.06	-0.97±0.31	-2.38±0.02 to -0.33±0.01
1,2,3,4-tetrachlorobenzene	-1.34	0.29±0.00	0.28±0.01	0.29±0.01	0.09±0.01 to 0.51±0.02
ethyl butanoate	-2.49	-4.66±0.01	-4.62±0.10	-4.54±0.09	-5.76±0.05 to -3.66±0.07
isobutylbenzene	0.16	-0.83±0.00	-0.83±0.01	-0.84±0.01	-1.08±0.02 to -0.59±0.02
isobutyl isobutanoate	-1.69	-3.87±0.00	-3.89±0.02	-3.56±0.06	-5.03±0.08 to -2.97±0.05
3-chloroaniline	-5.82	-6.11±0.00	-6.09±0.06	-6.11±0.05	-7.44±0.09 to -5.28±0.04
3-methylbutanoic acid	-6.09	-6.25±0.15	-7.93±1.57	-6.17±0.07	-9.50±1.36 to -4.80±0.05
4-nitroaniline	-10.27	-15.01±0.00	-15.18±0.21	-14.51±0.12	-17.50±0.08 to -13.54±0.08
3-methylhexane	2.71	2.34±0.00	2.34±0.00	2.35±0.01	2.26±0.00 to 2.39±0.00
nitrobenzene	-4.12	-9.90±0.01	-9.91±0.12	-9.56±0.06	-12.05±0.16 to -8.64±0.04
butanoic acid	-6.35	-6.47±0.00	-6.44±0.05	-6.33±0.08	-8.44±0.08 to -5.19±0.04
2-ethoxyethanol	-6.69	-4.43±0.01	-4.71±0.47	-3.97±0.17	-9.13±0.05 to -3.06±0.06
benzamide	-11.00	-11.00±0.00	-11.27±0.17	-10.61±0.15	-12.65±0.10 to -9.60±0.05
bromobenzene	-1.46	-1.96±0.00	-1.97±0.01	-1.98±0.02	-2.19±0.01 to -1.74±0.01
2,6-dimethylaniline	-5.21	-5.42±0.00	-5.36±0.06	-5.20±0.07	-6.65±0.06 to -4.56±0.03
tetrahydropyran	-3.12	-0.68±0.02	-0.79±0.05	-0.75±0.05	-1.36±0.04 to -0.13±0.00
n-butyl acetate	-2.64	-4.96±0.00	-5.09±0.06	-4.95±0.07	-6.11±0.07 to -4.03±0.02
diisopropyl ether	-0.53	0.14±0.00	0.15±0.07	0.15±0.07	-0.84±0.05 to 0.93±0.05
n-propyl formate	-2.48	-6.38±0.00	-6.62±0.06	-6.28±0.09	-7.49±0.06 to -5.41±0.04
ethyl propanoate	-2.68	-4.96±0.00	-4.98±0.07	-4.81±0.07	-5.97±0.04 to -3.97±0.03
p-dibromobenzene	-2.30	-1.50±0.00	-1.51±0.04	-1.52±0.02	-1.78±0.01 to -1.23±0.01
n-propyl butyrate	-2.28	-4.32±0.00	-4.37±0.06	-4.14±0.09	-5.42±0.03 to -3.44±0.03
1,1,1-trichloroethane	-0.19	-0.06±0.00	-0.04±0.01	-0.07±0.01	-0.36±0.02 to 0.20±0.01
2-iodophenol	-6.20	-5.38±0.01	-5.24±0.11	-5.17±0.03	-10.03±0.03 to -4.40±0.03
2,3-dimethylbuta-1,3-diene	0.40	0.37±0.00	0.34±0.02	0.27±0.01	0.05±0.01 to 0.70±0.01
pyrrolidine	-5.48	-1.99±0.01	-2.19±0.09	-1.79±0.12	-3.38±0.03 to -1.00±0.06
2-methyl-but-2-ene	1.31	1.17±0.00	1.18±0.02	1.18±0.01	1.03±0.01 to 1.33±0.01
2,3-dimethylpentane	2.52	2.32±0.00	2.32±0.00	2.32±0.00	2.24±0.00 to 2.37±0.00
p-cresol	-6.13	-6.14±0.00	-6.04±0.03	-6.06±0.17	-7.11±0.03 to -5.46±0.03
2-chloro-1,1,1-trimethoxyethane	-4.59	-4.08±0.01	-4.61±0.33	-3.40±0.07	-7.05±0.13 to -2.52±0.07
1-bromo-2-methylpropane	-0.03	-0.12±0.01	-0.15±0.03	-0.16±0.02	-0.41±0.02 to 0.14±0.01
4-cyanopyridine	-6.02	-8.31±0.00	-8.35±0.03	-8.22±0.06	-9.16±0.05 to -7.54±0.02
toluene	-0.89	-1.60±0.00	-1.62±0.01	-1.61±0.01	-1.75±0.01 to -1.45±0.00
2,2-dimethylpentane	2.88	2.33±0.00	2.34±0.01	2.34±0.01	2.25±0.00 to 2.38±0.00
1,2,4-trimethylbenzene	-0.86	-0.79±0.00	-0.79±0.02	-0.80±0.02	-1.01±0.01 to -0.57±0.01
1-chloro-2,2,2-trifluoroethane	0.06	-3.13±0.00	-3.22±0.03	-3.11±0.04	-4.06±0.04 to -2.49±0.05
3-nitrophenol	-9.62	-13.95±0.01	-13.97±0.14	-13.73±0.10	-16.28±0.11 to -12.73±0.04
dimethoxymethane	-2.93	-3.75±0.02	-4.53±0.73	-3.09±0.09	-7.85±0.10 to -2.51±0.03
non-1-ene	2.06	1.81±0.00	1.80±0.02	1.86±0.01	1.64±0.00 to 1.95±0.01
propionaldehyde	-3.43	-5.48±0.00	-5.50±0.05	-5.36±0.07	-6.37±0.06 to -4.76±0.04
cyclohexanol	-5.46	-3.16±0.00	-3.07±0.17	-2.86±0.13	-4.11±0.04 to -2.37±0.01
2,3-dimethylpyridine	-4.82	-4.39±0.00	-4.37±0.05	-4.31±0.09	-5.28±0.03 to -3.70±0.03
3-methyl-1h-indole	-5.88	-5.93±0.00	-6.04±0.02	-5.96±0.02	-6.33±0.01 to -5.46±0.03
2-methylpropene	1.16	0.97±0.00	0.97±0.01	0.97±0.01	0.82±0.00 to 1.09±0.00
diethyl malonate	-6.00	-9.41±0.01	-9.61±0.24	-8.90±0.15	-11.88±0.04 to -8.06±0.07
1-naphthylamine	-7.28	-8.04±0.00	-8.17±0.06	-7.84±0.10	-9.31±0.05 to -7.13±0.05
Z-1,2-dichloroethene	-1.17	-1.24±0.00	-1.25±0.02	-1.21±0.02	-1.55±0.01 to -0.95±0.02
but-1-ene	1.38	0.99±0.00	0.99±0.02	1.00±0.01	0.83±0.01 to 1.13±0.00
trans-1,4-dimethylcyclohexane	2.11	2.39±0.00	2.39±0.00	2.40±0.01	2.32±0.00 to 2.45±0.00
4-n-propylphenol	-5.90	-5.59±0.00	-5.42±0.05	-5.44±0.04	-6.59±0.01 to -4.92±0.02
2-methoxyethanamine	-6.55	-5.87±0.01	-5.76±0.07	-5.58±0.13	-9.84±0.05 to -4.60±0.02
dimethyl sulfoxide	-8.71	-8.49±0.00	-8.81±0.11	-8.22±0.10	-9.92±0.03 to -7.20±0.03
n-butylbenzene	-0.40	-0.88±0.00	-0.86±0.01	-0.87±0.01	-1.07±0.00 to -0.67±0.02

3-phenylpropanol	-6.92	-6.09±0.02	-6.66±0.11	-4.49±0.10	-7.98±0.11 to -4.09±0.04
propan-2-ol	-4.74	-3.65±0.00	-4.00±0.06	-3.32±0.10	-4.73±0.02 to -2.79±0.04
1-nitropropane	-3.34	-9.17±0.01	-9.40±0.16	-8.80±0.17	-10.90±0.05 to -7.80±0.08
m-bis(trifluoromethyl) benzene	1.07	-5.33±0.00	-5.46±0.06	-5.37±0.04	-6.24±0.06 to -4.64±0.01
3-methylbut-1-ene	1.82	1.17±0.00	1.17±0.01	1.16±0.01	1.01±0.01 to 1.32±0.00
1-bromoheptane	0.34	0.37±0.00	0.35±0.04	0.39±0.04	0.07±0.01 to 0.65±0.03
butanone	-3.71	-5.24±0.00	-5.25±0.06	-5.26±0.05	-6.15±0.04 to -4.41±0.07
1,1,1-trimethoxyethane	-4.42	-3.59±0.00	-3.64±0.10	-3.19±0.20	-6.17±0.16 to -2.22±0.05
3-ethylpyridine	-4.59	-4.45±0.00	-4.46±0.04	-4.44±0.08	-5.19±0.02 to -3.76±0.03
anisole	-2.45	-3.71±0.00	-3.91±0.09	-3.67±0.09	-4.43±0.03 to -3.16±0.03
propane	1.96	1.78±0.00	1.78±0.00	1.78±0.00	1.75±0.00 to 1.80±0.00
3-chlorophenol	-6.62	-6.05±0.00	-6.90±0.03	-5.78±0.05	-7.15±0.01 to -5.22±0.01
dichloromethane	-1.31	-1.29±0.00	-1.32±0.01	-1.29±0.02	-1.66±0.02 to -0.94±0.01
2,5-dimethylphenol	-5.91	-5.12±0.02	-5.49±0.42	-4.69±0.03	-6.84±0.01 to -4.16±0.02
biphenyl	-2.66	-4.22±0.00	-4.28±0.07	-4.27±0.03	-4.75±0.01 to -3.54±0.02
nonan-1-ol	-3.88	-2.79±0.00	-3.07±0.08	-2.63±0.21	-3.92±0.08 to -1.70±0.08
methylcyclohexane	1.70	2.19±0.00	2.20±0.01	2.20±0.01	2.11±0.00 to 2.26±0.00
3,4-dimethylphenol	-6.50	-5.72±0.01	-5.71±0.19	-5.56±0.02	-6.70±0.03 to -5.01±0.04
tert-butylbenzene	-0.44	-0.86±0.00	-0.88±0.02	-0.82±0.02	-1.08±0.01 to -0.61±0.02
diethoxymethoxybenzene	-5.23	-4.75±0.00	-4.83±0.18	-4.19±0.20	-8.78±0.10 to -3.21±0.09
pent-1-yne	0.01	0.15±0.00	0.17±0.02	0.19±0.03	-0.06±0.01 to 0.33±0.01
n-butylamine	-4.24	-3.73±0.00	-3.79±0.14	-3.43±0.16	-5.49±0.04 to -2.44±0.07
1-chloropentane	-0.07	0.32±0.00	0.29±0.03	0.31±0.04	0.06±0.01 to 0.57±0.01
iodoethane	-0.74	-3.04±0.00	-3.07±0.01	-3.04±0.02	-3.44±0.01 to -2.54±0.02
1,2-dibromoethane	-2.33	-2.22±0.00	-2.69±0.05	-1.65±0.01	-3.46±0.04 to -1.42±0.02
2-nitrophenol	-4.58	-10.32±0.03	-11.47±1.40	-8.85±0.11	-17.00±0.05 to -8.30±0.06
undecan-2-one	-2.15	-3.59±0.00	-3.69±0.10	-3.59±0.10	-4.42±0.02 to -2.81±0.03
ethylbenzene	-0.79	-1.29±0.00	-1.31±0.01	-1.28±0.02	-1.47±0.01 to -1.12±0.00
2,5-dimethylpyridine	-4.72	-4.28±0.00	-4.38±0.09	-4.21±0.13	-5.13±0.07 to -3.50±0.04
n-octylamine	-3.65	-2.83±0.00	-2.83±0.17	-2.65±0.22	-4.60±0.08 to -1.46±0.11
o-xylene	-0.90	-1.25±0.00	-1.28±0.02	-1.25±0.01	-1.45±0.01 to -1.07±0.01
4-tert-butylphenol	-5.91	-5.36±0.01	-5.66±0.23	-5.17±0.05	-6.34±0.02 to -4.59±0.04
benzyl chloride	-1.93	-2.93±0.00	-3.05±0.03	-3.01±0.04	-3.38±0.01 to -2.45±0.01
n-butanethiol	-0.99	-0.99±0.00	-0.95±0.04	-0.89±0.05	-1.40±0.02 to -0.59±0.02
piperidine	-5.11	-1.48±0.04	-1.56±0.17	-1.41±0.18	-3.05±0.21 to -0.57±0.03
n-octane	2.88	2.51±0.00	2.53±0.01	2.53±0.01	2.42±0.00 to 2.58±0.00
2,2,5-trimethylhexane	2.93	2.64±0.00	2.65±0.01	2.64±0.01	2.57±0.00 to 2.70±0.00
acetophenone	-4.58	-7.07±0.00	-7.07±0.07	-6.96±0.06	-8.00±0.04 to -6.17±0.04
2-bromo-2-methylpropane	0.84	-0.58±0.00	-0.52±0.03	-0.63±0.02	-0.84±0.01 to -0.31±0.02
trimethylamine	-3.20	-1.22±0.01	-1.38±0.08	-0.93±0.11	-2.45±0.02 to -0.28±0.06
pentan-3-one	-3.41	-4.31±0.00	-4.38±0.05	-4.30±0.04	-5.12±0.02 to -3.48±0.03
n-propylbenzene	-0.53	-1.06±0.00	-1.06±0.01	-1.08±0.02	-1.27±0.01 to -0.87±0.01
cyclohexylamine	-4.59	-2.93±0.01	-3.20±0.12	-2.66±0.11	-4.70±0.06 to -1.64±0.06
butan-1-ol	-4.72	-3.63±0.00	-3.79±0.17	-3.58±0.22	-4.83±0.05 to -2.58±0.03
1,1-diethoxyethane	-3.28	-1.25±0.01	-0.96±0.23	-0.74±0.11	-4.46±0.13 to -0.08±0.03
hexanal	-2.81	-4.88±0.00	-4.92±0.07	-4.74±0.06	-5.79±0.02 to -4.18±0.01
E-hept-2-ene	1.68	1.62±0.00	1.62±0.02	1.64±0.01	1.46±0.01 to 1.75±0.01
chlorobenzene	-1.12	-1.60±0.00	-1.61±0.02	-1.62±0.01	-1.79±0.00 to -1.39±0.02
isobutyl acetate	-2.36	-4.87±0.00	-4.82±0.05	-4.70±0.06	-6.00±0.06 to -3.94±0.03
2-chlorotoluene	-1.14	-1.30±0.00	-1.32±0.02	-1.27±0.02	-1.53±0.01 to -1.08±0.01
1,2-dimethoxyethane	-4.84	-3.74±0.01	-4.66±0.26	-3.02±0.09	-6.26±0.06 to -2.33±0.06
iodomethane	-0.89	-3.22±0.00	-3.30±0.01	-3.25±0.01	-3.64±0.01 to -2.75±0.01
anthracene	-3.95	-4.91±0.00	-4.94±0.00	-4.91±0.03	-5.13±0.02 to -4.70±0.01
hexafluoropropene	-3.76	-1.92±0.00	-1.87±0.04	-1.82±0.04	-2.50±0.02 to -1.42±0.02
n-butane	2.07	1.91±0.00	1.92±0.00	1.92±0.00	1.85±0.00 to 1.95±0.00
2,4-dimethylpentane	2.83	2.33±0.00	2.34±0.00	2.33±0.01	2.28±0.00 to 2.39±0.00
2-nitropropane	-3.13	-8.74±0.01	-8.76±0.09	-8.49±0.07	-10.52±0.09 to -7.37±0.14
n-heptylamine	-3.79	-3.02±0.01	-3.44±0.22	-2.91±0.22	-4.76±0.12 to -1.79±0.04
trimethyl phosphate	-8.70	-13.47±0.01	-14.55±0.51	-12.47±0.34	-20.02±0.21 to -11.24±0.07
1-bromohexane	0.18	0.23±0.00	0.17±0.03	0.24±0.04	-0.06±0.01 to 0.52±0.02
hept-1-ene	1.66	1.50±0.00	1.47±0.02	1.52±0.01	1.34±0.01 to 1.63±0.00

dibromomethane	-1.96	-0.72±0.00	-0.75±0.01	-0.74±0.00	-1.04±0.01 to -0.43±0.02
pentan-3-ol	-4.35	-2.83±0.00	-3.19±0.12	-2.54±0.16	-4.10±0.03 to -1.83±0.07
n-propylamine	-4.39	-3.77±0.00	-3.97±0.16	-3.43±0.06	-5.70±0.10 to -2.63±0.03
n-decane	3.16	2.82±0.00	2.83±0.01	2.83±0.01	2.70±0.01 to 2.89±0.00
methyl formate	-2.78	-9.58±0.05	-12.84±0.07	-7.68±0.10	-13.98±0.04 to -7.16±0.03
teflurane	0.50	-3.65±0.00	-3.67±0.06	-3.63±0.07	-4.52±0.04 to -2.89±0.05
1,2-diethoxyethane	-3.54	-2.48±0.01	-3.17±0.16	-1.65±0.08	-4.97±0.06 to -1.04±0.05
4-chloro-3-methylphenol	-6.79	-5.84±0.00	-5.97±0.19	-5.58±0.04	-6.82±0.02 to -5.09±0.03
2-iodopropane	-0.46	-2.77±0.00	-2.81±0.05	-2.83±0.02	-3.14±0.01 to -2.31±0.02
methyl trifluoroacetate	-1.10	-5.93±0.00	-5.88±0.06	-5.80±0.07	-6.94±0.04 to -5.03±0.04
o-toluidine	-5.53	-6.12±0.00	-6.13±0.08	-6.07±0.10	-7.40±0.12 to -5.30±0.03
E-hex-2-enal	-3.68	-5.70±0.00	-5.76±0.08	-5.56±0.05	-6.57±0.03 to -4.99±0.02
2-methylthiophene	-1.38	-0.96±0.00	-0.97±0.02	-0.99±0.01	-1.13±0.01 to -0.79±0.01
buta-1,3-diene	0.61	-0.08±0.02	-0.06±0.01	-0.05±0.01	-0.33±0.05 to 0.13±0.01
methyl pentanoate	-2.56	-4.94±0.00	-5.03±0.15	-4.84±0.10	-6.10±0.05 to -4.09±0.03
2-ethyltoluene	-1.04	-0.95±0.00	-0.93±0.01	-0.93±0.03	-1.16±0.01 to -0.73±0.01
chlorofluoromethane	-0.77	-2.63±0.00	-2.65±0.02	-2.61±0.02	-3.23±0.06 to -2.14±0.02
1,4-dimethylnaphthalene	-2.82	-2.75±0.00	-2.70±0.04	-2.76±0.02	-3.00±0.01 to -2.50±0.01
1-iodohexane	0.08	-2.14±0.00	-2.19±0.04	-2.17±0.04	-2.62±0.02 to -1.63±0.02
octan-1-ol	-4.09	-2.96±0.00	-3.00±0.24	-2.65±0.10	-4.05±0.04 to -1.81±0.05
phenyl formate	-3.82	-8.99±0.02	-9.42±0.16	-8.71±0.18	-10.70±0.25 to -7.56±0.08
benzyl alcohol	-6.62	-6.18±0.01	-6.61±0.53	-5.72±0.14	-8.93±0.04 to -4.92±0.03
1,3-dichlorobenzene	-0.98	-0.94±0.00	-0.94±0.02	-0.96±0.02	-1.15±0.00 to -0.72±0.01
octan-2-one	-2.88	-4.08±0.00	-4.13±0.09	-4.15±0.12	-5.00±0.05 to -3.25±0.03
cyclopentanone	-4.70	-4.60±0.00	-4.64±0.08	-4.51±0.09	-5.37±0.04 to -3.90±0.03
sec-butylbenzene	-0.45	-0.76±0.00	-0.75±0.01	-0.77±0.02	-1.02±0.01 to -0.51±0.01
1-bromopentane	-0.10	0.08±0.00	0.03±0.05	0.06±0.05	-0.25±0.02 to 0.34±0.01
iodobenzene	-1.74	-2.34±0.00	-2.34±0.02	-2.38±0.01	-2.55±0.01 to -2.10±0.00
N-methyl-N-2,2,2-trifluoroethyl-aniline	-1.92	-6.01±0.01	-6.42±0.38	-5.53±0.19	-8.35±0.08 to -4.41±0.06
n-hexylbenzene	-0.04	-0.54±0.00	-0.59±0.02	-0.58±0.03	-0.77±0.01 to -0.25±0.02
2-chloroaniline	-4.91	-6.07±0.01	-6.14±0.06	-5.99±0.08	-7.91±0.08 to -5.06±0.04
propan-1-ol	-4.85	-3.84±0.00	-4.38±0.06	-3.50±0.06	-4.95±0.03 to -2.86±0.03
isoflurane	0.10	-6.59±0.01	-6.77±0.14	-6.29±0.17	-9.96±0.07 to -5.26±0.08
p-toluidine	-5.57	-6.30±0.00	-6.24±0.09	-6.33±0.08	-7.72±0.12 to -5.44±0.03
isopropyl acetate	-2.64	-5.03±0.00	-5.06±0.14	-4.73±0.12	-6.12±0.02 to -4.06±0.07
3-cyanophenol	-9.65	-9.34±0.00	-9.31±0.13	-9.34±0.13	-10.23±0.02 to -8.77±0.02
2-bromopropane	-0.48	-0.52±0.00	-0.52±0.03	-0.48±0.03	-0.78±0.01 to -0.27±0.01
butyraldehyde	-3.18	-5.23±0.00	-5.37±0.08	-5.18±0.09	-6.09±0.03 to -4.41±0.04
methyl acetate	-3.13	-6.03±0.00	-6.09±0.07	-5.87±0.05	-7.24±0.07 to -5.16±0.02
1-methyl-pyrrole	-2.89	-3.30±0.00	-3.34±0.02	-3.26±0.02	-3.57±0.01 to -3.03±0.01
pyrene	-4.52	-5.70±0.00	-5.77±0.03	-5.74±0.02	-5.91±0.01 to -5.49±0.01
2-methylpyridine	-4.63	-4.95±0.00	-4.93±0.05	-4.97±0.14	-5.80±0.04 to -4.12±0.07
heptanal	-2.67	-4.72±0.00	-4.67±0.10	-4.50±0.05	-5.57±0.03 to -3.92±0.07
pentachloroethane	-1.39	-0.57±0.01	-0.62±0.01	-0.56±0.03	-0.95±0.02 to -0.23±0.01
n-hexyl acetate	-2.26	-4.62±0.00	-4.57±0.15	-4.39±0.05	-5.79±0.09 to -3.73±0.05
ethyl formate	-2.56	-6.74±0.00	-7.01±0.11	-6.65±0.13	-7.94±0.07 to -5.81±0.02
4-ethylphenol	-6.13	-5.82±0.01	-5.99±0.23	-5.80±0.20	-6.78±0.01 to -5.13±0.03
2,4-dimethylpyridine	-4.86	-4.54±0.00	-4.58±0.09	-4.45±0.06	-5.37±0.04 to -3.75±0.02
methyl methanesulfonate	-4.87	-12.20±0.01	-13.46±0.32	-11.72±0.09	-16.41±0.22 to -10.47±0.04
1,1,1,2-tetrachloroethane	-1.28	-0.97±0.00	-0.89±0.04	-0.91±0.04	-1.36±0.02 to -0.59±0.02
tribromomethane	-2.13	0.41±0.00	0.40±0.01	0.41±0.01	0.25±0.01 to 0.59±0.01
hex-1-yne	0.29	0.32±0.00	0.31±0.02	0.33±0.01	0.11±0.01 to 0.49±0.01
3-hydroxybenzaldehyde	-9.50	-12.15±0.01	-12.31±0.22	-12.00±0.07	-13.94±0.02 to -11.00±0.07
3-chloroprop-1-ene	-0.57	-0.76±0.00	-0.72±0.10	-0.65±0.04	-1.22±0.01 to -0.34±0.01
n-heptane	2.67	2.36±0.00	2.38±0.00	2.37±0.01	2.28±0.01 to 2.42±0.00
ethylamine	-4.50	-4.15±0.01	-4.15±0.10	-3.77±0.10	-5.90±0.05 to -2.89±0.08
4-isopropyltoluene	-0.68	-0.56±0.00	-0.55±0.02	-0.55±0.01	-0.81±0.02 to -0.33±0.01
2-chloro-2-methylpropane	1.09	-0.11±0.00	-0.17±0.02	-0.08±0.02	-0.40±0.01 to 0.17±0.01
diethyl sulfide	-1.46	-0.67±0.00	-0.64±0.03	-0.57±0.03	-1.16±0.03 to -0.24±0.01
n-propyl propanoate	-2.44	-4.62±0.00	-4.60±0.13	-4.62±0.06	-5.70±0.08 to -3.62±0.07
2,3-dimethylphenol	-6.16	-5.67±0.00	-5.63±0.03	-5.66±0.10	-6.33±0.03 to -5.05±0.03

4-chlorophenol	-7.03	-6.19±0.01	-6.38±0.20	-6.00±0.06	-7.16±0.01 to -5.53±0.03
1-bromobutane	-0.40	-0.07±0.00	-0.08±0.02	0.01±0.01	-0.41±0.02 to 0.20±0.00
dimethyl sulfate	-5.10	-13.87±0.01	-14.22±0.24	-13.53±0.13	-17.27±0.14 to -12.26±0.05
n-pentyl propanoate	-2.11	-4.21±0.00	-4.34±0.05	-3.82±0.05	-5.34±0.04 to -3.29±0.02
3-ethylphenol	-6.25	-5.81±0.00	-6.09±0.20	-5.65±0.04	-6.76±0.01 to -5.06±0.04
3-nitroaniline	-8.84	-13.83±0.00	-13.83±0.11	-13.55±0.17	-16.36±0.07 to -12.54±0.04
propanone	-3.80	-5.30±0.00	-5.36±0.05	-5.30±0.07	-6.16±0.03 to -4.51±0.05
tetrafluoromethane	3.12	-2.27±0.00	-2.25±0.01	-2.22±0.01	-2.60±0.01 to -1.96±0.01
di-n-propyl sulfide	-1.28	-0.14±0.00	-0.15±0.04	-0.11±0.05	-0.68±0.01 to 0.31±0.02
1-methyl-imidazole	-8.41	-7.42±0.00	-7.49±0.07	-7.49±0.08	-8.33±0.03 to -6.64±0.04
ethane	1.83	1.66±0.00	1.66±0.00	1.66±0.00	1.64±0.00 to 1.68±0.00
2-chloropyridine	-4.39	-5.52±0.00	-5.51±0.08	-5.53±0.04	-6.36±0.05 to -4.74±0.04
4-hydroxybenzaldehyde	-8.83	-12.37±0.01	-12.38±0.05	-12.07±0.07	-13.75±0.06 to -11.27±0.04
halothane	-0.11	-2.46±0.00	-2.55±0.04	-2.40±0.05	-3.14±0.02 to -1.84±0.03
2-ethylpyrazine	-5.45	-8.28±0.00	-8.21±0.10	-8.25±0.08	-9.41±0.05 to -7.33±0.03
benzotrifluoride	-4.21	-5.18±0.00	-5.19±0.02	-5.16±0.02	-5.49±0.02 to -4.88±0.01
diiodomethane	-2.49	-4.54±0.00	-4.54±0.02	-4.53±0.02	-5.07±0.02 to -4.09±0.03
2-chlorophenol	-4.55	-4.86±0.01	-4.80±0.05	-4.44±0.07	-8.92±0.02 to -3.88±0.04
2-methoxyaniline	-6.12	-7.71±0.00	-7.80±0.21	-7.34±0.16	-10.20±0.12 to -6.35±0.06
chloroethane	-0.63	-0.23±0.00	-0.24±0.01	-0.25±0.01	-0.48±0.01 to -0.01±0.01
3,5-dimethylpyridine	-4.84	-4.16±0.00	-4.18±0.04	-4.25±0.08	-4.90±0.04 to -3.50±0.05
methyl trimethylacetate	-2.40	-4.65±0.00	-4.53±0.08	-4.44±0.08	-5.68±0.06 to -3.80±0.03
4-methylbenzaldehyde	-4.27	-7.39±0.00	-7.42±0.08	-7.29±0.06	-8.28±0.03 to -6.65±0.05
benzaldehyde	-4.02	-7.79±0.00	-7.78±0.11	-7.66±0.12	-8.70±0.03 to -7.04±0.03
1,4-dichlorobenzene	-1.01	-1.06±0.00	-1.07±0.02	-1.06±0.02	-1.32±0.01 to -0.79±0.02
n-pentylamine	-4.09	-3.34±0.01	-3.30±0.08	-3.05±0.09	-5.16±0.13 to -2.10±0.08
2-methylpentane	2.51	2.20±0.00	2.21±0.00	2.21±0.00	2.12±0.01 to 2.24±0.00
pentan-1-ol	-4.57	-3.44±0.00	-3.46±0.22	-2.89±0.06	-4.53±0.02 to -2.46±0.06
cyclopentanol	-5.49	-3.32±0.00	-3.25±0.12	-3.22±0.05	-4.28±0.05 to -2.43±0.05
1,2-dichloroethane	-1.79	-1.75±0.01	-2.11±0.04	-1.31±0.22	-2.88±0.03 to -0.72±0.02
1,3-dichloropropane	-1.89	-1.93±0.00	-2.02±0.12	-1.73±0.04	-3.56±0.05 to -1.29±0.03
1-chloroheptane	0.29	0.66±0.00	0.70±0.03	0.67±0.03	0.37±0.00 to 0.91±0.01
1,3,5-trichlorobenzene	-0.78	-0.00±0.00	-0.00±0.00	0.00±0.01	-0.08±0.00 to 0.07±0.00
3-methoxyaniline	-7.29	-8.37±0.00	-8.68±0.12	-8.19±0.09	-9.90±0.06 to -7.37±0.04
hexanoic acid	-6.21	-6.27±0.19	-7.60±1.44	-5.83±0.05	-9.61±1.43 to -4.77±0.09
chlorodifluoromethane	-0.50	-3.53±0.00	-3.60±0.03	-3.52±0.05	-4.29±0.03 to -2.82±0.01
1,3-dimethylnaphthalene	-2.47	-2.69±0.00	-2.69±0.03	-2.71±0.02	-2.94±0.02 to -2.46±0.01
N,N-dimethyl p-nitrobenzamide	-11.95	-16.38±0.04	-16.59±0.32	-15.90±0.35	-19.02±0.14 to -14.59±0.09
1-bromopropane	-0.56	-0.26±0.00	-0.21±0.03	-0.24±0.04	-0.57±0.01 to 0.02±0.02
2,4-dimethylpentan-3-one	-2.74	-3.65±0.00	-3.66±0.10	-3.64±0.07	-4.50±0.03 to -2.84±0.03
ethyl phenyl ether	-2.22	-3.16±0.00	-3.13±0.10	-3.04±0.05	-3.92±0.02 to -2.58±0.02
isobutyraldehyde	-2.86	-5.03±0.00	-5.12±0.07	-5.00±0.05	-5.94±0.04 to -4.26±0.02
styrene	-1.24	-2.43±0.00	-2.45±0.01	-2.42±0.02	-2.64±0.01 to -2.23±0.01
dimethyl-disulfide	-1.83	-1.29±0.00	-1.30±0.05	-1.32±0.03	-1.87±0.02 to -0.76±0.02
1H-imidazole	-9.63	-9.30±0.00	-9.27±0.05	-9.28±0.04	-10.30±0.04 to -8.47±0.05
4-methylpentan-2-one	-3.05	-4.34±0.00	-4.60±0.08	-4.29±0.07	-5.27±0.06 to -3.53±0.03
tetrachloromethane	0.08	1.05±0.00	1.06±0.00	1.06±0.00	0.97±0.00 to 1.12±0.00
diethylamine	-4.07	-1.20±0.02	-1.21±0.19	-1.15±0.16	-2.66±0.08 to -0.16±0.03
propene	1.32	0.79±0.00	0.79±0.01	0.78±0.00	0.67±0.00 to 0.91±0.01
1,1-dichloroethane	-0.84	-0.83±0.00	-0.89±0.02	-0.83±0.02	-1.21±0.01 to -0.47±0.02
1,1,1-trifluoro-2,2,2-trimethoxyethane	-0.80	-4.44±0.01	-4.51±0.13	-4.41±0.23	-6.80±0.08 to -3.20±0.03
methyl-propyl-ether	-1.66	-0.86±0.00	-0.81±0.09	-0.75±0.05	-1.58±0.02 to -0.24±0.04
2,5-dimethyltetrahydrofuran	-2.92	-0.45±0.00	-0.55±0.07	-0.43±0.05	-1.25±0.03 to 0.25±0.04
triethylamine	-3.22	1.33±0.01	1.49±0.09	1.44±0.14	-0.09±0.04 to 2.33±0.04
benzotrifluoride	-0.25	-3.33±0.00	-3.33±0.03	-3.32±0.07	-3.89±0.02 to -2.85±0.04
2,6-dimethylnaphthalene	-2.63	-2.64±0.00	-2.64±0.02	-2.67±0.02	-2.87±0.01 to -2.42±0.01
fluorobenzene	-0.80	-1.71±0.00	-1.75±0.02	-1.69±0.02	-1.91±0.00 to -1.50±0.01
2-naphthol	-8.11	-8.04±0.01	-8.15±0.12	-8.03±0.13	-8.69±0.01 to -7.37±0.04
methyl cyanoacetate	-6.72	-10.21±0.01	-10.65±0.15	-9.93±0.08	-11.96±0.05 to -9.07±0.07
hexan-1-ol	-4.40	-3.27±0.01	-3.53±0.19	-3.39±0.18	-4.38±0.05 to -2.20±0.07
n-butylacetamide	-9.31	-8.40±0.01	-8.39±0.23	-7.96±0.17	-10.11±0.07 to -7.07±0.06

2-nitroaniline	-7.37	-12.75±0.04	-13.60±0.36	-11.55±0.10	-18.27±0.17 to -10.65±0.07
aniline	-5.49	-6.83±0.00	-6.90±0.08	-6.65±0.05	-8.06±0.06 to -6.05±0.04
4-ethyltoluene	-0.95	-0.84±0.00	-0.86±0.02	-0.83±0.04	-1.04±0.01 to -0.63±0.01
n-pentylbenzene	-0.23	-0.71±0.00	-0.73±0.01	-0.73±0.03	-0.93±0.01 to -0.39±0.02
naphthalene	-2.40	-3.62±0.00	-3.66±0.02	-3.62±0.01	-3.80±0.01 to -3.44±0.01
nitromethane	-4.02	-11.09±0.01	-11.30±0.14	-10.94±0.09	-13.04±0.06 to -9.72±0.11
benzyl bromide	-2.38	-3.27±0.00	-3.30±0.02	-3.29±0.03	-3.68±0.03 to -2.81±0.02
1,2-ethanediol	-9.30	-8.57±0.00	-8.49±0.12	-7.77±0.08	-13.49±0.09 to -6.99±0.04
trichloromethane	-1.08	-0.76±0.00	-0.79±0.02	-0.74±0.01	-1.12±0.02 to -0.39±0.02
3,3-dimethylpentane	2.56	2.30±0.00	2.32±0.01	2.31±0.00	2.24±0.00 to 2.35±0.00
N,N-dimethyl-p-methylbenzamide	-9.76	-8.22±0.02	-8.55±0.26	-8.13±0.05	-9.92±0.10 to -6.97±0.02
Z-pent-2-ene	1.31	1.14±0.00	1.14±0.01	1.14±0.01	0.99±0.01 to 1.27±0.01
diethyl ether	-1.59	-0.59±0.00	-0.77±0.02	-0.41±0.09	-1.33±0.02 to 0.10±0.04
4-methoxyaniline	-7.48	-8.32±0.00	-8.50±0.09	-8.10±0.05	-9.82±0.06 to -7.31±0.08
3-methylpentane	2.51	2.18±0.00	2.19±0.01	2.18±0.01	2.10±0.01 to 2.23±0.00
1-naphthol	-7.67	-7.74±0.00	-8.93±0.02	-7.03±0.08	-9.26±0.02 to -6.42±0.08
methyl p-methoxybenzoate	-5.33	-8.84±0.00	-9.08±0.15	-8.69±0.15	-10.34±0.08 to -7.70±0.09
hexan-3-ol	-4.06	-2.70±0.00	-2.86±0.09	-2.44±0.11	-3.78±0.05 to -1.77±0.07
hydrazine	-9.30	-10.04±0.01	-10.32±0.09	-9.72±0.10	-13.82±0.20 to -8.43±0.14
2-methoxy-1,1,1-trimethoxyethane	-5.73	-6.15±0.01	-6.44±0.24	-5.23±0.28	-10.58±0.16 to -4.13±0.10
phenyl trifluoroethyl ether	-1.29	-6.95±0.02	-7.78±0.23	-6.21±0.17	-9.93±0.08 to -4.83±0.08
pentanenitrile	-3.52	-3.63±0.00	-3.69±0.02	-3.63±0.02	-3.94±0.01 to -3.30±0.02
3,4-dimethylpyridine	-5.22	-4.48±0.00	-4.55±0.05	-4.51±0.09	-5.33±0.06 to -3.77±0.03
o-cresol	-5.87	-6.09±0.00	-6.21±0.05	-6.01±0.05	-6.70±0.02 to -5.47±0.04
acetonitrile	-3.88	-4.74±0.00	-4.76±0.01	-4.73±0.01	-5.08±0.02 to -4.41±0.02
cyclohexane	1.23	2.00±0.00	2.00±0.00	2.02±0.01	1.94±0.00 to 2.06±0.00
methyl chloroacetate	-4.00	-6.43±0.00	-6.63±0.21	-6.40±0.17	-7.79±0.08 to -5.23±0.06
2-methyltetrahydrofuran	-3.30	-0.89±0.00	-0.94±0.05	-0.97±0.05	-1.66±0.03 to -0.26±0.03
isoamyl formate	-2.13	-5.92±0.00	-5.94±0.09	-5.90±0.11	-7.16±0.07 to -4.89±0.07
bromotrifluoromethane	1.79	-1.63±0.00	-1.63±0.01	-1.61±0.03	-2.12±0.02 to -1.26±0.02
n-pentane	2.32	2.06±0.00	2.07±0.01	2.07±0.01	1.99±0.00 to 2.10±0.00
1,2,3,5-tetrachlorobenzene	-1.62	0.58±0.00	0.57±0.02	0.58±0.01	0.47±0.00 to 0.69±0.00
methylcyclopentane	1.59	2.04±0.00	2.04±0.01	2.05±0.00	1.97±0.00 to 2.09±0.00
cyclohexanone	-4.91	-4.46±0.01	-4.45±0.07	-4.51±0.11	-5.22±0.06 to -3.72±0.03
4-methylpyridine	-4.93	-5.04±0.00	-5.00±0.03	-5.01±0.04	-5.83±0.05 to -4.37±0.03
1,2-diacetoxyethane	-6.34	-11.69±0.01	-11.96±0.32	-11.02±0.05	-14.27±0.13 to -9.96±0.10
2-methylbuta-1,3-diene	0.68	0.09±0.00	0.05±0.01	0.11±0.02	-0.16±0.01 to 0.35±0.02
dimethyl sulfide	-1.61	-0.75±0.00	-0.75±0.02	-0.72±0.04	-1.17±0.02 to -0.40±0.02
heptan-4-one	-2.92	-3.87±0.00	-3.96±0.07	-3.73±0.10	-4.70±0.02 to -3.10±0.02
3-methoxyphenol	-7.66	-8.15±0.01	-8.34±0.17	-7.95±0.13	-9.45±0.03 to -7.11±0.05
quinoline	-5.72	-6.21±0.00	-6.13±0.05	-6.29±0.04	-7.04±0.03 to -5.50±0.02
trimethoxy methane	-4.42	-4.37±0.01	-4.70±0.35	-3.81±0.10	-9.19±0.23 to -2.73±0.06
2-methylhexane	2.93	2.35±0.00	2.37±0.00	2.36±0.01	2.26±0.01 to 2.39±0.00
formaldehyde	-2.75	-6.92±0.00	-6.98±0.01	-6.87±0.01	-7.79±0.04 to -6.15±0.08
acenaphthene	-3.15	-3.28±0.00	-3.31±0.03	-3.32±0.03	-3.56±0.02 to -3.02±0.01
methyl benzoate	-3.92	-7.24±0.00	-7.41±0.10	-7.03±0.07	-8.60±0.07 to -6.25±0.03
azetidine	-5.56	-3.12±0.02	-3.29±0.16	-3.19±0.13	-4.34±0.06 to -2.06±0.05
methanethiol	-1.24	-1.50±0.00	-1.50±0.03	-1.42±0.01	-1.93±0.01 to -1.13±0.02
oct-1-yne	0.71	0.62±0.00	0.65±0.02	0.63±0.02	0.42±0.01 to 0.81±0.02
1-chlorobutane	-0.16	0.21±0.00	0.19±0.03	0.24±0.02	-0.10±0.01 to 0.46±0.01
3-chloropyridine	-4.01	-4.49±0.00	-4.63±0.07	-4.46±0.06	-5.28±0.04 to -3.86±0.04
2-fluorophenol	-5.29	-5.03±0.00	-5.05±0.06	-4.77±0.10	-9.30±0.02 to -3.95±0.09
methane	1.99	1.53±0.00	1.53±0.00	1.53±0.00	1.53±0.00 to 1.53±0.00
N-methylacetamide	-10.00	-9.39±0.00	-9.54±0.07	-8.84±0.12	-11.11±0.03 to -7.92±0.06
cyclohexene	0.37	1.01±0.00	1.01±0.01	1.00±0.02	0.85±0.01 to 1.15±0.01
morpholine	-7.17	-4.42±0.06	-4.33±0.09	-4.18±0.13	-6.06±0.17 to -3.50±0.06
1-nitrobutane	-3.09	-8.85±0.01	-8.97±0.23	-8.64±0.10	-10.61±0.08 to -7.47±0.10
methanesulfonyl chloride	-4.87	-12.54±0.00	-12.81±0.19	-12.33±0.10	-14.78±0.08 to -10.99±0.08
1-iodopentane	-0.14	-2.30±0.00	-2.27±0.05	-2.33±0.04	-2.80±0.03 to -1.84±0.01
methyl ethyl ether	-2.10	-1.15±0.00	-1.16±0.06	-0.99±0.04	-1.85±0.02 to -0.56±0.02
N,N-dimethyl-p-methoxybenzamide	-11.01	-10.07±0.02	-10.35±0.07	-9.94±0.21	-11.84±0.16 to -8.69±0.06

2-isobutylpyrazine	-5.04	-7.65±0.01	-7.86±0.09	-7.47±0.07	-8.84±0.07 to -6.71±0.05
methyl hexanoate	-2.49	-4.78±0.00	-4.87±0.09	-4.76±0.10	-5.88±0.06 to -3.90±0.04
2,3-dimethylnaphthalene	-2.78	-2.72±0.00	-2.74±0.01	-2.78±0.02	-2.94±0.01 to -2.51±0.01
n-propanethiol	-1.06	-1.11±0.00	-1.20±0.05	-1.07±0.05	-1.61±0.02 to -0.72±0.02
methanol	-5.10	-4.74±0.00	-4.71±0.07	-4.49±0.04	-5.60±0.05 to -4.02±0.02
3-acetylpyridine	-8.26	-10.65±0.21	-10.60±0.24	-10.50±0.17	-11.97±0.19 to -9.58±0.27
4-methoxyacetophenone	-4.40	-8.60±0.00	-8.71±0.12	-8.65±0.09	-9.73±0.04 to -7.60±0.04
2,6-dimethylpyridine	-4.59	-4.41±0.00	-4.41±0.12	-4.41±0.06	-5.48±0.04 to -3.55±0.03
2,2-dimethylbutane	2.51	2.15±0.00	2.16±0.00	2.15±0.00	2.08±0.00 to 2.20±0.00
1,1,2-trichloroethane	-1.99	-1.62±0.02	-2.43±0.04	-1.46±0.23	-2.85±0.03 to -0.72±0.01
3-formylpyridine	-7.10	-11.30±0.00	-11.46±0.06	-11.11±0.13	-12.61±0.05 to -10.23±0.05
1-iodopropane	-0.53	-2.66±0.00	-2.65±0.01	-2.65±0.02	-3.13±0.02 to -2.23±0.02
cycloheptanol	-5.48	-2.81±0.00	-3.07±0.17	-2.58±0.17	-3.98±0.03 to -1.60±0.04
butanenitrile	-3.64	-3.83±0.00	-3.84±0.02	-3.82±0.03	-4.18±0.02 to -3.46±0.02
4-fluorophenol	-6.19	-6.34±0.01	-6.39±0.16	-6.11±0.04	-7.38±0.02 to -5.63±0.03
4-methylpentan-2-ol	-3.73	-2.76±0.01	-2.94±0.14	-2.53±0.07	-3.94±0.02 to -1.67±0.04
isobutyl formate	-2.22	-6.07±0.01	-6.21±0.12	-6.03±0.06	-7.30±0.03 to -4.92±0.09
4-methyl-1h-imidazole	-10.27	-9.00±0.01	-9.14±0.05	-8.98±0.04	-10.00±0.02 to -8.04±0.03
3-methylheptane	2.97	2.51±0.00	2.52±0.01	2.51±0.01	2.41±0.01 to 2.57±0.01
3-methylpyridine	-4.77	-4.80±0.00	-4.84±0.05	-4.81±0.06	-5.59±0.03 to -4.19±0.01
decan-2-one	-2.34	-3.75±0.00	-3.66±0.08	-3.62±0.10	-4.63±0.02 to -2.92±0.07
3-methylbutan-1-ol	-4.42	-3.41±0.00	-3.77±0.07	-3.14±0.10	-4.52±0.05 to -2.22±0.06
2,4-dimethylphenol	-6.01	-5.60±0.00	-5.68±0.06	-5.51±0.05	-6.23±0.02 to -4.90±0.03
methyl cyclopropanecarboxylate	-4.10	-5.81±0.00	-5.71±0.18	-5.61±0.08	-8.92±0.16 to -4.60±0.02
2-naphthylamine	-7.47	-8.22±0.00	-8.29±0.06	-8.18±0.12	-9.54±0.06 to -7.37±0.04
2-methoxyethanol	-6.76	-5.22±0.01	-5.04±0.21	-4.51±0.11	-9.84±0.08 to -3.83±0.04
2-chlorobutane	0.00	0.10±0.00	0.04±0.04	0.17±0.03	-0.20±0.01 to 0.37±0.01
methyl-tert-butyl ether	-2.21	-0.66±0.00	-0.80±0.11	-0.50±0.08	-1.49±0.03 to 0.03±0.04
3-cyanopyridine	-6.75	-8.33±0.00	-8.39±0.10	-8.31±0.07	-9.22±0.05 to -7.64±0.02
methyl butanoate	-2.83	-5.21±0.00	-5.30±0.06	-5.08±0.10	-6.32±0.06 to -4.27±0.06
octanal	-2.29	-4.57±0.00	-4.61±0.04	-4.44±0.12	-5.46±0.03 to -3.79±0.03
cyclopentane	1.20	1.87±0.00	1.87±0.00	1.87±0.00	1.81±0.00 to 1.92±0.00
2-phenylethanol	-6.79	-6.04±0.01	-6.24±0.37	-5.11±0.16	-8.78±0.08 to -4.42±0.04
bromomethane	-0.82	-0.47±0.00	-0.48±0.00	-0.48±0.00	-0.69±0.01 to -0.22±0.01
tetrachloroethene	0.10	2.17±0.00	2.17±0.00	2.17±0.00	2.16±0.00 to 2.18±0.00
1-bromooctane	0.52	0.53±0.00	0.48±0.02	0.50±0.04	0.21±0.01 to 0.79±0.01
1,1,2-trichloro-1,2,2-trifluoroethane	1.77	-0.95±0.00	-0.93±0.03	-0.97±0.04	-1.41±0.02 to -0.57±0.01
pyridine	-4.69	-5.43±0.00	-5.47±0.03	-5.41±0.06	-6.19±0.01 to -4.77±0.02
4-ethylpyridine	-4.73	-4.72±0.00	-4.69±0.05	-4.69±0.08	-5.54±0.04 to -4.02±0.03
alpha-methylstyrene	-1.24	-2.16±0.00	-2.19±0.02	-2.17±0.02	-2.41±0.01 to -1.91±0.01
isopropyl formate	-2.02	-6.23±0.00	-6.30±0.09	-6.03±0.10	-7.45±0.03 to -5.22±0.04
methyl t-butyl ether	-2.21	-0.67±0.00	-0.86±0.06	-0.75±0.05	-1.46±0.02 to 0.08±0.05
N,N-dimethylformamide	-7.81	-8.49±0.00	-8.55±0.17	-8.06±0.15	-9.90±0.03 to -7.38±0.08
heptan-1-ol	-4.21	-3.11±0.00	-3.36±0.15	-2.98±0.15	-4.27±0.06 to -2.06±0.04
2,2-dimethylpropane	2.51	2.00±0.00	2.01±0.00	2.00±0.00	1.95±0.00 to 2.05±0.00
1,3,5-trimethylbenzene	-0.90	-0.69±0.00	-0.73±0.02	-0.69±0.02	-0.92±0.01 to -0.49±0.01
methylamine	-4.55	-5.13±0.01	-5.37±0.12	-4.84±0.10	-6.83±0.02 to -3.98±0.04
2-methylpropan-1-ol	-4.50	-3.45±0.01	-3.70±0.15	-3.16±0.17	-4.59±0.04 to -2.39±0.03
propyne	-0.48	-0.34±0.00	-0.34±0.01	-0.34±0.01	-0.49±0.01 to -0.18±0.00
2,2,4-trimethylpentane	2.89	2.46±0.00	2.46±0.01	2.47±0.01	2.38±0.00 to 2.52±0.00
cyclopropane	0.75	1.34±0.00	1.34±0.00	1.34±0.00	1.28±0.00 to 1.39±0.00
pentan-2-ol	-4.39	-3.05±0.00	-3.08±0.14	-2.97±0.07	-3.96±0.02 to -2.20±0.04
2-methylbutan-1-ol	-4.42	-3.19±0.01	-3.65±0.12	-2.73±0.08	-4.38±0.04 to -2.09±0.05
1-iodobutane	-0.25	-2.44±0.00	-2.49±0.04	-2.44±0.04	-2.92±0.02 to -2.01±0.01
2-ethylpyridine	-4.33	-4.65±0.00	-4.71±0.06	-4.57±0.08	-5.56±0.03 to -3.86±0.05
propanenitrile	-3.84	-4.12±0.00	-4.12±0.03	-4.13±0.02	-4.45±0.03 to -3.82±0.01
N,N-dimethyl piperazine	-7.58	-0.74±0.00	-0.74±0.10	-0.63±0.24	-2.57±0.13 to 0.71±0.06
triacetyl glycerol	-8.84	-16.02±0.40	-20.20±0.88	-11.86±0.24	-35.58±1.80 to -12.61±0.71
n-nonane	3.13	2.67±0.00	2.68±0.01	2.69±0.01	2.54±0.01 to 2.72±0.00
benzene	-0.86	-2.04±0.00	-2.05±0.01	-2.05±0.01	-2.12±0.00 to -1.94±0.01
1-methylcyclohexene	0.67	1.33±0.00	1.33±0.01	1.35±0.02	1.16±0.01 to 1.51±0.01

1-iodoheptane	0.27	-2.00±0.00	-1.98±0.03	-2.01±0.02	-2.51±0.03 to -1.44±0.02
isoamyl acetate	-2.21	-5.34±0.00	-5.30±0.19	-4.76±0.08	-10.67±0.04 to -4.13±0.04
phenanthrene	-3.88	-4.97±0.00	-5.00±0.02	-5.01±0.02	-5.21±0.01 to -4.72±0.01
2-methylpent-1-ene	1.47	1.37±0.00	1.37±0.01	1.36±0.02	1.18±0.01 to 1.54±0.00
cis-1,2-dimethylcyclohexane	1.58	2.33±0.00	2.34±0.01	2.34±0.01	2.26±0.01 to 2.39±0.00
cyclopentene	0.56	0.69±0.00	0.67±0.00	0.70±0.01	0.57±0.01 to 0.82±0.01
n-propylcyclopentane	2.13	2.38±0.00	2.39±0.01	2.39±0.00	2.29±0.01 to 2.44±0.00
3,5-dimethylphenol	-6.27	-5.65±0.00	-6.12±0.20	-5.48±0.05	-6.66±0.02 to -4.92±0.02
bromoethane	-0.74	-0.51±0.00	-0.51±0.01	-0.49±0.01	-0.74±0.01 to -0.27±0.00
chloromethane	-0.55	-0.37±0.00	-0.36±0.01	-0.35±0.01	-0.59±0.01 to -0.15±0.00
hexan-2-one	-3.28	-4.37±0.00	-4.45±0.08	-4.43±0.10	-5.18±0.02 to -3.48±0.03
phenyl methyl sulfide	-2.73	-2.13±0.00	-2.04±0.02	-2.12±0.04	-2.70±0.03 to -1.76±0.02
2-propoxyethanol	-6.40	-4.06±0.00	-3.94±0.17	-3.53±0.05	-8.58±0.16 to -2.63±0.03
2,6-dimethylphenol	-5.26	-5.19±0.01	-5.07±0.18	-4.89±0.09	-6.38±0.01 to -4.27±0.02
methyl cyclopropyl ketone	-4.61	-5.35±0.00	-5.58±0.13	-5.26±0.04	-6.52±0.05 to -4.31±0.09
diisopropylamine	-3.22	0.12±0.01	-0.20±0.15	0.50±0.10	-1.60±0.09 to 1.30±0.04
n-propyl acetate	-2.79	-5.18±0.00	-5.33±0.10	-5.13±0.14	-6.29±0.06 to -4.23±0.04
hydrogen sulfide	-0.70	-2.62±0.00	-2.64±0.00	-2.59±0.00	-3.30±0.02 to -2.09±0.02
methyl cyclohexyl ketone	-3.90	-3.88±0.01	-4.02±0.07	-3.85±0.08	-4.75±0.03 to -3.14±0.02
2-methylbutane	2.38	2.03±0.00	2.04±0.00	2.03±0.00	1.97±0.01 to 2.08±0.00
methyl ethyl sulfide	-1.50	-0.73±0.00	-0.72±0.03	-0.75±0.04	-1.17±0.02 to -0.35±0.02
butan-2-ol	-4.62	-3.25±0.00	-3.34±0.16	-3.00±0.09	-4.36±0.03 to -2.27±0.04
ethanamide	-9.71	-9.76±0.00	-9.97±0.13	-9.67±0.14	-11.47±0.06 to -8.30±0.10
1,1-dichloroethene	0.25	0.38±0.00	0.37±0.01	0.37±0.01	0.17±0.01 to 0.58±0.02
trimethoxymethylbenzene	-4.04	-5.67±0.03	-5.85±0.18	-5.21±0.09	-7.44±0.05 to -4.34±0.09
diethyl succinate	-5.71	-11.33±0.02	-12.09±0.34	-10.55±0.14	-15.10±0.06 to -9.45±0.10
4-formylpyridine	-7.00	-11.05±0.00	-11.16±0.06	-10.89±0.13	-12.33±0.05 to -10.02±0.04
4-nitrophenol	-10.64	-14.45±0.01	-14.40±0.13	-13.90±0.15	-17.19±0.05 to -12.97±0.08
2-methylpropan-2-ol	-4.47	-3.28±0.00	-3.31±0.14	-3.20±0.08	-4.22±0.05 to -2.49±0.04
1-ethylnaphthalene	-2.40	-2.85±0.00	-2.86±0.03	-2.85±0.02	-3.09±0.01 to -2.61±0.01
ethanol	-5.00	-4.21±0.00	-4.46±0.05	-4.19±0.15	-5.16±0.03 to -3.40±0.01
propanoic acid	-6.46	-7.14±0.33	-8.51±1.49	-6.51±0.13	-10.20±1.44 to -5.58±0.14
methoxyflurane	-1.12	-2.94±0.02	-2.95±0.10	-2.82±0.04	-5.84±0.29 to -2.14±0.04
di-n-butylamine	-3.24	0.07±0.03	0.17±0.09	0.62±0.16	-1.77±0.13 to 1.35±0.06
methyl-isopropyl-ether	-2.01	-0.84±0.00	-0.87±0.07	-0.63±0.10	-1.63±0.05 to -0.16±0.05
diethyl disulfide	-1.64	-1.30±0.00	-1.36±0.09	-1.27±0.05	-1.91±0.04 to -0.75±0.02
4-acetylpyridine	-7.62	-10.24±0.00	-10.29±0.02	-10.06±0.08	-11.46±0.05 to -9.29±0.04
nonanal	-2.07	-4.41±0.00	-4.57±0.10	-4.33±0.16	-5.34±0.02 to -3.58±0.04
N-methylaniline	-4.69	-5.44±0.00	-5.57±0.11	-5.29±0.07	-6.41±0.03 to -4.55±0.04
nonan-5-one	-2.64	-3.51±0.00	-3.52±0.05	-3.36±0.06	-4.39±0.03 to -2.73±0.02
ethyl acetate	-2.94	-5.51±0.00	-5.43±0.14	-5.44±0.10	-6.63±0.04 to -4.67±0.04
E-oct-2-enal	-3.43	-5.36±0.00	-5.34±0.05	-5.37±0.04	-6.17±0.04 to -4.61±0.05
indane	-1.46	-1.26±0.00	-1.28±0.02	-1.25±0.02	-1.48±0.02 to -1.02±0.01
1,1-diacetoxyethane	-4.97	-10.58±0.07	-10.72±0.12	-10.03±0.17	-13.10±0.15 to -9.31±0.05
thiophenol	-2.55	-2.57±0.00	-2.63±0.06	-2.53±0.03	-3.04±0.01 to -2.18±0.03
4-bromophenol	-7.13	-6.51±0.00	-6.62±0.23	-6.27±0.04	-7.48±0.02 to -5.80±0.03
n-hexylamine	-3.95	-3.16±0.00	-3.37±0.16	-2.95±0.10	-4.93±0.07 to -1.96±0.05
p-xylene	-0.80	-1.15±0.00	-1.14±0.01	-1.18±0.01	-1.35±0.01 to -0.95±0.01
pentan-2-one	-3.52	-4.56±0.00	-4.55±0.06	-4.46±0.07	-5.48±0.03 to -3.78±0.07
triethyl phosphate	-7.54	-11.02±0.01	-11.51±0.29	-9.49±0.65	-17.26±0.21 to -8.41±0.25
E-but-2-enal	-4.22	-6.18±0.00	-6.23±0.06	-6.14±0.05	-7.02±0.02 to -5.43±0.05
heptan-2-one	-3.04	-4.23±0.00	-4.40±0.06	-4.10±0.06	-5.12±0.02 to -3.44±0.03
N-methylpiperazine	-7.77	-3.11±0.00	-3.26±0.08	-2.79±0.05	-4.76±0.12 to -1.80±0.07
3-methyl-but-1-ene	1.83	1.17±0.00	1.19±0.01	1.16±0.01	1.01±0.01 to 1.32±0.01
1-nitropentane	-2.82	-8.64±0.00	-8.80±0.08	-8.64±0.10	-10.47±0.09 to -7.32±0.04
bis(2-chloroethyl) ether	-4.23	-3.54±0.01	-4.88±0.41	-2.21±0.05	-7.06±0.07 to -1.82±0.05
1,2,4-trichlorobenzene	-1.12	-0.39±0.00	-0.41±0.01	-0.40±0.01	-0.60±0.01 to -0.18±0.01
E-1,2-dichloroethene	-0.78	-0.21±0.00	-0.21±0.00	-0.21±0.00	-0.32±0.01 to -0.11±0.00
3-methylbutan-2-one	-3.24	-4.37±0.00	-4.16±0.09	-4.34±0.06	-5.28±0.01 to -3.65±0.01
chloroethylene	-0.59	-0.36±0.00	-0.37±0.01	-0.34±0.01	-0.61±0.01 to -0.12±0.01
2-methylpropane	2.32	1.89±0.00	1.89±0.00	1.90±0.00	1.85±0.00 to 1.93±0.00

N,N-dimethylaniline	-3.45	-3.64±0.00	-3.90±0.14	-3.67±0.18	-4.84±0.04 to -2.57±0.04
2-methylpyrazine	-5.51	-8.79±0.00	-8.86±0.08	-8.70±0.13	-9.95±0.06 to -7.93±0.03
pentanoic acid	-6.16	-6.29±0.03	-9.30±1.80	-6.01±0.13	-10.99±1.66 to -4.85±0.06
ethyl hexanoate	-2.23	-4.29±0.00	-4.46±0.13	-4.16±0.08	-5.45±0.03 to -3.34±0.04
3,3,3-trimethoxypropionitrile	-6.40	-7.37±0.01	-8.01±0.45	-6.35±0.19	-11.11±0.11 to -5.72±0.05
phenol	-6.61	-6.62±0.01	-6.66±0.18	-6.38±0.06	-7.57±0.01 to -5.80±0.02
cyclohepta-1,3,5-triene	-0.99	-1.40±0.01	-1.43±0.03	-1.35±0.03	-1.82±0.03 to -1.06±0.01
methyl propanoate	-2.93	-5.45±0.00	-5.44±0.08	-5.29±0.08	-6.67±0.04 to -4.55±0.05
1,2-dichlorobenzene	-1.36	-1.21±0.00	-1.21±0.02	-1.20±0.02	-1.43±0.01 to -0.98±0.02
2-methylpentan-3-ol	-3.88	-2.45±0.01	-2.73±0.13	-2.28±0.18	-3.70±0.03 to -1.49±0.04
oct-1-ene	1.92	1.65±0.00	1.62±0.02	1.65±0.02	1.47±0.01 to 1.82±0.01
2-nitrotoluene	-3.58	-9.72±0.00	-9.82±0.20	-9.25±0.22	-11.45±0.06 to -8.31±0.06
di-isopropyl sulfide	-1.21	-0.58±0.01	-0.46±0.04	-0.44±0.05	-1.17±0.02 to -0.01±0.04
2,3-dimethylbutane	2.34	2.16±0.00	2.16±0.00	2.16±0.01	2.10±0.00 to 2.20±0.00
thiophene	-1.42	-1.35±0.00	-1.36±0.00	-1.35±0.01	-1.47±0.00 to -1.24±0.00
piperazine	-7.40	-5.58±0.03	-5.81±0.14	-5.32±0.17	-7.61±0.18 to -4.31±0.05
prop-2-en-1-ol	-5.03	-4.52±0.01	-4.50±0.19	-4.14±0.08	-6.55±0.04 to -3.48±0.04
isopropylbenzene	-0.30	-1.02±0.00	-1.05±0.01	-1.03±0.02	-1.22±0.01 to -0.79±0.01
2,2,2-trifluoroethanol	-4.31	-6.99±0.01	-7.37±0.47	-6.64±0.21	-10.30±0.11 to -5.09±0.10
n-pentylcyclopentane	2.55	2.69±0.00	2.71±0.01	2.70±0.01	2.59±0.01 to 2.78±0.01
2-butoxyethanol	-6.25	-4.03±0.01	-3.91±0.19	-3.59±0.11	-9.00±0.04 to -2.55±0.05
N,N-dimethylbenzamide	-9.29	-8.73±0.01	-8.58±0.17	-8.42±0.07	-10.40±0.06 to -7.54±0.03
but-1-yne	-0.16	-0.05±0.00	-0.05±0.02	-0.06±0.01	-0.20±0.00 to 0.12±0.01
N-methylpiperidine	-3.88	0.64±0.03	0.57±0.08	0.68±0.22	-0.58±0.06 to 1.70±0.08
4-methylacetophenone	-4.70	-6.67±0.00	-6.56±0.10	-6.64±0.06	-7.61±0.05 to -5.92±0.03
fluoromethane	-0.22	-0.92±0.00	-0.92±0.01	-0.91±0.01	-1.19±0.02 to -0.64±0.01
1,2,3-trichlorobenzene	-1.24	-0.54±0.00	-0.53±0.00	-0.53±0.01	-0.78±0.02 to -0.29±0.01
2-chloropropane	-0.25	-0.12±0.00	-0.13±0.01	-0.12±0.02	-0.39±0.01 to 0.13±0.01
4-chloroaniline	-5.90	-6.35±0.00	-6.28±0.06	-6.11±0.09	-7.60±0.05 to -5.52±0.01
hexa-1,5-diene	1.01	0.53±0.00	0.48±0.05	0.54±0.03	0.15±0.01 to 0.73±0.01
2-methylbut-2-ene	1.31	1.17±0.00	1.17±0.01	1.17±0.01	1.04±0.01 to 1.31±0.00
di-n-propyl ether	-1.16	0.04±0.00	0.10±0.06	0.04±0.06	-0.80±0.02 to 0.82±0.05
m-cresol	-5.49	-6.13±0.01	-6.21±0.23	-5.94±0.03	-7.06±0.01 to -5.38±0.02
trichloroethene	-0.44	0.49±0.00	0.50±0.01	0.47±0.00	0.36±0.01 to 0.65±0.01
ethene	1.28	0.62±0.00	0.62±0.01	0.62±0.01	0.48±0.02 to 0.72±0.01
n-hexane	2.48	2.21±0.00	2.21±0.01	2.22±0.00	2.12±0.01 to 2.25±0.00
hept-1-yne	0.60	0.47±0.00	0.48±0.02	0.48±0.01	0.24±0.01 to 0.64±0.01
1-methylnaphthalene	-2.44	-3.19±0.00	-3.22±0.02	-3.19±0.01	-3.44±0.02 to -2.97±0.01
dimethyl ether	-1.91	-1.68±0.00	-1.73±0.05	-1.54±0.05	-2.33±0.04 to -1.10±0.02
methyl cyclohexanecarboxylate	-3.30	-4.31±0.05	-4.22±0.08	-4.16±0.11	-5.45±0.06 to -3.39±0.07
pentanal	-3.03	-5.04±0.01	-5.17±0.05	-4.93±0.05	-5.89±0.05 to -4.21±0.04
1H-pyrrole	-4.78	-5.09±0.00	-5.13±0.02	-5.09±0.02	-5.35±0.02 to -4.80±0.01
penta-1,4-diene	0.93	0.28±0.00	0.30±0.02	0.32±0.05	-0.02±0.02 to 0.59±0.01
3-nitrotoluene	-3.45	-9.25±0.01	-9.24±0.11	-8.61±0.08	-11.44±0.07 to -8.06±0.05
cyanobenzene	-4.10	-5.18±0.00	-5.23±0.02	-5.16±0.01	-5.49±0.02 to -4.89±0.01

TABLE 4: Comparison of hydration free energies computed with different implicit solvent models versus experiment.

Molecule name	Expt. (kcal/mol)	IGB=1 ²³ (kcal/mol)	IGB=5 ²⁴ (kcal/mol)	IGB=7 ²⁵ (kcal/mol)	PB (ZAP) (kcal/mol)
2-methylpentan-2-ol	-3.92	-4.06±0.01	-2.67±0.00	-2.21±0.01	-3.74±0.01
nitroethane	-3.71	-8.79±0.01	-9.78±0.01	-9.29±0.01	-9.23±0.01
tetrahydrofuran	-3.47	-1.03±0.00	-1.32±0.00	-2.06±0.00	-2.05±0.00
N-methylmorpholine	-6.32	-2.64±0.01	-2.21±0.01	-5.25±0.01	-5.37±0.01
3,3-dimethylbutan-2-one	-3.11	-3.60±0.00	-4.16±0.00	-4.01±0.00	-4.40±0.00
acetaldehyde	-3.50	-5.45±0.00	-6.08±0.00	-5.74±0.00	-5.72±0.00
N-acetylpyrrolidine	-9.80	-6.75±0.00	-7.27±0.00	-7.88±0.00	-7.91±0.00
ethyl pentanoate	-2.49	-3.86±0.00	-4.46±0.00	-4.49±0.00	-5.08±0.00
di-n-butyl ether	-0.83	0.53±0.00	0.47±0.00	0.03±0.00	-0.65±0.02
acetic acid	-6.69	-10.84±0.18	-7.69±0.15	-7.28±0.18	-8.08±0.15
dimethylamine	-4.29	-2.42±0.00	-3.21±0.00	-3.49±0.00	-3.75±0.01
1,4-dioxane	-5.06	-3.03±0.00	-3.55±0.00	-4.54±0.00	-4.90±0.00
di-n-propylamine	-3.65	-0.35±0.02	-0.40±0.02	-0.93±0.02	-2.35±0.02
1,1-difluoroethane	-0.11	-1.63±0.00	-2.03±0.00	-2.57±0.00	-1.90±0.00
2-methoxyphenol	-5.57	-8.41±0.01	-6.09±0.01	-6.62±0.01	-6.26±0.01
methyl-octanoate	-2.04	-3.79±0.00	-4.46±0.00	-4.32±0.00	-4.93±0.00
1-bromo-2-chloroethane	-1.95	-1.63±0.01	-2.06±0.01	-2.14±0.01	-1.33±0.01
hex-1-ene	1.58	1.47±0.00	1.35±0.00	1.55±0.00	1.38±0.00
m-xylene	-0.83	-0.86±0.00	-1.16±0.00	-1.93±0.00	-1.11±0.00
ammonia	-4.29	-7.07±0.00	-7.24±0.00	-5.38±0.00	-6.69±0.01
1,2,4,5-tetrachlorobenzene	-1.34	0.82±0.00	0.47±0.00	0.02±0.00	0.71±0.00
decane-1-ol	-3.64	-4.41±0.00	-2.66±0.00	-1.98±0.00	-3.54±0.00
1,1,1-trifluoropropan-2-ol	-4.16	-8.59±0.00	-5.53±0.00	-6.79±0.00	-6.00±0.00
pent-1-ene	1.68	1.30±0.00	1.18±0.00	1.38±0.00	1.26±0.00
ethyl benzoate	-3.64	-5.89±0.01	-6.74±0.01	-7.71±0.01	-6.93±0.01
1-chlorohexane	0.00	0.65±0.00	0.47±0.00	0.57±0.00	0.45±0.00
2,3,4-trimethylpentane	2.56	2.39±0.00	2.46±0.00	2.52±0.00	2.34±0.00
4-cyanophenol	-10.17	-12.73±0.01	-9.89±0.00	-10.23±0.01	-9.62±0.00
nonan-2-one	-2.49	-3.33±0.01	-3.92±0.01	-3.81±0.01	-4.18±0.01
fluorene	-3.35	-3.71±0.00	-4.22±0.00	-6.10±0.00	-4.21±0.00
4-bromotoluene	-1.39	-1.12±0.00	-1.54±0.00	-2.16±0.00	-1.08±0.00
ethanethiol	-1.14	-1.71±0.00	-1.44±0.00	-1.32±0.00	-1.90±0.00
2-methylbutan-2-ol	-4.43	-4.36±0.01	-2.96±0.01	-2.49±0.01	-3.92±0.01
1-chloropropane	-0.33	0.18±0.00	-0.01±0.00	0.05±0.00	0.04±0.00
1,4-dichlorobutane	-2.32	-1.26±0.00	-1.64±0.00	-1.60±0.00	-1.57±0.00
1,2,3-trimethylbenzene	-1.21	-0.70±0.00	-0.90±0.00	-1.77±0.00	-1.00±0.00
n-pentyl acetate	-2.51	-4.13±0.00	-4.78±0.00	-4.87±0.00	-5.30±0.00
dimethyl sulfone	-10.08	-10.77±0.01	-12.30±0.01	-13.53±0.01	-12.37±0.01
1,1,2,2-tetrachloroethane	-2.47	-1.37±0.01	-1.81±0.01	-2.79±0.01	-0.96±0.01
methyl p-nitrobenzoate	-6.88	-13.09±0.01	-14.76±0.01	-15.24±0.01	-13.68±0.01
1,2-dichloropropane	-1.27	-1.06±0.01	-1.41±0.01	-1.53±0.01	-1.29±0.01
1,2,3,4-tetrachlorobenzene	-1.34	0.61±0.00	0.29±0.00	-0.02±0.00	0.49±0.00
ethyl butanoate	-2.49	-4.06±0.01	-4.66±0.01	-4.71±0.01	-5.32±0.03
isobutylbenzene	0.16	-0.54±0.00	-0.83±0.00	-1.51±0.00	-0.87±0.00
isobutyl isobutanoate	-1.69	-3.41±0.00	-3.87±0.00	-3.85±0.00	-4.65±0.00
3-chloroaniline	-5.82	-5.44±0.00	-6.11±0.00	-7.00±0.00	-6.10±0.01
3-methylbutanoic acid	-6.09	-9.36±0.18	-6.25±0.15	-5.62±0.18	-7.13±0.15
4-nitroaniline	-10.27	-13.72±0.00	-15.01±0.00	-16.04±0.00	-15.20±0.00
3-methylhexane	2.71	2.32±0.00	2.34±0.00	2.43±0.00	2.28±0.00
nitrobenzene	-4.12	-8.80±0.01	-9.90±0.01	-10.34±0.01	-9.02±0.01
butanoic acid	-6.35	-9.49±0.01	-6.47±0.00	-5.96±0.01	-7.21±0.01
2-ethoxyethanol	-6.69	-5.88±0.01	-4.43±0.01	-4.25±0.01	-5.82±0.01
benzamide	-11.00	-10.14±0.00	-11.00±0.00	-12.64±0.00	-11.59±0.00
bromobenzene	-1.46	-1.47±0.00	-1.96±0.00	-2.56±0.00	-1.33±0.00
2,6-dimethylaniline	-5.21	-4.88±0.00	-5.42±0.00	-6.30±0.00	-5.78±0.01
tetrahydropyran	-3.12	-0.46±0.02	-0.68±0.02	-1.34±0.02	-1.43±0.02
n-butyl acetate	-2.64	-4.31±0.00	-4.96±0.00	-5.05±0.00	-5.44±0.00

diisopropyl ether	-0.53	0.07±0.00	0.14±0.00	-0.62±0.00	-1.01±0.00
n-propyl formate	-2.48	-5.55±0.00	-6.38±0.00	-5.73±0.00	-6.31±0.00
ethyl propanoate	-2.68	-4.33±0.00	-4.96±0.00	-5.04±0.00	-5.46±0.00
p-dibromobenzene	-2.30	-0.98±0.00	-1.50±0.00	-2.08±0.00	-0.80±0.00
n-propyl butyrate	-2.28	-3.77±0.00	-4.32±0.00	-4.35±0.00	-5.04±0.03
1,1,1-trichloroethane	-0.19	0.16±0.00	-0.06±0.00	-0.43±0.00	0.32±0.00
2-iodophenol	-6.20	-8.45±0.01	-5.38±0.01	-5.77±0.01	-4.39±0.01
2,3-dimethylbuta-1,3-diene	0.40	0.56±0.00	0.37±0.00	0.35±0.00	0.45±0.00
pyrrolidine	-5.48	-1.70±0.01	-1.99±0.01	-3.20±0.01	-3.54±0.01
2-methyl-but-2-ene	1.31	1.29±0.00	1.17±0.00	1.14±0.00	1.19±0.00
2,3-dimethylpentane	2.52	2.28±0.00	2.32±0.00	2.38±0.00	2.25±0.00
p-cresol	-6.13	-8.82±0.00	-6.14±0.00	-6.58±0.00	-6.30±0.00
2-chloro-1,1,1-trimethoxyethane	-4.59	-3.76±0.01	-4.08±0.01	-4.70±0.01	-5.59±0.01
1-bromo-2-methylpropane	-0.03	0.06±0.01	-0.12±0.01	0.03±0.01	0.44±0.01
4-cyanopyridine	-6.02	-7.46±0.00	-8.31±0.00	-9.80±0.00	-7.52±0.00
toluene	-0.89	-1.22±0.00	-1.60±0.00	-2.30±0.00	-1.33±0.00
2,2-dimethylpentane	2.88	2.29±0.00	2.33±0.00	2.36±0.00	2.26±0.00
1,2,4-trimethylbenzene	-0.86	-0.58±0.00	-0.79±0.00	-1.67±0.00	-0.94±0.00
1-chloro-2,2,2-trifluoroethane	0.06	-2.63±0.00	-3.13±0.00	-5.16±0.00	-1.90±0.00
3-nitrophenol	-9.62	-16.53±0.01	-13.95±0.01	-14.07±0.01	-13.26±0.01
dimethoxymethane	-2.93	-3.03±0.02	-3.75±0.02	-4.03±0.02	-4.89±0.02
non-1-ene	2.06	1.92±0.00	1.81±0.00	2.05±0.00	1.75±0.00
propionaldehyde	-3.43	-4.87±0.00	-5.48±0.00	-5.08±0.00	-5.30±0.00
cyclohexanol	-5.46	-4.83±0.00	-3.16±0.00	-2.63±0.00	-4.07±0.00
2,3-dimethylpyridine	-4.82	-3.86±0.00	-4.39±0.00	-5.99±0.00	-4.18±0.00
3-methyl-1h-indole	-5.88	-5.55±0.00	-5.93±0.00	-8.36±0.00	-6.20±0.00
2-methylpropene	1.16	1.09±0.00	0.97±0.00	1.04±0.00	1.08±0.00
diethyl malonate	-6.00	-8.36±0.01	-9.41±0.01	-9.64±0.01	-10.64±0.10
1-naphthylamine	-7.28	-7.27±0.00	-8.04±0.00	-9.58±0.00	-8.30±0.01
Z-1,2-dichloroethene	-1.17	-0.86±0.00	-1.24±0.00	-1.64±0.00	-0.93±0.00
but-1-ene	1.38	1.12±0.00	0.99±0.00	1.17±0.00	1.11±0.00
trans-1,4-dimethylcyclohexane	2.11	2.31±0.00	2.39±0.00	2.34±0.00	2.23±0.00
4-n-propylphenol	-5.90	-8.32±0.00	-5.59±0.00	-6.04±0.00	-5.98±0.00
2-methoxyethanamine	-6.55	-4.94±0.01	-5.87±0.01	-5.27±0.01	-6.96±0.01
dimethyl sulfoxide	-8.71	-7.81±0.00	-8.49±0.00	-9.58±0.00	-9.74±0.00
n-butylbenzene	-0.40	-0.56±0.00	-0.88±0.00	-1.56±0.00	-0.88±0.00
3-phenylpropanol	-6.92	-7.55±0.02	-6.09±0.02	-6.23±0.02	-6.80±0.02
propan-2-ol	-4.74	-5.30±0.01	-3.65±0.00	-3.17±0.01	-4.44±0.01
1-nitropropane	-3.34	-8.23±0.01	-9.17±0.01	-8.61±0.01	-8.77±0.01
m-bistrifluoromethyl benzene	1.07	-4.72±0.00	-5.33±0.00	-9.36±0.00	-4.02±0.00
3-methylbut-1-ene	1.82	1.29±0.00	1.17±0.00	1.33±0.00	1.24±0.00
1-bromoheptane	0.34	0.56±0.00	0.37±0.00	0.54±0.00	0.88±0.00
butanone	-3.71	-4.62±0.00	-5.24±0.00	-4.79±0.00	-5.12±0.00
1,1,1-trimethoxyethane	-4.42	-3.38±0.00	-3.59±0.00	-4.27±0.00	-5.34±0.00
3-ethylpyridine	-4.59	-3.88±0.00	-4.45±0.00	-6.02±0.00	-4.23±0.00
anisole	-2.45	-3.10±0.00	-3.71±0.00	-4.48±0.00	-3.49±0.00
propane	1.96	1.79±0.00	1.78±0.00	1.84±0.00	1.82±0.00
3-chlorophenol	-6.62	-8.95±0.00	-6.05±0.00	-6.40±0.00	-6.09±0.00
dichloromethane	-1.31	-0.97±0.00	-1.29±0.00	-1.57±0.00	-0.80±0.00
2,5-dimethylphenol	-5.91	-7.72±0.02	-5.12±0.02	-5.68±0.02	-5.52±0.02
biphenyl	-2.66	-3.54±0.00	-4.22±0.00	-5.73±0.00	-4.08±0.00
nonan-1-ol	-3.88	-4.52±0.00	-2.79±0.00	-2.11±0.00	-3.68±0.00
methylcyclohexane	1.70	2.16±0.00	2.19±0.00	2.17±0.00	2.12±0.00
3,4-dimethylphenol	-6.50	-8.48±0.01	-5.72±0.01	-6.23±0.01	-6.07±0.01
tert-butylbenzene	-0.44	-0.61±0.00	-0.86±0.00	-1.61±0.00	-0.99±0.00
diethoxymethoxybenzene	-5.23	-4.63±0.00	-4.75±0.00	-6.26±0.00	-7.43±0.00
pent-1-yne	0.01	0.38±0.00	0.15±0.00	0.16±0.00	0.42±0.00
n-butylamine	-4.24	-3.00±0.00	-3.73±0.00	-2.73±0.00	-4.28±0.01
1-chloropentane	-0.07	0.50±0.00	0.32±0.00	0.41±0.00	0.32±0.00
iodoethane	-0.74	-2.70±0.00	-3.04±0.00	-2.86±0.00	-1.56±0.00
1,2-dibromoethane	-2.33	-1.77±0.00	-2.22±0.00	-2.21±0.00	-1.04±0.00

2-nitrophenol	-4.58	-13.46±0.03	-10.32±0.03	-10.34±0.03	-9.86±0.03
undecan-2-one	-2.15	-3.02±0.00	-3.59±0.00	-3.47±0.00	-3.91±0.00
ethylbenzene	-0.79	-0.94±0.00	-1.29±0.00	-1.99±0.00	-1.16±0.00
2,5-dimethylpyridine	-4.72	-3.77±0.00	-4.28±0.00	-5.89±0.00	-4.12±0.00
n-octylamine	-3.65	-2.13±0.00	-2.83±0.00	-1.81±0.00	-3.60±0.01
o-xylene	-0.90	-0.96±0.00	-1.25±0.00	-2.05±0.00	-1.17±0.00
4-tert-butylphenol	-5.91	-8.16±0.01	-5.36±0.01	-5.89±0.01	-5.96±0.01
benzyl chloride	-1.93	-2.37±0.00	-2.93±0.00	-3.73±0.00	-2.70±0.00
n-butanethiol	-0.99	-1.23±0.00	-0.99±0.00	-0.79±0.00	-1.54±0.00
piperidine	-5.11	-1.31±0.04	-1.48±0.04	-2.64±0.04	-2.96±0.06
n-octane	2.88	2.51±0.00	2.51±0.00	2.64±0.00	2.44±0.00
2,2,5-trimethylhexane	2.93	2.56±0.00	2.64±0.00	2.67±0.00	2.48±0.00
acetophenone	-4.58	-6.16±0.00	-7.07±0.00	-7.98±0.00	-6.78±0.00
2-bromo-2-methylpropane	0.84	-0.39±0.00	-0.58±0.00	-0.39±0.00	0.10±0.00
trimethylamine	-3.20	-1.11±0.01	-1.22±0.01	-3.19±0.01	-2.91±0.01
pentan-3-one	-3.41	-3.75±0.00	-4.31±0.00	-4.22±0.00	-4.50±0.00
n-propylbenzene	-0.53	-0.73±0.00	-1.06±0.00	-1.75±0.00	-1.01±0.00
cyclohexylamine	-4.59	-2.29±0.01	-2.93±0.01	-2.06±0.01	-3.97±0.01
butan-1-ol	-4.72	-5.34±0.00	-3.63±0.00	-2.98±0.00	-4.32±0.00
1,1-diethoxyethane	-3.28	-1.25±0.01	-1.25±0.01	-2.23±0.01	-3.16±0.01
hexanal	-2.81	-4.26±0.00	-4.88±0.00	-4.40±0.00	-4.84±0.00
E-hept-2-ene	1.68	1.73±0.00	1.62±0.00	1.73±0.00	1.52±0.00
chlorobenzene	-1.12	-1.14±0.00	-1.60±0.00	-2.23±0.00	-1.25±0.00
isobutyl acetate	-2.36	-4.26±0.00	-4.87±0.00	-4.98±0.00	-5.39±0.00
2-chlorotoluene	-1.14	-0.90±0.00	-1.30±0.00	-1.89±0.00	-1.06±0.00
1,2-dimethoxyethane	-4.84	-3.06±0.01	-3.74±0.01	-4.26±0.01	-5.01±0.01
iodomethane	-0.89	-2.88±0.00	-3.22±0.00	-3.07±0.00	-1.72±0.00
anthracene	-3.95	-4.26±0.00	-4.91±0.00	-6.81±0.00	-5.00±0.00
hexafluoropropene	-3.76	-1.85±0.00	-1.92±0.00	-6.01±0.00	-0.21±0.00
n-butane	2.07	1.92±0.00	1.91±0.00	1.99±0.00	1.94±0.00
2,4-dimethylpentane	2.83	2.31±0.00	2.33±0.00	2.41±0.00	2.27±0.00
2-nitropropane	-3.13	-7.88±0.01	-8.74±0.01	-8.25±0.01	-8.59±0.01
n-heptylamine	-3.79	-2.31±0.01	-3.02±0.01	-2.01±0.01	-3.74±0.01
trimethyl phosphate	-8.70	-11.88±0.01	-13.47±0.01	-11.42±0.01	-14.70±0.02
1-bromohexane	0.18	0.41±0.00	0.23±0.00	0.39±0.00	0.75±0.00
hept-1-ene	1.66	1.62±0.00	1.50±0.00	1.72±0.00	1.50±0.00
dibromomethane	-1.96	-0.42±0.00	-0.72±0.00	-0.79±0.00	0.04±0.00
pentan-3-ol	-4.35	-4.33±0.00	-2.83±0.00	-2.27±0.00	-3.86±0.00
n-propylamine	-4.39	-3.04±0.00	-3.77±0.00	-2.79±0.00	-4.25±0.01
n-decane	3.16	2.80±0.00	2.82±0.00	2.96±0.00	2.69±0.00
methyl formate	-2.78	-8.54±0.05	-9.58±0.05	-8.71±0.05	-9.41±0.05
teflurane	0.50	-3.24±0.00	-3.65±0.00	-7.13±0.00	-1.48±0.00
1,2-diethoxyethane	-3.54	-2.13±0.01	-2.48±0.01	-3.39±0.01	-5.18±0.21
4-chloro-3-methylphenol	-6.79	-8.69±0.01	-5.84±0.00	-6.19±0.01	-5.99±0.01
2-iodopropane	-0.46	-2.46±0.00	-2.77±0.00	-2.55±0.00	-1.35±0.00
methyl trifluoroacetate	-1.10	-5.45±0.00	-5.93±0.00	-8.10±0.00	-4.36±0.00
o-toluidine	-5.53	-5.49±0.00	-6.12±0.00	-6.92±0.00	-6.15±0.01
E-hex-2-enal	-3.68	-5.09±0.00	-5.70±0.00	-5.59±0.00	-5.31±0.00
2-methylthiophene	-1.38	-0.66±0.00	-0.96±0.00	-1.97±0.00	-0.86±0.00
buta-1,3-diene	0.61	0.16±0.02	-0.08±0.02	0.06±0.02	0.13±0.02
methyl pentanoate	-2.56	-4.25±0.00	-4.94±0.00	-4.82±0.00	-5.39±0.02
2-ethyltoluene	-1.04	-0.70±0.00	-0.95±0.00	-1.75±0.00	-1.00±0.00
chlorofluoromethane	-0.77	-2.25±0.00	-2.63±0.00	-3.09±0.00	-1.98±0.00
1,4-dimethylnaphthalene	-2.82	-2.40±0.00	-2.75±0.00	-4.12±0.00	-2.95±0.00
1-iodohexane	0.08	-1.82±0.00	-2.14±0.00	-1.87±0.00	-0.77±0.00
octan-1-ol	-4.09	-4.68±0.00	-2.96±0.00	-2.28±0.00	-3.81±0.00
phenyl formate	-3.82	-7.93±0.02	-8.99±0.02	-8.95±0.02	-8.43±0.02
benzyl alcohol	-6.62	-7.76±0.01	-6.18±0.01	-6.61±0.01	-6.76±0.01
1,3-dichlorobenzene	-0.98	-0.48±0.00	-0.94±0.00	-1.56±0.00	-0.65±0.00
octan-2-one	-2.88	-3.49±0.00	-4.08±0.00	-3.99±0.00	-4.36±0.02
cyclopentanone	-4.70	-4.08±0.00	-4.60±0.00	-4.60±0.00	-4.53±0.00

sec-butylbenzene	-0.45	-0.50±0.00	-0.76±0.00	-1.46±0.00	-0.87±0.00
1-bromopentane	-0.10	0.26±0.00	0.08±0.00	0.22±0.00	0.63±0.00
iodobenzene	-1.74	-1.83±0.00	-2.34±0.00	-2.82±0.00	-1.48±0.00
N-methyl-N-2,2,2-trifluoroethyl-aniline	-1.92	-5.89±0.01	-6.01±0.01	-10.61±0.01	-6.46±0.01
n-hexylbenzene	-0.04	-0.25±0.00	-0.54±0.00	-1.22±0.00	-0.64±0.00
2-chloroaniline	-4.91	-5.41±0.01	-6.07±0.01	-7.22±0.01	-5.90±0.01
propan-1-ol	-4.85	-5.55±0.01	-3.84±0.00	-3.20±0.01	-4.46±0.01
isoflurane	0.10	-6.01±0.01	-6.59±0.01	-10.78±0.01	-4.86±0.01
p-toluidine	-5.57	-5.68±0.00	-6.30±0.00	-7.18±0.00	-6.26±0.00
isopropyl acetate	-2.64	-4.41±0.00	-5.03±0.00	-5.23±0.00	-5.60±0.01
3-cyanophenol	-9.65	-12.17±0.01	-9.34±0.00	-9.67±0.01	-9.07±0.01
2-bromopropane	-0.48	-0.33±0.00	-0.52±0.00	-0.41±0.00	0.11±0.00
butyraldehyde	-3.18	-4.62±0.00	-5.23±0.00	-4.78±0.00	-5.11±0.00
methyl acetate	-3.13	-5.23±0.00	-6.03±0.00	-6.00±0.00	-6.11±0.00
1-methyl-pyrrole	-2.89	-2.79±0.00	-3.30±0.00	-3.98±0.00	-2.73±0.00
pyrene	-4.52	-5.07±0.00	-5.70±0.00	-7.76±0.00	-5.86±0.00
2-methylpyridine	-4.63	-4.32±0.00	-4.95±0.00	-6.58±0.00	-4.56±0.00
heptanal	-2.67	-4.11±0.00	-4.72±0.00	-4.24±0.00	-4.78±0.03
pentachloroethane	-1.39	-0.33±0.01	-0.57±0.01	-1.83±0.01	0.49±0.01
n-hexyl acetate	-2.26	-3.98±0.00	-4.62±0.00	-4.70±0.00	-5.18±0.00
ethyl formate	-2.56	-5.88±0.00	-6.74±0.00	-6.11±0.00	-6.57±0.00
4-ethylphenol	-6.13	-8.53±0.01	-5.82±0.01	-6.28±0.01	-6.12±0.01
2,4-dimethylpyridine	-4.86	-4.00±0.00	-4.54±0.00	-6.21±0.00	-4.34±0.00
methyl methanesulfonate	-4.87	-10.47±0.01	-12.20±0.01	-11.47±0.01	-11.39±0.01
1,1,1,2-tetrachloroethane	-1.28	-0.65±0.00	-0.97±0.00	-1.72±0.00	-0.21±0.00
tribromomethane	-2.13	0.63±0.00	0.41±0.00	0.24±0.00	1.02±0.00
hex-1-yne	0.29	0.55±0.00	0.32±0.00	0.34±0.00	0.57±0.00
3-hydroxybenzaldehyde	-9.50	-14.51±0.01	-12.15±0.01	-12.41±0.01	-11.84±0.01
3-chloroprop-1-ene	-0.57	-0.45±0.00	-0.76±0.00	-0.78±0.00	-0.58±0.00
n-heptane	2.67	2.36±0.00	2.36±0.00	2.47±0.00	2.32±0.00
ethylamine	-4.50	-3.41±0.01	-4.15±0.01	-3.24±0.01	-4.45±0.01
4-isopropyltoluene	-0.68	-0.36±0.00	-0.56±0.00	-1.38±0.00	-0.81±0.00
2-chloro-2-methylpropane	1.09	0.08±0.00	-0.11±0.00	0.02±0.00	-0.13±0.00
diethyl sulfide	-1.46	-0.36±0.00	-0.67±0.00	-0.60±0.00	-1.13±0.00
n-propyl propanoate	-2.44	-4.04±0.00	-4.62±0.00	-4.70±0.00	-5.21±0.00
2,3-dimethylphenol	-6.16	-8.24±0.00	-5.67±0.00	-6.12±0.00	-5.92±0.00
4-chlorophenol	-7.03	-8.99±0.01	-6.19±0.01	-6.57±0.01	-6.19±0.01
1-bromobutane	-0.40	0.12±0.00	-0.07±0.00	0.06±0.00	0.50±0.00
dimethyl sulfate	-5.10	-11.83±0.01	-13.87±0.01	-9.75±0.01	-10.99±0.01
n-pentyl propanoate	-2.11	-3.66±0.00	-4.21±0.00	-4.27±0.00	-4.99±0.03
3-ethylphenol	-6.25	-8.53±0.00	-5.81±0.00	-6.20±0.00	-6.09±0.00
3-nitroaniline	-8.84	-12.61±0.00	-13.83±0.00	-14.71±0.00	-13.60±0.01
propanone	-3.80	-4.65±0.00	-5.30±0.00	-5.38±0.00	-5.23±0.00
tetrafluoromethane	3.12	-2.05±0.00	-2.27±0.00	-5.17±0.00	0.74±0.00
di-n-propyl sulfide	-1.28	0.15±0.00	-0.14±0.00	-0.01±0.00	-0.71±0.00
1-methyl-imidazole	-8.41	-6.66±0.00	-7.42±0.00	-9.09±0.00	-7.30±0.00
ethane	1.83	1.66±0.00	1.66±0.00	1.71±0.00	1.70±0.00
2-chloropyridine	-4.39	-4.87±0.00	-5.52±0.00	-7.57±0.00	-4.79±0.00
4-hydroxybenzaldehyde	-8.83	-14.85±0.01	-12.37±0.01	-12.69±0.01	-12.09±0.01
halothane	-0.11	-2.06±0.00	-2.46±0.00	-4.95±0.00	-0.52±0.00
2-ethylpyrazine	-5.45	-7.44±0.00	-8.28±0.00	-10.65±0.00	-8.17±0.00
benzonitrile	-4.21	-4.57±0.00	-5.18±0.00	-5.78±0.00	-4.58±0.00
diiodomethane	-2.49	-4.02±0.00	-4.54±0.00	-4.55±0.00	-2.28±0.00
2-chlorophenol	-4.55	-7.79±0.01	-4.86±0.01	-5.60±0.01	-4.61±0.01
2-methoxyaniline	-6.12	-6.96±0.00	-7.71±0.00	-8.65±0.00	-7.85±0.01
chloroethane	-0.63	-0.04±0.00	-0.23±0.00	-0.21±0.00	-0.16±0.00
3,5-dimethylpyridine	-4.84	-3.67±0.00	-4.16±0.00	-5.70±0.00	-4.04±0.00
methyl trimethylacetate	-2.40	-4.04±0.00	-4.65±0.00	-4.42±0.00	-5.10±0.00
4-methylbenzaldehyde	-4.27	-6.56±0.00	-7.39±0.00	-8.01±0.00	-6.91±0.00
benzaldehyde	-4.02	-6.89±0.00	-7.79±0.00	-8.40±0.00	-7.12±0.00
1,4-dichlorobenzene	-1.01	-0.58±0.00	-1.06±0.00	-1.68±0.00	-0.77±0.00

n-pentylamine	-4.09	-2.63±0.01	-3.34±0.01	-2.35±0.01	-3.98±0.01
2-methylpentane	2.51	2.19±0.00	2.20±0.00	2.28±0.00	2.17±0.00
pentan-1-ol	-4.57	-5.15±0.00	-3.44±0.00	-2.79±0.00	-4.19±0.00
cyclopentanol	-5.49	-5.00±0.00	-3.32±0.00	-2.86±0.00	-4.19±0.00
1,2-dichloroethane	-1.79	-1.36±0.01	-1.75±0.01	-1.92±0.01	-1.48±0.01
1,3-dichloropropane	-1.89	-1.50±0.00	-1.93±0.00	-1.96±0.00	-1.73±0.00
1-chloroheptane	0.29	0.83±0.00	0.66±0.00	0.77±0.00	0.61±0.00
1,3,5-trichlorobenzene	-0.78	0.43±0.00	-0.00±0.00	-0.61±0.00	0.27±0.00
3-methoxyaniline	-7.29	-7.56±0.00	-8.37±0.00	-9.35±0.00	-8.51±0.01
hexanoic acid	-6.21	-9.38±0.21	-6.27±0.19	-5.74±0.21	-7.10±0.19
chlorodifluoromethane	-0.50	-3.12±0.00	-3.53±0.00	-5.18±0.00	-2.10±0.00
1,3-dimethylnaphthalene	-2.47	-2.33±0.00	-2.69±0.00	-4.09±0.00	-2.91±0.00
N,N-dimethyl p-nitrobenzamide	-11.95	-14.76±0.04	-16.38±0.04	-17.11±0.04	-15.79±0.04
1-bromopropane	-0.56	-0.07±0.00	-0.26±0.00	-0.14±0.00	0.33±0.00
2,4-dimethylpentan-3-one	-2.74	-3.09±0.00	-3.65±0.00	-3.34±0.00	-3.93±0.00
ethyl phenyl ether	-2.22	-2.67±0.00	-3.16±0.00	-4.13±0.00	-3.25±0.02
isobutyraldehyde	-2.86	-4.42±0.00	-5.03±0.00	-4.60±0.00	-5.03±0.00
styrene	-1.24	-1.94±0.00	-2.43±0.00	-3.18±0.00	-2.23±0.00
dimethyl-disulfide	-1.83	-0.99±0.00	-1.29±0.00	-1.65±0.00	-1.55±0.00
1H-imidazole	-9.63	-8.52±0.00	-9.30±0.00	-11.53±0.00	-9.21±0.00
4-methylpentan-2-one	-3.05	-3.75±0.00	-4.34±0.00	-4.20±0.00	-4.55±0.00
tetrachloromethane	0.08	1.10±0.00	1.05±0.00	0.35±0.00	1.95±0.00
diethylamine	-4.07	-0.97±0.02	-1.20±0.02	-1.95±0.02	-2.77±0.03
propene	1.32	0.92±0.00	0.79±0.00	0.96±0.00	0.96±0.00
1,1-dichloroethane	-0.84	-0.54±0.00	-0.83±0.00	-1.05±0.00	-0.59±0.00
1,1,1-trifluoro-2,2,2-trimethoxyethane	-0.80	-4.22±0.01	-4.44±0.01	-5.85±0.01	-5.32±0.01
methyl-propyl-ether	-1.66	-0.53±0.00	-0.86±0.00	-1.18±0.00	-1.42±0.00
2,5-dimethyltetrahydrofuran	-2.92	-0.45±0.00	-0.45±0.00	-1.49±0.00	-1.61±0.00
triethylamine	-3.22	0.32±0.01	1.33±0.01	-1.01±0.01	-1.63±0.02
benzotrifluoride	-0.25	-2.73±0.00	-3.33±0.00	-5.48±0.00	-2.63±0.00
2,6-dimethylnaphthalene	-2.63	-2.27±0.00	-2.64±0.00	-4.07±0.00	-2.89±0.00
fluorobenzene	-0.80	-1.25±0.00	-1.71±0.00	-2.33±0.00	-1.41±0.00
2-naphthol	-8.11	-10.62±0.01	-8.04±0.01	-9.04±0.01	-8.25±0.01
methyl cyanoacetate	-6.72	-9.19±0.01	-10.21±0.01	-10.44±0.01	-9.55±0.01
hexan-1-ol	-4.40	-4.99±0.01	-3.27±0.01	-2.61±0.01	-4.06±0.01
n-butylacetamide	-9.31	-7.78±0.01	-8.40±0.01	-8.79±0.01	-9.62±0.07
2-nitroaniline	-7.37	-11.77±0.04	-12.75±0.04	-14.22±0.04	-13.97±0.04
aniline	-5.49	-6.12±0.00	-6.83±0.00	-7.59±0.00	-6.51±0.01
4-ethyltoluene	-0.95	-0.58±0.00	-0.84±0.00	-1.63±0.00	-0.94±0.00
n-pentylbenzene	-0.23	-0.40±0.00	-0.71±0.00	-1.39±0.00	-0.76±0.00
naphthalene	-2.40	-3.07±0.00	-3.62±0.00	-4.93±0.00	-3.42±0.00
nitromethane	-4.02	-9.92±0.01	-11.09±0.01	-10.52±0.01	-10.13±0.01
benzyl bromide	-2.38	-2.67±0.00	-3.27±0.00	-3.93±0.00	-2.46±0.00
1,2-ethanediol	-9.30	-12.30±0.01	-8.57±0.00	-7.27±0.01	-9.71±0.00
trichloromethane	-1.08	-0.47±0.00	-0.76±0.00	-1.43±0.00	0.04±0.00
3,3-dimethylpentane	2.56	2.25±0.00	2.30±0.00	2.33±0.00	2.24±0.00
N,N-dimethyl-p-methylbenzamide	-9.76	-7.46±0.02	-8.22±0.02	-9.35±0.02	-8.72±0.02
Z-pent-2-ene	1.31	1.28±0.00	1.14±0.00	1.22±0.00	1.22±0.00
diethyl ether	-1.59	-0.36±0.00	-0.59±0.00	-1.13±0.00	-1.32±0.00
4-methoxyaniline	-7.48	-7.47±0.00	-8.32±0.00	-9.27±0.00	-8.28±0.00
3-methylpentane	2.51	2.17±0.00	2.18±0.00	2.26±0.00	2.16±0.00
1-naphthol	-7.67	-10.32±0.01	-7.74±0.00	-8.86±0.01	-7.92±0.01
methyl p-methoxybenzoate	-5.33	-7.72±0.00	-8.84±0.00	-9.74±0.00	-8.97±0.00
hexan-3-ol	-4.06	-4.18±0.01	-2.70±0.00	-2.12±0.01	-3.75±0.00
hydrazine	-9.30	-9.50±0.01	-10.04±0.01	-8.56±0.01	-9.94±0.01
2-methoxy-1,1,1-trimethoxyethane	-5.73	-5.78±0.01	-6.15±0.01	-6.82±0.01	-10.63±0.44
phenyl trifluoroethyl ether	-1.29	-6.18±0.02	-6.95±0.02	-10.00±0.02	-6.89±0.02
pentanenitrile	-3.52	-3.34±0.00	-3.63±0.00	-3.59±0.00	-3.26±0.00
3,4-dimethylpyridine	-5.22	-3.94±0.00	-4.48±0.00	-6.09±0.00	-4.28±0.00
o-cresol	-5.87	-8.61±0.00	-6.09±0.00	-6.45±0.00	-6.16±0.00
acetonitrile	-3.88	-4.40±0.00	-4.74±0.00	-4.88±0.00	-4.21±0.00

cyclohexane	1.23	2.00±0.00	2.00±0.00	2.00±0.00	2.01±0.00
methyl chloroacetate	-4.00	-5.57±0.00	-6.43±0.00	-6.65±0.00	-6.06±0.00
2-methyltetrahydrofuran	-3.30	-0.73±0.00	-0.89±0.00	-1.77±0.00	-1.83±0.00
isoamyl formate	-2.13	-5.11±0.00	-5.92±0.00	-5.23±0.00	-5.99±0.01
bromotrifluoromethane	1.79	-1.45±0.00	-1.63±0.00	-3.79±0.00	0.85±0.00
n-pentane	2.32	2.07±0.00	2.06±0.00	2.15±0.00	2.07±0.00
1,2,3,5-tetrachlorobenzene	-1.62	0.91±0.00	0.58±0.00	0.15±0.00	0.81±0.00
methylcyclopentane	1.59	2.02±0.00	2.04±0.00	2.01±0.00	2.00±0.00
cyclohexanone	-4.91	-3.93±0.01	-4.46±0.01	-4.34±0.01	-4.49±0.01
4-methylpyridine	-4.93	-4.39±0.00	-5.04±0.00	-6.66±0.00	-4.65±0.00
1,2-diacetoxyethane	-6.34	-10.31±0.01	-11.69±0.01	-11.59±0.01	-12.61±0.01
2-methylbuta-1,3-diene	0.68	0.32±0.00	0.09±0.00	0.15±0.00	0.23±0.01
dimethyl sulfide	-1.61	-0.46±0.00	-0.75±0.00	-0.73±0.00	-0.97±0.00
heptan-4-one	-2.92	-3.31±0.00	-3.87±0.00	-3.68±0.00	-4.14±0.00
3-methoxyphenol	-7.66	-10.85±0.01	-8.15±0.01	-8.62±0.01	-8.38±0.01
quinoline	-5.72	-5.42±0.00	-6.21±0.00	-8.24±0.00	-5.78±0.00
trimethoxy methane	-4.42	-3.94±0.01	-4.37±0.01	-4.74±0.01	-6.55±0.01
2-methylhexane	2.93	2.33±0.00	2.35±0.00	2.43±0.00	2.29±0.00
formaldehyde	-2.75	-6.57±0.00	-6.92±0.00	-6.12±0.00	-6.08±0.00
acenaphthene	-3.15	-2.97±0.00	-3.28±0.00	-5.05±0.00	-3.41±0.00
methyl benzoate	-3.92	-6.29±0.00	-7.24±0.00	-8.03±0.00	-7.17±0.00
azetidine	-5.56	-2.52±0.02	-3.12±0.02	-3.92±0.02	-4.11±0.06
methanethiol	-1.24	-1.84±0.00	-1.50±0.00	-1.48±0.00	-1.81±0.00
oct-1-yne	0.71	0.85±0.00	0.62±0.00	0.67±0.00	0.81±0.00
1-chlorobutane	-0.16	0.39±0.00	0.21±0.00	0.28±0.00	0.23±0.00
3-chloropyridine	-4.01	-3.83±0.00	-4.49±0.00	-6.12±0.00	-3.90±0.00
2-fluorophenol	-5.29	-7.93±0.00	-5.03±0.00	-5.79±0.00	-5.00±0.00
methane	1.99	1.53±0.00	1.53±0.00	1.56±0.00	1.55±0.00
N-methylacetamide	-10.00	-8.60±0.00	-9.39±0.00	-9.92±0.00	-9.78±0.01
cyclohexene	0.37	1.14±0.00	1.01±0.00	0.90±0.00	1.07±0.00
morpholine	-7.17	-3.94±0.06	-4.42±0.06	-5.93±0.06	-6.36±0.11
1-nitrobutane	-3.09	-7.93±0.01	-8.85±0.01	-8.25±0.01	-8.50±0.01
methanesulfonyl chloride	-4.87	-11.09±0.00	-12.54±0.00	-13.30±0.00	-8.72±0.00
1-iodopentane	-0.14	-1.97±0.00	-2.30±0.00	-2.04±0.00	-0.90±0.00
methyl ethyl ether	-2.10	-0.78±0.00	-1.15±0.00	-1.50±0.00	-1.62±0.00
N,N-dimethyl-p-methoxybenzamide	-11.01	-9.07±0.02	-10.07±0.02	-11.29±0.02	-11.04±0.13
2-isobutylpyrazine	-5.04	-6.86±0.01	-7.65±0.01	-9.86±0.01	-7.78±0.01
methyl hexanoate	-2.49	-4.09±0.00	-4.78±0.00	-4.65±0.00	-5.18±0.00
2,3-dimethylnaphthalene	-2.78	-2.36±0.00	-2.72±0.00	-4.16±0.00	-2.94±0.00
n-propanethiol	-1.06	-1.38±0.00	-1.11±0.00	-0.97±0.00	-1.63±0.00
methanol	-5.10	-6.58±0.00	-4.74±0.00	-4.08±0.00	-4.98±0.00
3-acetylpyridine	-8.26	-9.46±0.21	-10.65±0.21	-12.41±0.21	-10.19±0.22
4-methoxyacetophenone	-4.40	-7.53±0.00	-8.60±0.00	-9.62±0.00	-8.54±0.00
2,6-dimethylpyridine	-4.59	-3.92±0.00	-4.41±0.00	-6.12±0.00	-4.22±0.00
2,2-dimethylbutane	2.51	2.12±0.00	2.15±0.00	2.17±0.00	2.13±0.00
1,1,2-trichloroethane	-1.99	-1.19±0.02	-1.62±0.02	-2.11±0.02	-1.11±0.02
3-formylpyridine	-7.10	-10.15±0.00	-11.30±0.00	-12.61±0.00	-10.26±0.01
1-iodopropane	-0.53	-2.33±0.00	-2.66±0.00	-2.44±0.00	-1.23±0.00
cycloheptanol	-5.48	-4.40±0.00	-2.81±0.00	-2.30±0.00	-3.94±0.00
butanenitrile	-3.64	-3.53±0.00	-3.83±0.00	-3.81±0.00	-3.44±0.00
4-fluorophenol	-6.19	-9.10±0.01	-6.34±0.01	-6.70±0.01	-6.38±0.01
4-methylpentan-2-ol	-3.73	-4.30±0.01	-2.76±0.01	-2.18±0.01	-3.87±0.01
isobutyl formate	-2.22	-5.27±0.01	-6.07±0.01	-5.40±0.01	-6.09±0.01
4-methyl-1h-imidazole	-10.27	-8.32±0.01	-9.00±0.01	-11.12±0.01	-9.07±0.01
3-methylheptane	2.97	2.48±0.00	2.51±0.00	2.60±0.00	2.41±0.00
3-methylpyridine	-4.77	-4.19±0.00	-4.80±0.00	-6.37±0.00	-4.46±0.00
decan-2-one	-2.34	-3.17±0.00	-3.75±0.00	-3.63±0.00	-4.04±0.00
3-methylbutan-1-ol	-4.42	-5.12±0.00	-3.41±0.00	-2.75±0.00	-4.19±0.00
2,4-dimethylphenol	-6.01	-8.18±0.01	-5.60±0.00	-6.07±0.01	-5.91±0.00
methyl cyclopropanecarboxylate	-4.10	-5.14±0.00	-5.81±0.00	-6.06±0.00	-6.91±0.01
2-naphthylamine	-7.47	-7.45±0.00	-8.22±0.00	-9.77±0.00	-8.50±0.06

2-methoxyethanol	-6.76	-6.54±0.01	-5.22±0.01	-4.86±0.01	-6.35±0.01
2-chlorobutane	0.00	0.28±0.00	0.10±0.00	0.19±0.00	0.06±0.00
methyl-tert-butyl ether	-2.21	-0.45±0.00	-0.66±0.00	-1.13±0.00	-1.33±0.00
3-cyanopyridine	-6.75	-7.52±0.00	-8.33±0.00	-9.93±0.00	-7.45±0.00
methyl butanoate	-2.83	-4.50±0.00	-5.21±0.00	-5.11±0.00	-5.55±0.00
octanal	-2.29	-3.96±0.00	-4.57±0.00	-4.08±0.00	-4.59±0.00
cyclopentane	1.20	1.88±0.00	1.87±0.00	1.87±0.00	1.89±0.00
2-phenylethanol	-6.79	-7.45±0.01	-6.04±0.01	-6.23±0.01	-6.68±0.01
bromomethane	-0.82	-0.27±0.00	-0.47±0.00	-0.41±0.00	0.13±0.00
tetrachloroethene	0.10	2.18±0.00	2.17±0.00	2.08±0.00	2.26±0.00
1-bromooctane	0.52	0.71±0.00	0.53±0.00	0.71±0.00	1.00±0.00
1,1,2-trichloro-1,2,2-trifluoroethane	1.77	-1.05±0.00	-0.95±0.00	-5.28±0.00	1.33±0.00
pyridine	-4.69	-4.71±0.00	-5.43±0.00	-7.04±0.00	-4.86±0.00
4-ethylpyridine	-4.73	-4.10±0.00	-4.72±0.00	-6.33±0.00	-4.45±0.00
alpha-methylstyrene	-1.24	-1.73±0.00	-2.16±0.00	-2.96±0.00	-2.10±0.00
isopropyl formate	-2.02	-5.42±0.00	-6.23±0.00	-5.64±0.00	-6.30±0.00
methyl t-butyl ether	-2.21	-0.45±0.00	-0.67±0.00	-1.14±0.00	-1.33±0.00
N,N-dimethylformamide	-7.81	-7.66±0.00	-8.49±0.00	-8.31±0.00	-8.44±0.00
heptan-1-ol	-4.21	-4.83±0.00	-3.11±0.00	-2.45±0.00	-3.94±0.00
2,2-dimethylpropane	2.51	1.99±0.00	2.00±0.00	2.02±0.00	2.02±0.00
1,3,5-trimethylbenzene	-0.90	-0.49±0.00	-0.69±0.00	-1.55±0.00	-0.87±0.00
methylamine	-4.55	-4.33±0.01	-5.13±0.01	-4.08±0.01	-4.99±0.01
2-methylpropan-1-ol	-4.50	-5.12±0.01	-3.45±0.01	-2.80±0.01	-4.21±0.01
propyne	-0.48	-0.09±0.00	-0.34±0.00	-0.38±0.00	0.05±0.00
2,2,4-trimethylpentane	2.89	2.39±0.00	2.46±0.00	2.50±0.00	2.34±0.00
cyclopropane	0.75	1.39±0.00	1.34±0.00	1.46±0.00	1.49±0.00
pentan-2-ol	-4.39	-4.64±0.00	-3.05±0.00	-2.50±0.00	-3.97±0.00
2-methylbutan-1-ol	-4.42	-4.86±0.01	-3.19±0.01	-2.51±0.01	-4.05±0.01
1-iodobutane	-0.25	-2.12±0.00	-2.44±0.00	-2.20±0.00	-1.03±0.00
2-ethylpyridine	-4.33	-4.05±0.00	-4.65±0.00	-6.11±0.00	-4.35±0.00
propanenitrile	-3.84	-3.81±0.00	-4.12±0.00	-4.15±0.00	-3.69±0.00
N,N-dimethyl piperazine	-7.58	-2.24±0.01	-0.74±0.00	-6.38±0.01	-6.24±0.01
triacetyl glycerol	-8.84	-24.56±0.42	-16.02±0.40	-14.05±0.42	-20.33±0.41
n-nonane	3.13	2.66±0.00	2.67±0.00	2.80±0.00	2.56±0.00
benzene	-0.86	-1.58±0.00	-2.04±0.00	-2.67±0.00	-1.54±0.00
1-methylcyclohexene	0.67	1.38±0.00	1.33±0.00	1.09±0.00	1.22±0.00
1-iodoheptane	0.27	-1.68±0.00	-2.00±0.00	-1.72±0.00	-0.65±0.00
isoamyl acetate	-2.21	-4.64±0.00	-5.34±0.00	-5.38±0.00	-8.39±0.58
phenanthrene	-3.88	-4.32±0.00	-4.97±0.00	-6.78±0.00	-5.04±0.00
2-methylpent-1-ene	1.47	1.47±0.00	1.37±0.00	1.46±0.00	1.37±0.00
cis-1,2-dimethylcyclohexane	1.58	2.26±0.00	2.33±0.00	2.28±0.00	2.22±0.00
cyclopentene	0.56	0.87±0.00	0.69±0.00	0.58±0.00	0.84±0.00
n-propylcyclopentane	2.13	2.33±0.00	2.38±0.00	2.36±0.00	2.25±0.00
3,5-dimethylphenol	-6.27	-8.41±0.00	-5.65±0.00	-6.12±0.00	-6.02±0.00
bromoethane	-0.74	-0.31±0.00	-0.51±0.00	-0.43±0.00	0.11±0.00
chloromethane	-0.55	-0.18±0.00	-0.37±0.00	-0.36±0.00	-0.20±0.00
hexan-2-one	-3.28	-3.77±0.00	-4.37±0.00	-4.29±0.00	-4.53±0.00
phenyl methyl sulfide	-2.73	-1.68±0.00	-2.13±0.00	-3.00±0.00	-2.18±0.00
2-propoxyethanol	-6.40	-5.57±0.01	-4.06±0.00	-3.85±0.01	-5.57±0.00
2,6-dimethylphenol	-5.26	-7.57±0.01	-5.19±0.01	-5.74±0.01	-5.50±0.01
methyl cyclopropyl ketone	-4.61	-4.72±0.00	-5.35±0.00	-5.60±0.00	-5.88±0.00
diisopropylamine	-3.22	-0.18±0.01	0.12±0.01	-0.83±0.01	-2.10±0.01
n-propyl acetate	-2.79	-4.52±0.00	-5.18±0.00	-5.30±0.00	-5.61±0.00
hydrogen sulfide	-0.70	-4.40±0.00	-2.62±0.00	-2.84±0.00	-3.00±0.00
methyl cyclohexyl ketone	-3.90	-3.33±0.01	-3.88±0.01	-3.74±0.01	-4.24±0.02
2-methylbutane	2.38	2.03±0.00	2.03±0.00	2.10±0.00	2.04±0.00
methyl ethyl sulfide	-1.50	-0.42±0.00	-0.73±0.00	-0.68±0.00	-1.05±0.00
butan-2-ol	-4.62	-4.82±0.00	-3.25±0.00	-2.73±0.00	-4.16±0.00
ethanamide	-9.71	-9.11±0.00	-9.76±0.00	-10.43±0.00	-10.38±0.00
1,1-dichloroethene	0.25	0.60±0.00	0.38±0.00	0.22±0.00	0.53±0.00
trimethoxymethylbenzene	-4.04	-5.33±0.03	-5.67±0.03	-7.10±0.03	-7.46±0.04

diethyl succinate	-5.71	-10.09±0.02	-11.33±0.02	-11.30±0.02	-13.59±0.26
4-formylpyridine	-7.00	-9.89±0.00	-11.05±0.00	-12.41±0.00	-10.13±0.00
4-nitrophenol	-10.64	-17.10±0.01	-14.45±0.01	-14.60±0.01	-13.95±0.01
2-methylpropan-2-ol	-4.47	-4.75±0.00	-3.28±0.00	-2.87±0.00	-4.18±0.00
1-ethylnaphthalene	-2.40	-2.45±0.00	-2.85±0.00	-4.18±0.00	-3.00±0.00
ethanol	-5.00	-5.96±0.00	-4.21±0.00	-3.63±0.00	-4.72±0.00
propanoic acid	-6.46	-10.27±0.35	-7.14±0.33	-6.67±0.35	-7.77±0.33
methoxyflurane	-1.12	-2.53±0.02	-2.94±0.02	-5.38±0.02	-2.60±0.02
di-n-butylamine	-3.24	0.06±0.03	0.07±0.03	-0.43±0.03	-2.17±0.09
methyl-isopropyl-ether	-2.01	-0.57±0.00	-0.84±0.00	-1.28±0.00	-1.49±0.00
diethyl disulfide	-1.64	-1.00±0.00	-1.30±0.00	-1.59±0.00	-1.73±0.00
4-acetylpyridine	-7.62	-9.06±0.00	-10.24±0.00	-11.98±0.00	-9.80±0.00
nonanal	-2.07	-3.81±0.00	-4.41±0.00	-3.91±0.00	-4.51±0.02
N-methylaniline	-4.69	-4.81±0.00	-5.44±0.00	-7.04±0.00	-5.47±0.01
nonan-5-one	-2.64	-2.96±0.00	-3.51±0.00	-3.29±0.00	-3.92±0.02
ethyl acetate	-2.94	-4.80±0.00	-5.51±0.00	-5.64±0.00	-5.85±0.00
E-oct-2-enal	-3.43	-4.76±0.00	-5.36±0.00	-5.24±0.00	-5.11±0.02
indane	-1.46	-1.02±0.00	-1.26±0.00	-2.30±0.00	-1.27±0.00
1,1-diacetoxyethane	-4.97	-9.39±0.07	-10.58±0.07	-10.55±0.07	-11.89±0.07
thiophenol	-2.55	-2.83±0.00	-2.57±0.00	-3.46±0.00	-2.70±0.00
4-bromophenol	-7.13	-9.35±0.00	-6.51±0.00	-6.85±0.00	-6.24±0.00
n-hexylamine	-3.95	-2.45±0.00	-3.16±0.00	-2.16±0.00	-4.23±0.10
p-xylene	-0.80	-0.85±0.00	-1.15±0.00	-1.93±0.00	-1.11±0.00
pentan-2-one	-3.52	-3.96±0.00	-4.56±0.00	-4.50±0.00	-4.69±0.00
triethyl phosphate	-7.54	-9.89±0.01	-11.02±0.01	-9.75±0.01	-15.29±0.50
E-but-2-enal	-4.22	-5.56±0.00	-6.18±0.00	-6.12±0.00	-5.67±0.00
heptan-2-one	-3.04	-3.63±0.00	-4.23±0.00	-4.14±0.00	-4.50±0.02
N-methylpiperazine	-7.77	-3.60±0.00	-3.11±0.00	-7.08±0.00	-7.02±0.00
3-methyl-but-1-ene	1.83	1.28±0.00	1.17±0.00	1.33±0.00	1.24±0.00
1-nitropentane	-2.82	-7.73±0.00	-8.64±0.00	-8.04±0.00	-8.34±0.01
bis(2-chloroethyl) ether	-4.23	-2.92±0.01	-3.54±0.01	-4.20±0.01	-3.92±0.01
1,2,4-trichlorobenzene	-1.12	0.04±0.00	-0.39±0.00	-0.91±0.00	-0.12±0.00
E-1,2-dichloroethene	-0.78	0.15±0.00	-0.21±0.00	-0.63±0.00	0.11±0.00
3-methylbutan-2-one	-3.24	-3.79±0.00	-4.37±0.00	-4.28±0.00	-4.56±0.00
chloroethylene	-0.59	-0.09±0.00	-0.36±0.00	-0.50±0.00	-0.13±0.00
2-methylpropane	2.32	1.90±0.00	1.89±0.00	1.95±0.00	1.93±0.00
N,N-dimethylaniline	-3.45	-3.67±0.00	-3.64±0.00	-6.50±0.00	-4.39±0.00
2-methylpyrazine	-5.51	-7.89±0.00	-8.79±0.00	-11.28±0.00	-8.53±0.00
pentanoic acid	-6.16	-9.35±0.05	-6.29±0.03	-5.77±0.05	-7.09±0.03
ethyl hexanoate	-2.23	-3.70±0.00	-4.29±0.00	-4.32±0.00	-5.05±0.03
3,3,3-trimethoxypropionitrile	-6.40	-6.91±0.01	-7.37±0.01	-7.70±0.01	-8.61±0.01
phenol	-6.61	-9.25±0.01	-6.62±0.01	-6.97±0.01	-6.54±0.01
cyclohepta-1,3,5-triene	-0.99	-1.00±0.01	-1.40±0.01	-1.85±0.01	-1.02±0.01
methyl propanoate	-2.93	-4.73±0.00	-5.45±0.00	-5.38±0.00	-5.70±0.00
1,2-dichlorobenzene	-1.36	-0.78±0.00	-1.21±0.00	-1.73±0.00	-0.93±0.00
2-methylpentan-3-ol	-3.88	-3.88±0.01	-2.45±0.01	-1.86±0.01	-3.59±0.01
oct-1-ene	1.92	1.76±0.00	1.65±0.00	1.88±0.00	1.62±0.00
2-nitrotoluene	-3.58	-8.69±0.00	-9.72±0.00	-10.02±0.00	-9.38±0.01
di-isopropyl sulfide	-1.21	-0.27±0.01	-0.58±0.01	-0.50±0.01	-1.30±0.01
2,3-dimethylbutane	2.34	2.13±0.00	2.16±0.00	2.21±0.00	2.14±0.00
thiophene	-1.42	-0.96±0.00	-1.35±0.00	-2.39±0.00	-1.09±0.00
piperazine	-7.40	-5.11±0.03	-5.58±0.03	-7.80±0.03	-8.25±0.09
prop-2-en-1-ol	-5.03	-6.17±0.01	-4.52±0.01	-4.04±0.01	-4.98±0.01
isopropylbenzene	-0.30	-0.72±0.00	-1.02±0.00	-1.74±0.00	-1.03±0.00
2,2,2-trifluoroethanol	-4.31	-10.05±0.01	-6.99±0.01	-8.22±0.01	-6.90±0.01
n-pentylcyclopentane	2.55	2.63±0.00	2.69±0.00	2.69±0.00	2.49±0.00
2-butoxyethanol	-6.25	-5.83±0.01	-4.03±0.01	-3.79±0.01	-7.48±0.72
N,N-dimethylbenzamide	-9.29	-7.88±0.01	-8.73±0.01	-9.82±0.01	-9.03±0.01
but-1-yne	-0.16	0.19±0.00	-0.05±0.00	-0.07±0.00	0.26±0.00
N-methylpiperidine	-3.88	-0.13±0.03	0.64±0.03	-2.10±0.03	-2.16±0.05
4-methylacetophenone	-4.70	-5.84±0.00	-6.67±0.00	-7.60±0.00	-6.57±0.00

fluoromethane	-0.22	-0.70±0.00	-0.92±0.00	-0.89±0.00	-0.76±0.00
1,2,3-trichlorobenzene	-1.24	-0.16±0.00	-0.54±0.00	-0.94±0.00	-0.31±0.00
2-chloropropane	-0.25	0.06±0.00	-0.12±0.00	-0.07±0.00	-0.13±0.00
4-chloroaniline	-5.90	-5.64±0.00	-6.35±0.00	-7.24±0.00	-6.27±0.00
hexa-1,5-diene	1.01	0.76±0.00	0.53±0.00	0.82±0.00	0.63±0.00
2-methylbut-2-ene	1.31	1.28±0.00	1.17±0.00	1.14±0.00	1.19±0.00
di-n-propyl ether	-1.16	0.14±0.00	0.04±0.00	-0.44±0.00	-0.97±0.02
m-cresol	-5.49	-8.82±0.01	-6.13±0.01	-6.51±0.01	-6.27±0.01
trichloroethene	-0.44	0.73±0.00	0.49±0.00	0.17±0.00	0.73±0.00
ethene	1.28	0.71±0.00	0.62±0.00	0.84±0.00	0.85±0.00
n-hexane	2.48	2.21±0.00	2.21±0.00	2.31±0.00	2.19±0.00
hept-1-yne	0.60	0.70±0.00	0.47±0.00	0.50±0.00	0.69±0.00
1-methylnaphthalene	-2.44	-2.73±0.00	-3.19±0.00	-4.52±0.00	-3.19±0.00
dimethyl ether	-1.91	-1.20±0.00	-1.68±0.00	-1.85±0.00	-1.93±0.00
methyl cyclohexanecarboxylate	-3.30	-3.69±0.05	-4.31±0.05	-4.08±0.05	-4.90±0.05
pentanal	-3.03	-4.43±0.01	-5.04±0.01	-4.58±0.01	-4.96±0.01
1H-pyrrole	-4.78	-4.55±0.00	-5.09±0.00	-6.25±0.00	-4.50±0.00
penta-1,4-diene	0.93	0.50±0.00	0.28±0.00	0.51±0.00	0.43±0.00
3-nitrotoluene	-3.45	-8.24±0.01	-9.25±0.01	-9.69±0.01	-8.58±0.01
cyanobenzene	-4.10	-4.57±0.00	-5.18±0.00	-5.77±0.00	-4.57±0.00

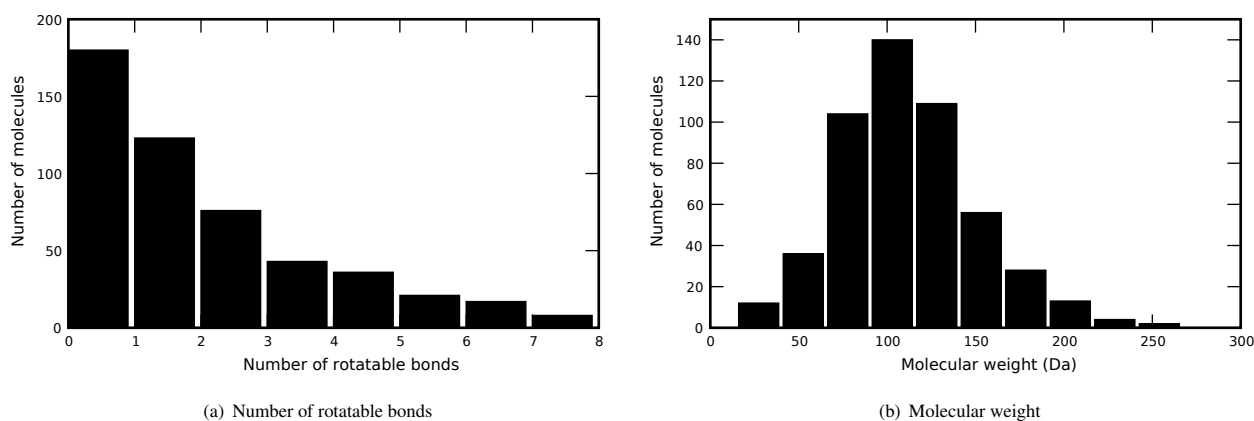


Figure 1. Distributions of the number of rotatable bonds and molecular weight for the 504 molecule test set.

References

- [1] Rizzo, R. C.; Aynechi, T.; Case, D. A.; Kuntz, I. D. *J. Chem. Theory Comput.* **2006**, *2*, 128-139.
- [2] Bordner, A. J.; Cavasotto, C. N.; Abagyan, R. A. *J. Phys. Chem. B.* **2002**, *106*, 11009-11015.
- [3] Shirts, M. R.; Pitner, J. W.; Swope, W. C.; Pande, V. S. *J. Chem. Phys.* **2003**, *119*, 5740-5761.
- [4] Guthrie, J. P. *Can. J. Chem.* **1991**, *69*, 1893-1903.
- [5] Guthrie, J. P. *Can. J. Chem.* **1976**, *54*, 202-209.
- [6] et al., J. P. G. *Can. J. Chem.* **1980**, *58*, 1281-1294.
- [7] et al., J. P. G. *Can. J. Chem.* **1992**, *70*, 1671-1683.
- [8] Guthrie, J. P. *Can. J. Chem.* **1992**, *70*, 1942-1054.
- [9] et al., C. H. R. *J. Chem. Soc. Faraday Trans. 1* **1973**, 1577-1585.
- [10] Guthrie, J. P. *J. Am. Chem. Soc.* **1973**, *95*, 6999-7003.
- [11] Lu, J. **1994**, Ph.D. Thesis, University of Western Ontario.
- [12] et al., J. P. G. *Can. J. Chem.* **1993**, *71*, 2109-2122.

- [13] Guthrie, J. P. manuscript in preparation.
- [14] Guthrie, J. P. Unpublished data.
- [15] et al., S. W. *Env. Tech. Lett.* **1987**, *8*, 483-486 Estimated by J. Peter Guthrie from Henry's law constant at 298 K by interpolation using the temperature dependence equation.
- [16] et al., J. P. G. *Can. J. Chem.* **1998**, *76*, 929-936.
- [17] et al., J. P. G. Manuscript in preparation.
- [18] et al., W. J. D. *J. Geophys. Res.* **1994**, *99D*, 16927-16932.
- [19] Guthrie, J. P. personal communication, based on Henry's law constant.
- [20] Guthrie, J. P. *Can. J. Chem.* **1978**, *56*, 2342-2354.
- [21] et al., M. H. A. *J. Chem. Soc. Perkin Trans. 2* **1994**, *2*, 1777-1791.
- [22] Wolfenden, R.; Williams, R. *J. Am. Chem. Soc.* **1983**, *105*, 1028-1031.
- [23] Tsui, V.; Case, D. A. *Biopolymers (Nucl. Acid. Sci.)* **2001**, *56*, 275-291.
- [24] Onufriev, A.; Bashford, D.; Case, D. A. *Proteins: Struct., Funct., Bioinf.* **2004**, *55*, 383-394.
- [25] Mongan, J.; Simmerling, C.; McCammon, J. A.; Case, D. A.; Onufriev, A. *J. Chem. Theor. Comput.* **2007**, *3*, 156 - 169.

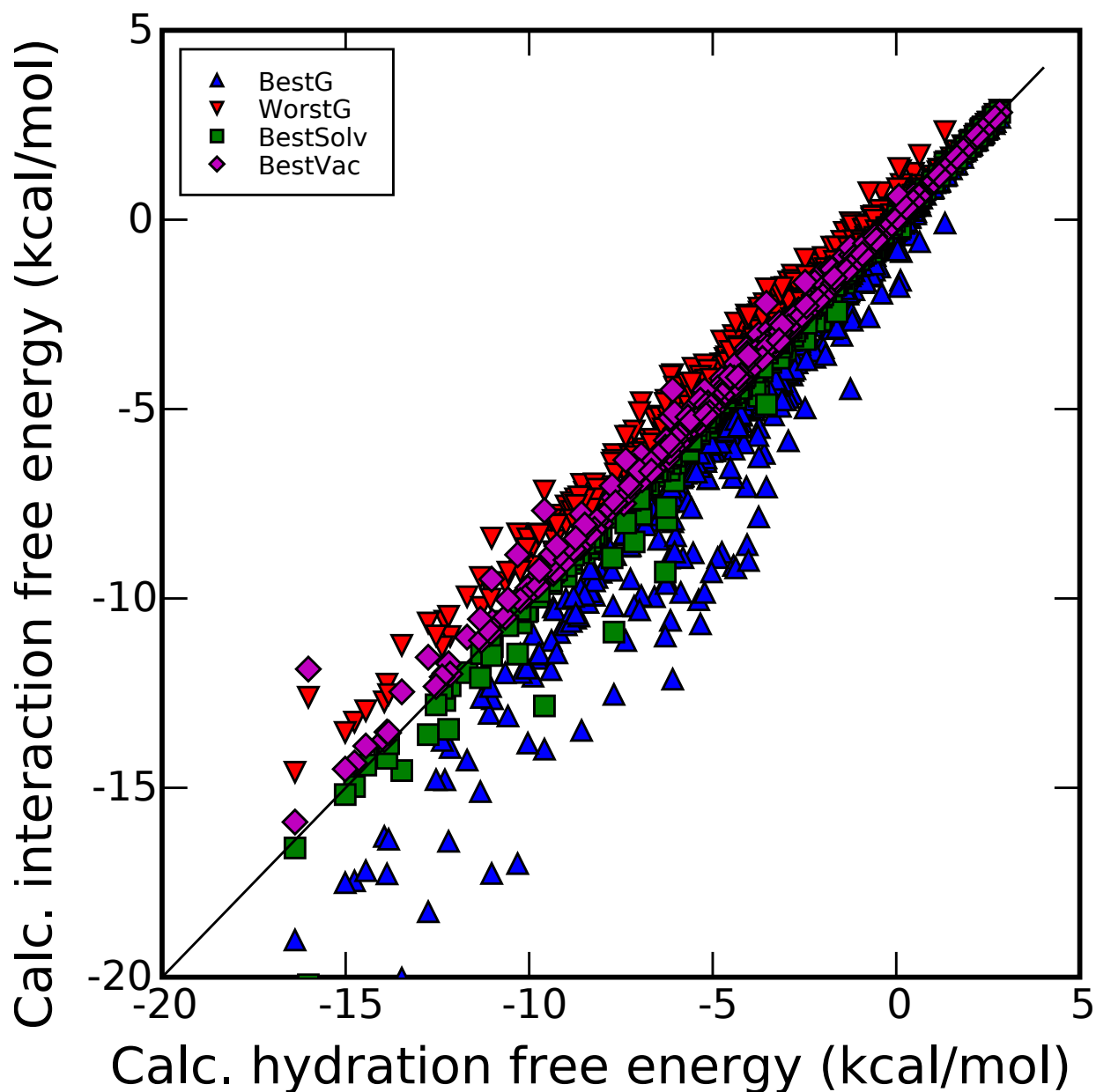


Figure 2. Calculated hydration free energies versus interaction free energies computed with different conformations. Calculated hydration free energies are plotted, versus single-conformation interaction free energies computed using the different schemes for selecting conformations: BestG, the conformation resulting in the most favorable interaction free energy; WorstG, the conformation resulting in the least favorable interaction free energy; BestVac, the conformation with the lowest potential energy in vacuum; BestSolv, the conformation with the lowest potential energy in solvent. The diagonal line is the $x = y$ line, and indicates exact agreement between calculated interaction free energies and calculated hydration free energies.