

WATER SOLUBILITY:

**COMPARISON OF TEST RESULTS AND
PREDICTIONS**

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [± log units]	Result
4	reacts (decomposes)	reacts	-	agree
6	hydrophobic	< 10 ⁻³	-	agree
16	> 700,000 [10,000]	> 700,000 [10,000]	0	agree
17	100,000 [10,000]	50,000 [10,000]	0	agree
21	< 0.8	< 0.01	-1.9	disagree
23	mixes with each other in all ratios	~200,000	-	agree
24	17.2	≤ 0.15 x 10 ⁻³ [0.01]	-3.2	disagree
26	0.1 - 0.5	< 1.6 x 10 ⁻³ [0.01]	-1.7	disagree
37	1	1	0	agree
44	< 5	0.01	-2.7	disagree
47	145.7	< 1	-2.2	disagree
49	1,450	~100,000 [10,000]	0.8	agree
50	5.3 +/- 3	< 0.1	-1.4	disagree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [± log units]	Result
53	nd	≤0.1	-	-
54	17.9	500	+1.4	disagree
61	<0.05	<0.1	+0.3	agree
68	145,000 [10,000]	>100,000 [10,000]	0	agree
69	>48,000 [10,000]	200,000 [10,000]	0	agree
70	30	<2	-1.1	disagree
76	7.7	<10	+ 0.1	agree
78	<0.05	<1	+ 1.3	disagree
79	<0.03	<0.1	+ 1.5	disagree
87	4,040	2,000	-0.3	agree
96	<500,000 [10,000]	100,000 [10,000]	0	agree
99	reacts	reacts	-	agree
101	32,000 [10,000]	<250,000 [10,000]	0	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [$\pm$ log units]	Result
102	0.17	<1	+0.7	agree
106	<0.2	$2.4 \cdot 10^{-3}$ [0.01]	-1.3	disagree
107	reacts	reacts	-	agree
108	0.19	≤ 0.1	-0.3	agree
110	<1	0.01	-2.0	disagree
113	0.065	5×10^{-3} [0.01]	-0.15	agree
118	58	<25,000 [10,000]	+2.2	disagree
124	182	900	+0.7	agree
128	<10	<1	-1.0	agree
133	2.3	2.3	0	agree
144	<0.01	<1	+2.0	disagree
148	<0.005 [0.01]	<0.1	+1.0	agree
151	5.61	0.1 - 10	-0.7	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [$\pm$ log units]	Result
155	<0.3	$\leq 10^{-4}$	-1.4	disagree
156	13	10 - 100	+0.5	agree
164	39	<5	-0.9	agree
170	69,190 [10,000]	140,000 [10,000]	0	agree
173	nd	≤ 5	-	-
176	<10	<10	0	agree
182	<10	<2,000	+2.3	disagree
186	0.9	9	+1.0	agree
192	hydrolyses	2,500	-	-
194	479,000 [10,000]	$\geq 100,000$ [10,000]	0	agree
196	>300,000 [10,000]	>200,000 [10,000]	0	agree
197	8.2	<1000	+2.1	disagree
200	0.071	0.0064 [0.01]	-0.8	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [$\pm$ log units]	Result
204	0.27	<0.1	-0.4	agree
214	<0.1	<1000	+4.0	disagree
216	4.2×10^3	<100	-1.6	disagree
217	<0.07	<100	+3.1	disagree
218	63+/-5	<50	-0.1	agree
219	363	<1000	+0.4	agree
222	1.52	reacts	-	-
224	180,000 [10,000]	60,000 [10,000]	0	agree
235	<10 (hydrolyses)	≤ 0.1	-2.0	agree
237	18	18 (reacts)	0	agree
239	<0.01	$\leq 10^{-3}$ [0.01]	0	agree
240	299,000 [10,000]	100,000-200,000 [10,000]	0	agree
241	4.55×10^6 [10,000]	>100,000 [10,000]	0	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [± log units]	Result
242	> 11.7 x 10 ⁶ [10,000]	100,000 [10,000]	0	agree
253	< 0.02	0.02	0	agree
256	470,000 [10,000]	10,000 - 50,000 [10,000]	0	agree
263	77,500 [10,000]	90,000 - 100,000 [10,000]	0	agree
265	712,900 [10,000]	1,000 - 5,000	-0.6	agree
267	nd	< 0.1	-	-
268	2.3	< 5	+0.3	agree
269	3	3	0	agree
270	730	1 - 1000	-	-
271	5,000 - 10,000	< 1000	-0.9	agree
275	< 0.04	0.2	+0.7	agree
278	< 30	≤ 10	-0.4	agree
281	3	< 10	+0.4	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [$\pm$ log units]	Result
283/ 429	<0.5	$\leq 10^{-3}$ [0.01]	-1.7	disagree
286	0.019	$< 10^{-3}$ [0.01]	-0.3	agree
287	0.005 - 0.009 [0.01]	<0.1	+1.0	agree
289	0.091	≤ 0.01	+0.04	agree
291	<60	<1	-1.8	agree
292	37	900 (pH 1.1) 45 (pH 7.8) (Lit. value)	-	-
300	56	<1000	+1.2	disagree
307	16	<1000	+1.8	disagree
309	0.022 - 0.042	<1	+1.5	disagree
312	214,000 [10,000]	>100,000 [10,000]	0	agree
318	53	<100	+0.3	agree
320	<0.007 [0.01]	<10	+3.0	disagree
321	57,000 [10,000]	5,000 - 15,000	0	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [$\pm \log$ units]	Result
330	1570	> 100,000 [10,000]	0.8	agree
335	n.d.	< 10	-	-
336	11,500 [10,000]	< 100	-2.0	disagree
337	660	< 7	-2.0	disagree
340	749	20,000 [10,000]	+1.1	disagree
341	66	1,000 - 10,000	+1.9	disagree
342	65,800	80,000	+0.08	agree
344	nd (subst. only stable in aqu. solution)	200,000	-	-
348	0.053	< 0.1	+0.3	agree
349	< 0.2	< 0.1	-0.3	agree
354	31	< 50	+0.2	agree
355	0.008 [0.01]	7.9×10^{-3} [0.01]	0	agree
360	1410	500 - 1,500	-0.1	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [$\pm$ log units]	Result
361	0.153	<10	+1.8	disagree
362	4.6 - 4.9	<150	+1.5	disagree
364	>300,000 [10,000]	$\geq$ 200,000 [10,000]	0	agree
366	11	<0.1	-2.0	disagree
368	14	reacts	-	-
369	479,000 [10,000]	370,000 [10,000]	0	agree
370	nd (decomposes)	8,000	-	-
373	12.7	5 - 15	-0.1	agree
376	0.04	0.03	-0.1	agree
379	1.45	9	+0.8	agree
381	<10 ⁻³ [0.01]	<0.01	0	agree
383	<0.03	<0.1	+0.5	agree
386	19 pH 5 18 pH 7 16 pH 9	<300	+1.2	disagree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [± log units]	Result
393	0.6	<10	+1.2	disagree
394	1140 x 10 ³ [10,000]	~500,000 [10,000]	-0	agree
396	61,400 [10,000]	1,000 - 2,000	-0.8	agree
398	hydrolyses	reacts	-	agree
401	137.5	500 - 1,000	0.7	agree
406	<0.01	0.1	+1	agree
411	<0.0015 [0.01]	≤0.1	+1	agree
413	<0.03	1	+1.5	disagree
414	3,300	100 - 10,000	-0.5	agree
415	≤0.005 [0.01]	<0.1	+1.0	agree
416	0.0048 [0.01]	<0.1	+1.0	agree
417	1.26 x 10 ⁻⁴ [0.01]	<1	+2.0	disagree
420	1.6 pH 5 1.4 pH 7 1.5 pH 9	<10	+0.8	agree

Chem. No.	MPD water sol. [mg/l]	SAR water sol. [mg/l]	Difference [± log units]	Result
421	50 x 10 ⁻⁶ [0.01]	<1	+2.0	disagree
425	>990,000 [10,000]	200,000 [10,000]	0	agree
431	0.078	<0.1	+0.1	agree
436	<10 ⁶	<100	-2.0	disagree
437	0.012	<1	+1.9	disagree
439	480	5,000 - 50,000	+1.3	disagree
441	9,550	≥40,000 [10,000]	+0.02	disagree
442	6,210	≤ 10,000	+0.2	agree
443	nd	1,000 - 10,000	-	-
444	61	100	+0.2	agree
445	<0.5	<1 (acid)	+0.3	agree
446	<0.02	<0.001 [0.01]	-0.3	agree
451	20,000 [10,000]	10,000 - 50,000 [10,000]	0	agree
472	16.2	<0.05	-2.5	disagree