ERRATA

Estimation of the Aqueous Solubility of Organic Molecules by the Group Contribution Approach [*J. Chem. Inf. Comput. Sci. 41*, 439−455 (2001)] By Gilles Klopman* and Hao Zhu. Department of Chemistry, Case Western Reserve University, 10900 Euclid Avenue, Cleveland, Ohio 44106

Pages 441 and 442. The data listed in Tables 5 and 6 were not correct. The correct tables are as follows.

Table 5. Basic Parameter Set of the Group Contribution Method[a]

no.	parameter	freq of use	coeff	*t* value	no.	parameter	freq of use	coeff	*t* value
1	-CH3 or CH4	2062	−1.212	60.051	27	-CH═O	12	0.909	5.477
2	-CH2-	1805	−0.658	75.944	28	-C(═O)OH aromatic	29	−0.501	3.928
3	-CH<	418	−0.126	3.331	29	-C(═O)OH aliphatic	56	0.688	9.886
4	=CH2	50	−1.261	14.447	30	-C(═O)O- ester	132	0.431	6.671
5	=CH- not in HC(═O)-	102	−0.38	6.762	31	-C(═O)O- ester, in a ring	6	−1.287	4.844
6	=C< non in -C(═O)-,-C(═S)-	54	0.262	3.158	32	-C(═O)N<	120	0.503	11.123
7	=C= in S═C═N-	3	−1.512	4.779	33	-C(O)N=	4	−0.782	2.743
8	C$CH (triple bond)	12	−0.922	6.116	34	-C(═O)-	29	0.48	2.607
9	-CH2- in a ring	443	−0.689	31.795	35	-C(═O)- in a ring	37	0.281	1.9
10	-CH< in a ring	235	−0.317	8.027	36	-S═O	8	0.813	4.04
11	>C< in a ring	173	0.406	8.802	37	-CH2-NH2	2	2.397	5.957
12	=CH- in a ring	2777	−0.533	52.819	38	Ph-NH2	28	−0.128	1.195
13	F- aliphatic	22	−1.295	14.761	39	-NH2 other	16	−0.364	2.333
14	F- aromatic	100	−0.57	15.508	40	-NH-	58	0.917	11.667
15	Cl- aromatic	423	−1.615	81.376	41	-N-	83	2.425	31.73
16	Cl- aliphatic	264	−1.054	36.763	42	-N$C aromatic	6	−0.464	2.367
17	Br- aromatic	43	−2.129	38.829	43	-N$C aliphatic	14	1.243	6.006
18	Br- aliphatic	49	−1.174	19.975	44	=NH or -N=	14	0.176	1.124
19	I- aromatic	17	−2.391	16.906	45	-N= in a ring	254	−0.354	10.213
20	I- aliphatic	11	−1.779	14.066	46	-NO2 aromatic	71	−1.406	20.649
21	-CH2-OH	53	1.794	20.409	47	-SH	8	−0.853	4.666
22	-CH -OH	59	1.652	14.171	48	-S-	69	−0.344	4.157
23	Ph -OH	30	2.574	16.354	49	-S- cyclic	17	−0.921	6.283
24	-OH other	61	0.911	8.708	50	-C(═S)-	11	−2.71	16.8
25	-O- in a ring	35	−0.529	4.8	51	P═O	19	1.753	9.24
26	-O- not in ester	250	0.749	14.147	52	P═S	38	−0.463	2.637

[a] The value of constant C_0 is 5.0924.

Table 6. Extended Parameters of the Group Contribution Approach[a]

no.	parameter	freq of use	coeff	*t* value	no.	parameter	freq of use	coeff	*t* value
53(1)	cH -n =c -NH2	18	−1.481	11.839	81(1)	O -C∧H -C∧H -O -	11	−1.607	12.118
53(2)	n =c -OH				81(2)	OH -C∧H -C∧H -OH			
54	F- C -c =c - ⟨2-F⟩	6	−0.405	2.627	81(3)	OH -C∧H -C∧H -NH -			
55	N∧ -C∧H2-C∧H2-N∧ -	10	−0.737	4.769	81(4)	OH -C∧H -C∧H -O -			
56	S -PS -O -CH3	14	−0.289	2.403	81(5)	OH -C∧H -C∧ -OH			
57	NH -c -n =c -n =c -NH - ⟨4-Cl⟩	4	−1.196	3.873	82(1)	CH3-CO -CH2-	13	1.103	6.43
58(1)	cH =cH -c -O -PS -O -CH3 ⟨5-O -CH3⟩	15	−1.408	11.491	82(2)	CO -CH2-CH3			
					83	c =c -N -CO -CH2-	14	1.022	8.979
58(2)	c -c -O -PS -O -CH3 ⟨4-O -CH3⟩				84(1)	N∧ -C∧" -CH3	8	0.624	4.67
58(3)	n =c -n =c -O -PS -O -CH3				84(2)	N∧ =C∧ -C∧H2-			
59(1)	Cl -C =CH - ⟨2-Cl⟩	15	−0.934	5.798	84(3)	N∧ =C∧ -C -CH3			
59(2)	Cl -C =C - ⟨2-Cl⟩				85	O -CO -CH2-	22	0.853	6.548
59(3)	Cl -C∧ -C∧ =C∧ - ⟨2-Cl⟩				86	N∧ =C∧ -c =	7	2.132	9.632
60(1)	Cl -c =c. -	26	−0.908	11.559	87(1)	CH3-CO -O -CH2-	13	0.958	5.338
60(2)	Cl -c =c -cH =c. -				87(2)	CH3-CO -O -CH -			
60(3)	Cl -c =c -c =cH -cH =cH - ⟨4-Cl⟩				87(3)	CH3-CO -O -CH3			
61(1)	O -CH2-CH2-	65	0.57	9.148	88	CO -CH -c =cH -cH =cH - ⟨3-c -⟩	8	0.426	3.882
61(2)	O -CH2-C =				89	cH -c -CH2-CO -	8	−0.104	0.702
61(3)	O -CH2-CH -				90	CO -O -c -cH =	23	−0.289	2.951
62	cH =cH -n =c. -cH =	9	1.993	9.642	91	C∧O -C∧H =C∧ -	5	1.502	5.122
63(1)	CH -CH2-CH2-CH -	156	−0.242	7.148	92(1)	OH -C -CH3	91	0.218	3.762
63(2)	CH3-CH -CH -CH2-CH2-				92(2)	OH -CH -CH3			
63(3)	CH3-CH2-CH -CH -CH3				92(3)	OH -CH2-C -			
63(4)	CH2-CH2-CH -CH2-CH -				92(4)	OH -C -CH2-CH3			
63(5)	CH3-CH2-CH -CH2-CH -				92(5)	OH -CH -CH -CH3			
63(6)	CH3-CH2-CH -CH2-CH2-				92(6)	OH -CH -CH2-CH3			
63(7)	CH3-CH -CH2-CH2-CH2- ⟨2-CH3⟩				92(7)	OH -CH2-CH -CH3			
63(8)	CH2-CH2-CH -CH2-CH2- ⟨3-CH2-⟩				92(8)	CH2-CH2-CH -CH2- ⟨3-OH⟩			
63(9)	CH3-CH2-CH2-CH2-CH -CH3				92(9)	OH -CH -CH2-CH2-CH2-			
63(10)	CH2-CH2-CH -CH - ⟨3-CH3⟩				93(1)	S -CH -CH3	28	0.082	1.074

Table 6 (Continued)

no.	parameter	freq of use	coeff	*t* value	no.	parameter	freq of use	coeff	*t* value
64(1)	CH3-C∧ -C∧ -C∧H2- ⟨2-CH3⟩	21	−0.34	4.517	93(2)	S -CH2-CH2-			
64(2)	C∧H2-C∧H2-C∧H -C∧H2- ⟨3-CH3⟩				93(3)	S∧ -C∧H2-C∧H2-			
64(3)	CH2-CH2-C∧H -C∧H2-C∧H2- ⟨3-C∧H2-⟩				93(4)	S -CH2-CH2-CH3			
					94	PO -S -	9	0.516	2.764
64(4)	C∧H2-C∧H2-C∧ -C∧H2-				95	CH2-N -CH2- ⟨2-CO -⟩	9	2.358	12.191
65(1)	cH =c. -cH =c. -cH =	30	−0.582	9.346	96	CH"-CH2-C∧ -CH -	4	0.656	2.185
65(2)	c =cH -cH =c. -cH =c -				97	cH =c -c =cH - ⟨2-OH⟩	14	−0.71	4.033
65(3)	cH =c. -cH =cH -cH =cH -c. =cH -				98	N -c =n -c -O -	4	−0.413	1.217
66(1)	N∧H -c. =c. -	18	−1.357	13.144	99(1)	c =cH -cH =c -C∧ -c =	5	0.363	2.39
66(2)	N∧H -C∧O -c. =				99(2)	cH =cH -c =c. -cH =c -			
66(3)	N∧H -C∧O -C∧. -				100(1)	Cl -c =c -OH	9	1.029	5.376
67(1)	C∧O -N∧H -C∧O -N∧ -	4	−2.082	7.592	100(2)	Cl -c =c -CH2-			
67(2)	C∧O -N∧H -C∧O -N∧H -C∧H =				101	C∧O -C∧ -CH2-CH2-	22	0.336	4.282
68	CO -C∧ -C. - ⟨3-OH⟩	9	−3.211	9.854	102	c -c =c - ⟨2-OH⟩	4	−0.722	2.02
69(1)	N -c =cH -cH =c -	25	−0.282	2.558	103(1)	CH2-O -CH -	6	1.119	5.658
69(2)	N∧ -c =cH -cH =c -				103(2)	CH2-O -C∧H -			
69(3)	NH2-c =c -cH =c -				104	c. -C∧H2-c. -	4	−0.982	3.61
69(4)	NH2-c =c. -				105	C∧O -N∧H -C∧S -N∧H -	4	0.84	3.911
69(5)	N -c =c -cH =c -c =				106	C∧H -C∧H2-C∧H2-C.H -C.H -C∧H2-C∧H2-C. =	6	1.048	3.667
69(6)	cH =c -cH =c - ⟨2-NH -⟩								
69(7)	NH2-c =c. -cH =				107	CH2-O -c =c -cH =c -cH = ⟨6-Cl⟩	4	−0.643	2.077
70(1)	N∧H -c. =n -	8	0.564	3.105	108	NO2-c -cH =c -NO2	6	0.695	3.074
70(2)	N -c =n -c =c -				109(1)	c -O -CH -CH3 ⟨3-CH3⟩	6	0.739	3.676
70(3)	N -c =n -c =n -				109(2)	CH3-CH2-O -CH2-			
71	OH -CO -c =cH -cH = c - ⟨4-cH=⟩	16	−0.336	2.953	110	cH =cH -n =c. -c =	6	1.359	5.429
72	C∧O -c. =cH -cH =cH -cH = c. -C∧O -	6	−0.979	5.399	111	cH =cH -c -O -c -cH =c -CH -	16	−1.205	7.908
					112(1)	CO -CH =CH -c =	4	−2.749	9.296
73(1)	OH -c =cH -cH =c -OH	11	−0.488	3.651	112(2)	CO -C∧ =C∧H -			
73(2)	OH -c =cH -cH =c -NH -				113	N∧H -C∧O -C∧ -CH - CH2- ⟨4-CH2-⟩	12	0.33	2.587
73(3)	OH -c =cH -cH =c -NH2								
73(4)	OH -c =cH -cH =c -C" -				114(1)	NH -CO -c =cH -	7	0.328	1.967
74	cH =cH -cH =c -c =	176	0.169	4.843	114(2)	CH3-NH -CO -CH2-			
75	N -CH -CH3	14	0.476	5.203	115	I -c =c -	6	0.113	0.473
76	CH2-NH -CH2-CH2-	4	1.057	5.473	116(1)	O∧ -C∧ -CH2-	9	1.04	6.857
77(1)	cH =c -c1 =cH -cH =c -c -	23	−0.354	5.04	116(2)	O∧ -C∧H -O∧ -			
77(2)	cH =c -cH =c -c = c1 - c =				116(3)	O∧ -C∧H2-C∧H2-O∧ -			
77(3)	cH =cH -c =cH -cH =c -c1 =cH -cH = ⟨7-cH=⟩				117(1)	c. -c,	262	−0.7	30.323
					117(2)	c. -c. -			
78(1)	cH =cH -cH =c -c1 =c -c = ⟨6-Cl⟩	23	−0.328	4.032	117(3)	c,-c,			
78(2)	Cl -c =cH -c =c1 - ⟨4-cH=⟩				118(1)	c -N -CO -NH -CH3	8	1.63	7.988
78(3)	cH =cH -c =cH -c. =cH - ⟨3-Cl⟩				118(2)	c -NH -CO -NH -SO2-			
79	C∧H =C∧H -C∧O -C∧H =C. -	8	−0.813	2.792	118(3)	c -NH -CO -NH -C∧H -			
80	CH2-CH2-O -c =	5	−0.667	2.416	118(4)	c -NH -CO -N -CH2-			

[a] ∧ element is included in one ring; . element is included in two rings; , element is included in three rings; c, o, n aromatic elements; " double bond attached.

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