

————— *Supporting Information* —————

**Feature selection in molecular graph neural  
networks based on quantum chemical approaches**

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## Supplementary Figures and Table

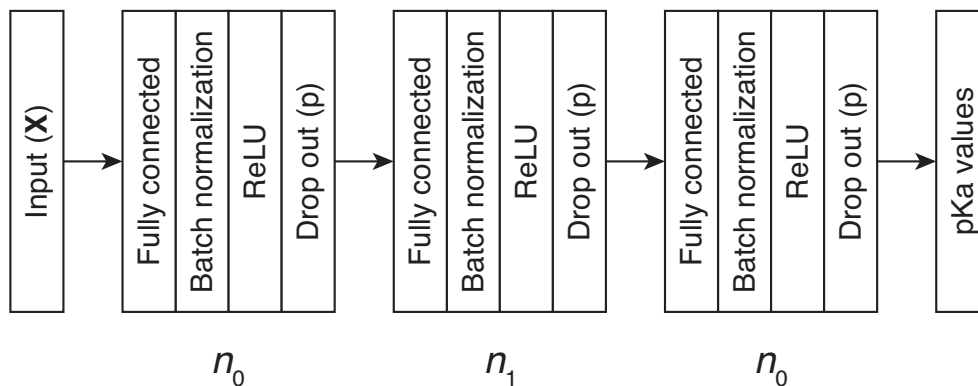


Figure S1: Details of machine learning process

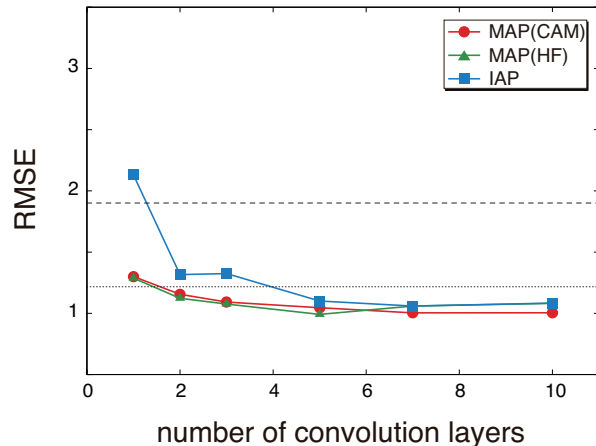


Figure S2: Root mean square errors (RMSEs) of the pKa values obtained by IGC and two types of atom features (IAP and MAP) with different number of convolution layers (1, 2, 3, 5, 7, and 10). The MAPs were computed at CAM-B3LYP/aug-cc-pVDZ level (CAM) and Hartree-Fock/6-31G\*\* level (HF). For comparison, the RMSEs computed with MolGpka and OPERA are also shown with black dashed and dotted lines, respectively.

Table S1: Comparison between experimental and calculated pKa values. In the cases of important graph convolution (IGC), simple graph convolution (SGC), and simple graph convolution network (SGCN), the data were computed with ten convolution layers ( $L = 10$ ).

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
617-97-0	-6.56	-6.73	0.58	-6.64	-4.58	-4.97	-4.82	4.36
463-56-9	0.85	3.75	6.60	4.12	2.33	2.25	2.42	2.47
5515-35-5	1.00	4.08	5.06	3.16	3.99	2.12	7.29	4.03
3112-46-7	1.34	1.75	1.24	1.75	1.85	2.22	1.74	2.68
38876-67-4	1.37	1.64	1.47	2.13	2.20	1.98	2.13	4.48
151-01-9	1.79	1.90	8.46	2.15	2.62	2.85	2.71	2.64
1199-67-3	1.86	1.39	1.02	0.47	1.49	1.08	1.29	1.81
6795-92-2	1.89	1.80	1.28	1.97	2.48	2.03	1.51	4.64
89324-43-6	1.94	1.75	2.04	2.49	2.78	3.05	2.03	8.34
99-60-5	1.96	2.36	2.06	2.28	2.92	2.17	3.11	2.56
1321-11-5	2.08	10.75	2.76	4.16	3.92	4.23	3.63	4.02
204326-31-8	2.13	3.25	3.96	3.83	3.15	3.15	5.44	5.80
2566-34-9	2.20	3.21	2.30	3.32	4.17	3.97	4.50	8.78
5683-31-8	2.21	2.23	3.54	2.54	4.19	2.65	3.21	5.07
552-16-9	2.23	2.51	2.49	2.86	2.85	2.68	3.02	3.72
601-99-0	2.24	6.47	2.34	-0.14	2.98	2.12	2.39	2.97
637-44-5	2.26	2.03	2.36	2.85	2.83	3.32	2.24	3.29
6787-46-8	2.51	3.77	2.61	3.27	3.03	3.24	3.34	3.59
74893-46-2	2.55	2.17	2.44	2.91	2.90	3.02	2.56	3.39
1483-67-6	2.61	2.17	2.71	2.99	2.77	3.15	2.54	4.48
590-93-2	2.63	2.14	2.73	3.07	3.01	3.05	2.57	3.54
80220-95-7	2.67	1.93	2.57	2.88	2.84	3.22	2.30	3.94
90259-31-7	2.71	2.30	2.42	2.69	2.76	2.89	2.96	4.94

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
769-40-4	2.75	1.91	6.04	4.40	4.24	4.22	2.74	4.58
40991-34-2	2.76	3.00	2.86	3.02	2.59	3.10	2.45	3.35
1975-51-5	2.91	3.53	3.01	3.11	3.58	2.95	3.89	2.76
54045-76-0	2.96	3.03	3.06	2.93	2.86	2.79	2.59	4.93
594-58-1	2.97	2.43	3.79	2.78	4.34	3.30	4.26	6.32
2164-61-6	3.00	2.59	2.90	2.87	2.44	3.30	2.22	5.59
6967-82-4	3.00	2.81	3.06	3.05	2.88	3.34	3.02	6.20
849067-18-1	3.10	4.77	1.06	2.72	3.11	3.03	3.27	3.13
133232-68-5	3.17	2.73	2.96	3.40	3.21	3.24	3.70	3.06
6345-67-1	3.22	2.54	2.45	2.90	3.12	2.54	3.31	3.22
866-32-0	3.22	3.12	3.12	3.59	3.41	3.86	3.34	2.85
632-46-2	3.23	3.38	3.47	3.90	3.71	4.13	3.97	4.28
6319-40-0	3.24	3.01	3.14	3.23	3.12	2.74	3.54	3.33
59337-97-2	3.30	8.09	3.20	2.60	3.17	2.28	3.11	3.06
453-71-4	3.37	3.06	3.47	3.37	3.22	3.36	3.62	3.67
32821-75-3	3.38	3.12	3.49	3.47	3.43	3.29	3.47	3.80
77133-27-8	3.41	3.31	3.31	3.61	3.19	3.47	3.44	4.08
2604-45-7	3.43	3.27	3.53	3.66	3.31	3.95	3.89	4.93
6926-49-4	3.44	3.88	3.67	3.45	3.73	3.76	3.91	4.10
50907-33-0	3.45	3.88	3.54	3.37	3.89	3.40	3.89	3.50
90259-35-1	3.51	3.22	3.41	3.63	3.42	3.89	3.33	11.89
4607-38-9	3.53	11.80	3.56	3.23	3.74	3.07	3.99	5.40
71515-74-7	3.55	3.85	3.84	3.82	3.75	3.60	3.84	3.85
56-91-7	3.59	3.97	3.69	4.47	4.09	4.38	3.99	3.38
14778-29-1	3.60	n/a	n/a	5.06	7.10	5.55	5.44	4.30
636-76-0	3.61	8.93	3.71	3.84	3.51	3.65	3.81	3.59

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
85-55-2	3.64	3.67	3.74	3.71	3.35	3.90	3.49	4.42
168902-34-9	3.66	3.48	3.56	3.39	3.64	3.43	3.64	4.03
50907-46-5	3.69	3.80	4.17	4.16	4.16	3.92	3.70	4.36
19182-29-7	3.70	1.60	3.60	1.82	2.02	2.73	2.51	4.63
603-79-2	3.73	3.76	3.83	4.06	3.72	4.13	3.98	3.76
88-97-1	3.75	9.46	4.00	3.53	3.13	3.69	3.45	4.24
102606-33-7	3.79	3.80	3.69	4.11	3.78	4.26	3.98	3.86
3440-99-1	3.82	3.88	3.99	3.72	3.51	3.77	3.86	3.92
612-20-4	3.84	3.79	3.94	3.37	3.95	3.50	3.85	4.23
112868-41-4	3.86	3.76	3.76	4.14	3.77	4.07	3.80	3.59
23384-04-5	3.90	3.23	4.00	4.87	4.03	4.89	3.72	4.61
25567-10-6	3.92	3.86	3.89	4.07	4.00	4.12	4.01	3.87
3739-38-6	3.95	4.23	4.05	3.92	3.76	3.94	3.81	4.26
5732-10-5	3.96	3.18	3.86	4.02	3.93	3.70	3.99	4.26
6336-70-5	4.02	11.25	4.12	4.31	3.77	4.20	3.94	3.87
127340-37-8	4.03	4.36	4.13	4.08	4.01	3.92	3.73	5.42
594-61-6	4.04	2.84	4.17	2.54	3.94	3.50	4.25	4.50
529-75-9	4.05	3.77	4.15	4.33	3.46	4.32	3.42	4.04
586-38-9	4.06	4.08	3.99	4.08	3.76	4.08	3.83	3.35
50685-26-2	4.09	3.91	4.11	4.06	3.92	3.85	3.99	3.51
1642-81-5	4.13	3.93	4.03	4.14	3.93	4.07	3.98	4.38
3780-93-6	4.15	n/a	4.25	7.08	5.73	5.42	5.69	5.46
88550-26-9	4.16	13.51	4.56	3.43	4.32	3.60	4.17	7.88
621-51-2	4.17	4.08	4.12	4.26	3.77	4.14	3.83	3.69
1123-28-0	4.18	13.46	4.21	3.91	4.01	3.66	4.31	4.53
134-11-2	4.18	3.77	4.08	4.28	3.63	4.34	3.40	3.86

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
93-09-4	4.20	3.95	3.93	4.35	3.87	4.19	3.92	4.09
6926-51-8	4.23	3.88	4.33	4.42	3.95	4.97	3.91	4.79
63635-26-7	4.24	3.73	4.19	4.33	3.71	4.39	3.38	4.08
93351-38-3	4.25	4.08	4.15	4.25	3.79	4.14	3.83	3.72
5651-47-8	4.27	3.99	4.17	3.81	4.04	4.03	3.98	3.76
1129-06-2	4.28	4.10	4.32	4.30	3.87	4.18	3.98	3.90
99-04-7	4.28	3.93	4.24	4.15	3.74	4.23	4.00	3.92
25022-55-3	4.30	3.35	4.20	3.89	3.42	3.85	2.97	4.09
88550-27-0	4.31	2.66	4.21	4.43	4.25	4.34	4.17	6.37
61363-71-1	4.34	6.27	5.52	4.37	5.55	4.49	8.73	7.41
634-97-9	4.35	14.18	4.45	4.37	4.19	4.35	3.40	4.16
723-47-7	4.40	11.26	4.50	6.62	5.68	6.17	4.79	6.35
20044-86-4	4.46	4.83	4.36	4.63	4.99	4.79	4.29	3.76
30762-00-6	4.48	4.17	4.19	4.65	4.09	4.50	3.93	4.22
103323-97-3	4.54	4.15	4.64	3.87	4.03	4.29	3.91	3.25
15058-72-7	4.55	4.63	4.65	5.06	3.93	4.33	3.28	6.51
13205-46-4	4.57	4.17	4.67	4.60	4.12	4.60	3.93	4.28
873376-02-4	4.59	3.66	3.90	4.49	3.99	4.31	4.53	4.93
5438-19-7	4.63	4.17	4.53	4.63	4.10	4.50	3.93	4.25
626-98-2	4.69	3.98	4.59	4.65	4.14	4.58	4.15	4.03
10375-04-9	4.70	8.22	4.65	5.17	5.44	4.63	5.37	7.03
6996-92-5	4.79	n/a	n/a	4.97	4.73	4.84	4.66	5.80
100043-29-6	4.84	5.40	6.88	2.50	4.02	3.48	4.42	3.07
273-39-2	4.88	6.45	5.36	5.50	5.33	5.35	4.99	5.55
89123-36-4	4.89	10.70	4.85	4.84	5.03	4.26	4.78	6.83
1885-22-9	5.00	n/a	n/a	6.63	6.59	6.98	4.75	5.81

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
75-98-9	5.04	4.18	4.94	4.71	4.05	4.83	5.19	5.05
69084-03-3	5.06	6.03	5.16	6.87	6.42	6.36	5.37	6.89
79100-71-3	5.15	6.82	5.27	2.11	4.49	4.30	6.88	5.17
52662-66-5	5.20	8.21	5.31	8.13	7.63	8.03	8.70	9.97
67465-26-3	5.25	n/a	n/a	5.00	4.78	5.02	4.66	5.52
600-40-8	5.28	n/a	n/a	5.25	5.41	5.74	5.44	5.25
127-73-1	5.46	6.04	6.26	6.98	6.52	7.29	6.63	7.36
5858-17-3	5.48	5.59	5.38	5.67	5.73	5.73	5.13	7.46
6017-47-6	5.50	n/a	5.56	5.60	5.85	5.70	5.84	5.95
6280-28-0	5.55	4.98	7.07	4.47	4.69	5.09	4.29	5.22
4636-39-9	5.64	6.23	6.35	8.13	8.91	6.92	8.77	7.63
64276-66-0	5.65	5.04	5.55	4.99	4.27	4.79	3.62	4.69
112989-11-4	5.70	4.12	5.80	5.34	4.56	5.53	5.60	8.58
2977-73-3	5.75	6.01	5.77	6.07	7.79	8.10	8.92	10.13
12770-97-7	5.84	6.46	6.27	5.74	6.03	5.99	5.81	2.93
1610-26-0	5.89	n/a	n/a	6.64	8.05	6.44	7.62	6.53
16699-12-0	5.91	5.84	n/a	6.88	6.64	7.40	6.57	7.16
15084-15-8	5.96	5.98	6.02	5.90	5.93	6.44	4.95	5.96
6059-10-5	6.00	n/a	5.90	6.62	5.76	5.26	5.77	5.16
97477-81-1	6.00	6.43	5.96	6.26	5.80	5.01	8.07	4.73
76076-35-2	6.13	4.91	4.38	6.21	6.34	6.40	5.14	7.67
882-32-6	6.15	n/a	6.25	6.33	6.16	6.48	5.84	6.13
603-72-5	6.20	4.83	6.30	7.87	7.87	6.19	6.65	5.89
515-67-3	6.23	7.45	7.79	7.47	8.27	7.45	7.74	7.26
15084-16-9	6.28	6.01	6.38	6.32	6.48	6.57	4.89	6.18
14832-59-8	6.30	9.35	n/a	5.34	4.63	5.17	4.33	5.78

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
118090-08-7	6.33	7.59	6.43	8.10	9.49	7.70	8.70	9.40
7693-52-9	6.36	6.19	6.26	6.27	6.49	6.22	6.17	6.36
93079-57-3	6.38	6.48	6.28	6.55	5.86	5.99	8.07	5.82
15570-12-4	6.39	6.08	7.25	6.39	6.34	6.40	5.82	6.16
89295-61-4	6.42	5.68	6.32	6.50	6.67	6.38	6.18	4.00
3182-75-0	6.48	n/a	6.30	6.33	6.39	6.37	6.43	6.64
17103-51-4	6.50	5.40	6.40	6.91	6.14	5.90	5.09	6.00
17103-48-9	6.62	6.20	6.52	7.42	6.85	7.40	7.03	6.63
23045-32-1	6.63	8.37	6.60	8.52	8.15	9.09	8.39	9.47
885-82-5	6.73	6.75	7.44	6.52	7.31	7.01	6.97	7.32
5471-69-2	6.75	n/a	6.85	6.74	6.22	6.60	5.84	6.76
13442-05-2	6.76	10.85	7.66	8.84	9.40	9.51	9.44	9.66
3251-56-7	6.83	5.73	6.93	6.96	6.39	6.60	8.42	8.16
2036-13-7	6.88	8.59	6.98	6.62	8.75	6.51	9.32	6.78
80-37-5	6.91	6.66	7.01	7.42	7.60	7.62	7.46	5.99
10452-78-5	6.92	5.84	7.53	8.04	8.91	8.31	9.23	8.30
58851-99-3	7.02	6.89	7.12	6.84	5.99	7.08	8.20	7.20
23045-33-2	7.05	7.97	7.15	9.55	8.22	8.80	8.53	9.12
515-59-3	7.12	5.69	7.02	6.76	6.46	7.02	5.93	7.20
100-02-7	7.13	6.61	7.06	6.99	6.53	7.02	8.59	7.34
24067-17-2	7.15	n/a	3.86	8.36	9.02	8.33	8.80	9.12
2423-71-4	7.22	5.83	7.12	7.37	7.76	7.61	9.56	7.98
13331-27-6	7.30	n/a	4.63	7.55	8.23	8.34	8.77	9.18
269727-10-8	7.31	n/a	7.21	8.26	8.87	7.03	8.68	8.05
2268-11-3	7.35	9.18	7.25	7.62	8.77	7.72	7.96	5.43
6665-86-7	7.39	6.64	7.49	7.96	6.98	8.07	8.12	7.86



CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
635-93-8	7.40	7.07	7.42	7.82	7.74	7.48	7.41	7.95
57-68-1	7.44	11.27	7.54	6.53	6.37	6.67	6.70	7.06
6958-78-7	7.46	7.15	8.10	6.52	6.79	8.42	6.64	7.41
74537-62-5	7.48	8.49	n/a	7.32	8.74	8.09	9.16	8.62
609-22-3	7.60	6.81	7.70	7.31	7.35	7.41	6.45	9.16
163136-69-4	7.60	6.53	7.50	8.06	6.50	7.37	8.57	6.65
91753-33-2	7.63	7.34	7.53	6.22	6.54	6.43	7.45	8.58
70661-86-8	7.64	7.42	7.74	7.92	7.47	7.86	9.65	8.21
20513-25-1	7.65	11.13	7.75	8.50	7.63	9.48	9.82	8.49
33426-53-8	7.67	7.03	7.77	8.58	8.82	8.85	9.51	8.61
38397-07-8	7.69	8.73	7.83	8.11	8.35	8.18	8.90	8.02
6953-61-3	7.70	7.97	n/a	8.76	8.29	8.75	8.30	9.36
80348-66-9	7.75	6.52	7.65	7.48	9.92	7.80	7.28	8.29
615-58-7	7.77	6.72	8.14	7.45	7.44	7.17	6.55	9.02
6468-96-8	7.80	7.05	7.70	7.11	7.18	7.77	8.21	7.66
4427-22-9	7.82	8.02	7.72	8.33	8.41	8.30	8.31	7.75
5978-34-7	7.86	8.59	9.22	8.14	8.46	7.85	8.55	7.96
769-79-9	7.89	7.82	8.10	7.73	7.96	7.29	8.77	7.67
7467-91-6	7.92	7.46	8.02	8.47	7.95	8.29	8.20	8.58
7454-47-9	7.98	7.32	8.08	8.04	8.10	7.82	7.94	7.95
14452-34-7	7.98	6.52	7.88	7.38	7.91	7.31	7.56	7.01
71288-96-5	8.00	8.31	8.10	8.89	8.66	8.86	7.85	8.41
6089-66-3	8.01	8.56	8.11	7.77	8.49	7.40	8.80	7.09
85-87-0	8.02	9.16	n/a	9.19	9.52	9.31	9.06	10.68
2446-50-6	8.07	8.41	n/a	8.66	8.25	8.93	8.73	7.73
4776-14-1	8.09	9.72	n/a	9.51	9.95	9.29	9.81	9.39

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
79-15-2	8.10	5.57	8.57	8.10	7.39	7.95	7.30	8.39
52515-76-1	8.12	8.39	8.22	8.43	7.65	8.54	8.63	9.28
13704-50-2	8.14	8.92	8.07	8.70	8.50	8.60	8.45	10.06
70027-43-9	8.20	5.29	8.10	7.40	6.61	7.88	5.77	7.77
79100-69-9	8.20	6.71	8.45	4.47	8.27	8.85	7.76	7.38
139097-73-7	8.25	8.54	8.35	7.82	8.51	8.09	9.63	7.59
5344-97-8	8.25	5.28	8.11	8.06	8.15	8.05	8.77	8.43
18362-30-6	8.26	5.73	7.96	7.22	6.95	7.88	7.41	7.57
4198-90-7	8.27	7.49	8.37	8.14	9.13	8.25	9.70	8.01
85403-59-4	8.30	8.11	8.20	8.51	8.19	8.73	8.84	9.14
17056-96-1	8.34	8.81	8.24	8.64	7.97	9.06	8.33	8.18
27761-48-4	8.36	8.41	8.05	7.09	7.73	8.11	8.53	7.64
27556-51-0	8.39	8.11	9.54	8.66	8.64	8.70	8.59	8.61
37790-28-6	8.44	8.04	8.54	8.64	8.68	8.68	8.67	9.72
68-34-8	8.46	7.76	8.56	8.52	8.51	8.48	8.02	8.88
2216-93-5	8.50	8.57	8.40	9.30	8.46	8.57	8.51	7.31
95-77-2	8.58	7.96	8.69	8.40	7.43	8.59	7.70	7.76
6311-65-5	8.63	7.96	8.11	8.56	8.81	8.56	8.00	8.97
604-44-4	8.64	8.72	9.00	8.75	8.54	8.77	8.13	8.66
1146-41-4	8.66	7.80	8.67	8.57	8.23	8.61	7.98	8.93
89-40-7	8.68	10.00	8.78	7.68	8.36	8.06	8.42	6.25
481-13-0	8.70	8.70	8.60	7.92	7.55	7.70	7.77	7.66
131060-07-6	8.70	9.25	8.60	9.05	7.70	7.76	7.73	9.56
87-64-9	8.70	8.31	8.80	8.38	8.37	8.85	8.30	8.32
122231-61-2	8.71	7.97	n/a	8.76	8.52	8.85	8.33	8.18
98-80-6	8.74	n/a	7.94	9.88	9.00	8.66	8.82	10.01

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
7405-23-4	8.77	7.47	8.67	8.55	8.14	8.49	7.90	8.66
17056-99-4	8.80	7.96	8.21	8.78	8.18	8.72	8.42	8.78
367-12-4	8.81	8.24	9.17	8.53	8.75	8.66	8.02	8.27
103-87-7	8.83	9.66	8.93	10.03	9.59	9.66	9.11	9.78
2993-20-6	8.87	8.45	8.77	8.48	8.48	8.90	8.07	7.22
2446-51-7	8.89	7.59	8.79	10.86	5.68	11.54	7.53	9.04
78564-54-2	8.90	9.52	n/a	8.85	8.81	8.82	9.41	7.44
77456-53-2	8.91	9.66	8.81	8.95	9.21	8.70	9.41	8.06
7385-87-7	8.94	8.45	8.84	8.61	8.38	8.93	8.34	9.11
58-56-0	8.98	9.14	9.08	9.49	9.22	9.14	9.10	9.92
17260-71-8	9.04	8.82	8.94	8.89	9.40	9.25	9.20	8.96
6665-83-4	9.09	6.93	9.19	8.87	8.46	8.81	8.15	8.90
4463-42-7	9.12	n/a	9.02	10.03	9.89	9.94	9.17	10.42
53059-30-6	9.14	8.75	8.57	8.81	9.14	9.03	9.02	9.30
89415-43-0	9.17	11.88	9.07	9.55	9.08	9.56	8.82	10.00
2039-66-9	9.19	9.95	9.09	10.09	9.69	9.71	9.54	9.82
37432-20-5	9.20	10.07	8.69	9.46	9.56	9.58	9.53	9.13
571-60-8	9.25	7.96	8.99	9.75	9.27	9.72	8.85	9.79
588-05-6	9.27	9.60	9.85	9.57	9.30	9.96	9.20	9.81
77-67-8	9.34	9.58	9.18	9.51	9.29	9.49	8.34	6.70
20296-09-7	9.36	10.05	9.46	9.35	9.65	9.60	9.96	7.14
59-50-7	9.40	9.55	9.50	9.37	8.82	9.30	8.35	9.24
5374-12-9	9.43	7.91	7.11	9.05	8.65	8.20	8.30	7.88
3463-03-4	9.47	9.82	9.37	8.55	8.79	9.25	8.76	9.48
7147-90-2	9.48	10.03	9.58	9.07	8.87	8.73	8.18	6.17
103-90-2	9.50	9.30	n/a	9.69	9.14	9.58	8.90	9.73

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
584-43-0	9.59	9.47	7.90	9.42	8.66	8.96	8.30	6.25
5111-66-0	9.64	9.08	9.74	9.62	9.18	9.54	8.90	9.63
89466-06-8	9.64	n/a	n/a	9.04	8.87	8.43	8.51	9.11
84452-98-2	9.66	8.96	8.47	8.95	9.17	9.13	8.30	7.73
3566-61-8	9.70	9.73	9.60	9.54	8.96	5.92	8.45	4.67
487-93-4	9.73	9.57	9.63	9.97	9.40	9.84	8.77	9.97
70460-18-3	9.75	8.85	9.15	8.58	8.98	8.67	8.83	9.04
2937-60-2	9.77	11.70	9.89	9.68	9.22	9.34	9.15	9.89
124603-61-8	9.80	10.56	9.70	10.70	9.96	9.89	8.87	6.48
6244-77-5	9.81	9.57	9.91	10.09	10.81	9.93	10.72	10.37
154286-35-8	9.85	9.67	9.32	9.76	9.30	9.92	8.92	10.00
10319-77-4	9.89	7.62	9.80	9.54	10.96	8.85	11.20	9.57
613-14-9	9.92	9.32	9.38	8.74	8.91	9.27	8.90	9.72
91-04-3	9.92	11.60	9.42	9.65	8.80	9.48	9.35	9.81
127351-11-5	9.96	9.31	9.86	9.77	9.98	10.14	10.18	10.05
61-67-6	9.98	9.39	9.88	9.35	9.70	9.65	9.33	8.80
3144-47-6	10.00	6.20	6.90	7.27	7.85	5.99	7.61	7.32
28128-30-5	10.00	9.92	10.10	10.37	9.78	10.10	9.58	8.63
34420-17-2	10.00	n/a	9.90	9.38	10.07	9.31	9.37	9.98
27289-33-4	10.01	9.63	10.19	10.04	9.30	10.10	9.25	9.88
26074-38-4	10.03	7.97	10.16	10.01	5.74	9.68	8.84	8.65
826-81-3	10.08	9.52	9.98	9.81	8.94	9.63	8.80	9.35
698-71-5	10.10	11.20	10.42	10.04	9.48	9.88	9.28	9.95
108-68-9	10.13	10.97	10.11	10.22	9.47	9.83	9.30	10.12
127351-05-7	10.18	9.65	10.17	9.98	10.17	10.19	10.08	10.07
1641-41-4	10.20	8.73	10.10	10.24	9.44	10.29	9.65	9.92

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
7343-35-3	10.22	11.10	n/a	12.66	11.16	12.27	11.51	9.89
122-94-1	10.23	10.11	10.13	10.09	9.49	10.06	8.79	9.93
622-62-8	10.23	10.12	10.33	10.05	9.46	9.95	8.80	9.92
14531-55-6	10.27	11.37	10.37	8.88	10.09	9.16	11.38	8.12
914296-27-8	10.30	10.93	10.37	10.92	10.84	10.17	11.06	9.82
90045-28-6	10.30	7.97	8.90	8.78	8.03	8.86	8.05	9.64
95-65-8	10.32	10.16	10.44	10.12	9.72	10.11	9.23	10.03
56768-47-9	10.35	10.14	10.25	10.00	9.86	10.07	9.99	8.96
3594-88-5	10.40	9.64	9.69	9.07	8.92	8.58	9.10	9.64
103-16-2	10.47	10.10	10.37	10.06	9.43	9.97	8.79	9.89
22440-82-0	10.50	9.44	9.67	9.76	10.00	9.79	9.03	9.74
854706-73-3	10.54	9.77	10.64	9.97	9.40	9.83	9.09	10.04
496-78-6	10.55	10.21	10.65	10.70	10.14	10.29	9.70	10.07
5919-26-6	10.60	11.55	n/a	10.64	7.90	10.33	5.12	6.30
91967-91-8	10.61	11.13	10.67	9.96	9.93	9.74	9.66	9.90
56577-68-5	10.70	n/a	n/a	9.53	9.87	9.21	10.34	10.61
6244-75-3	10.76	9.87	10.66	10.63	10.71	10.82	10.69	10.57
3144-09-0	10.80	9.13	9.09	9.72	9.86	10.08	9.94	8.74
74926-85-5	10.82	10.63	10.93	10.88	10.16	10.49	9.61	9.97
20484-31-5	10.84	10.38	n/a	10.87	9.81	10.64	9.37	10.05
3228-04-4	10.85	10.74	10.80	10.22	10.26	10.33	10.10	10.18
636-04-4	10.86	10.17	10.83	10.71	10.81	10.89	10.73	10.64
170245-15-5	10.88	10.92	11.93	10.52	10.84	9.59	10.95	9.20
10569-71-8	10.90	10.89	10.70	10.66	10.35	10.49	10.09	10.25
127351-04-6	10.95	10.20	10.85	10.54	10.13	10.76	10.40	10.49
120-65-0	10.96	10.00	9.63	9.86	9.57	9.63	9.39	9.93

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
127351-08-0	10.99	9.89	10.89	10.75	10.36	10.90	10.52	10.53
7684-18-6	11.00	11.13	9.44	9.20	8.16	9.38	9.43	9.18
95236-95-6	11.18	10.18	11.08	10.62	10.69	10.91	10.68	10.58
13207-66-4	11.24	10.54	10.65	8.73	9.00	8.65	8.60	9.46
95236-94-5	11.26	10.25	11.34	10.88	10.61	11.05	10.64	10.57
942-32-5	11.30	12.27	n/a	11.14	10.93	11.72	11.43	10.06
5326-80-7	11.30	10.46	n/a	10.60	10.27	10.43	10.09	9.70
5310-26-9	11.36	10.50	11.71	10.97	10.83	11.17	10.68	10.60
23562-77-8	11.48	10.43	n/a	10.78	9.79	10.73	9.08	9.98
3031-73-0	11.50	10.77	11.40	11.72	11.39	11.43	10.56	11.03
119059-70-0	11.53	9.93	11.43	10.22	9.95	8.51	9.98	9.84
637-53-6	11.56	9.75	11.41	10.88	11.11	10.87	11.50	11.05
55252-75-0	11.77	8.81	10.43	9.71	9.89	9.93	9.52	9.67
97317-28-7	11.81	10.56	11.62	11.29	10.92	11.61	10.71	10.55
34535-90-5	11.91	12.00	11.59	12.36	11.68	12.55	11.86	10.11
19854-93-4	12.09	12.40	12.60	11.70	11.79	11.75	11.36	9.80
89267-19-6	12.10	12.87	11.75	13.05	12.24	13.90	12.91	11.90
14575-62-3	12.14	12.08	6.75	11.39	10.62	11.14	11.31	10.43
3696-23-9	12.30	9.23	11.74	10.60	10.13	10.34	7.47	8.55
2646-30-2	12.35	9.34	12.25	10.33	9.72	10.17	8.11	9.00
582-60-5	12.52	12.09	n/a	12.86	12.24	12.99	11.79	11.52
128-37-0	12.55	9.98	11.80	10.41	10.33	9.93	9.79	10.09
80-15-9	12.64	11.10	12.37	10.95	10.80	10.86	10.88	10.20
19322-71-5	12.80	11.34	9.47	12.54	11.54	11.73	11.72	11.84
105868-53-9	13.10	11.01	7.69	11.85	11.24	11.84	11.83	10.95
116866-63-8	13.33	12.06	n/a	12.88	12.12	12.89	11.72	11.52

CAS No.	exp.	MolGpKa	OPERA	IGC		SGC		SGCN
				MAP	IAP	MAP	IAP	MAP
122992-92-1	13.46	14.41	n/a	14.20	12.83	14.28	11.64	12.99
271-42-1	13.86	13.51	13.58	11.74	12.92	12.84	12.86	12.18
3589-73-9	14.54	14.72	n/a	13.94	13.24	13.86	12.37	11.25
3073-77-6	14.70	11.38	10.72	11.31	16.05	10.34	13.24	7.47
42845-45-4	15.54	13.85	12.31	15.32	15.16	15.33	14.76	14.81
71-31-8	15.97	14.02	13.00	14.87	14.39	15.05	14.61	14.35
130190-71-5	16.65	9.85	8.12	9.45	9.91	8.66	9.24	8.70