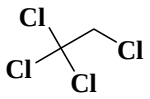
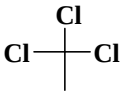
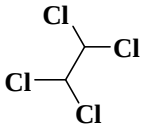
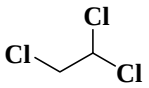
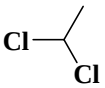
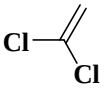
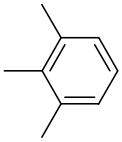
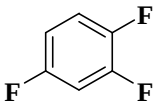
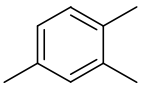
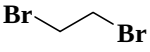
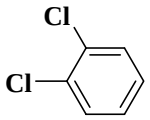
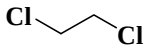
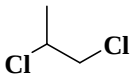
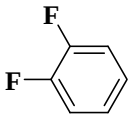
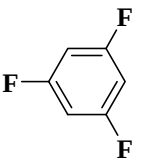
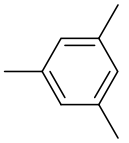
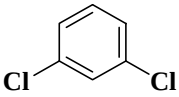
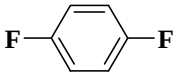
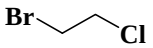
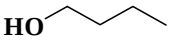
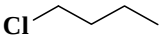
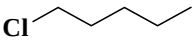
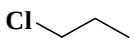
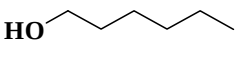
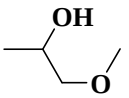
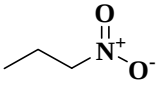
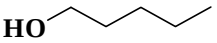
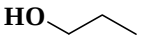
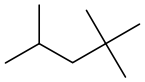
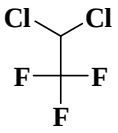
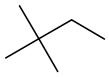
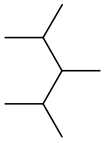
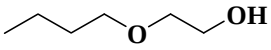
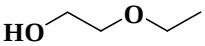
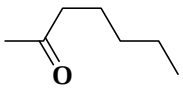
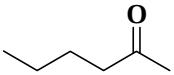
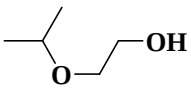
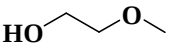
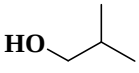
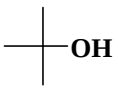
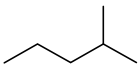
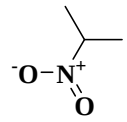
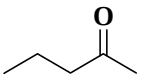
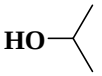
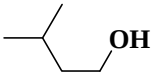
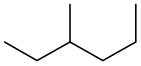
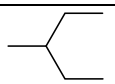
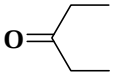
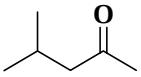
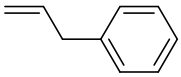
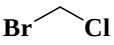
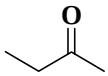
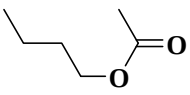
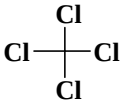
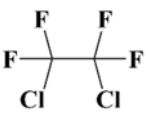
Supporting Information

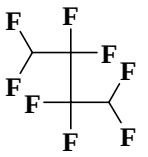
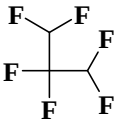
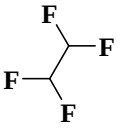
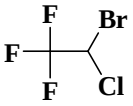
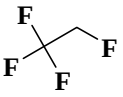
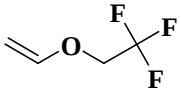
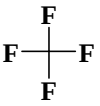
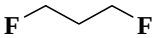
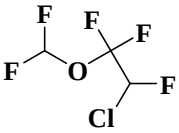
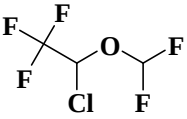
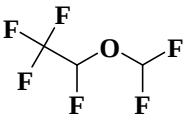
Table S1. Log $K_{lip/w}$ values, molecular descriptors and structures of all studied compounds

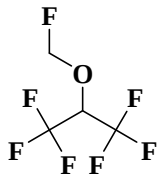
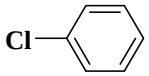
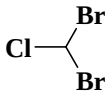
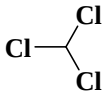
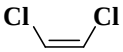
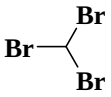
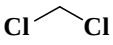
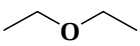
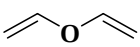
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
1	630-20-6	2.85	2.90	2.93		165.891	-0.022	
2	71-55-6	2.66	2.81	2.68	2.49	131.930	-0.018	
3[a]	79-34-5	2.46	2.03	2.19	2.39	165.891	-0.024	
4	79-00-5	2.09	1.97	2.01	1.89	131.930	-0.027	
5	1717-00-6	1.34	2.48	2.37		115.960	-0.025	
6	75-34-3	1.74	1.85	1.76	1.79	97.969	-0.027	
7	75-35-4	2.19	2.36	2.12	2.13	95.953	-0.016	
8[a]	526-73-8	3.32	3.84	3.63	3.66	120.094	-0.036	
9	367-23-7	2.67	2.63	2.59	2.52	132.019	-0.028	
10[a]	95-63-6	3.43	3.84	3.63	3.63	120.094	-0.035	
11	106-93-4	1.67	1.61	2.01	1.96	185.868	-0.037	

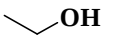
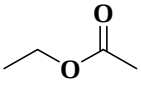
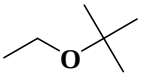
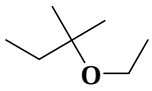
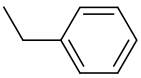
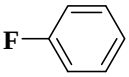
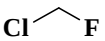
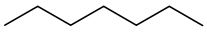
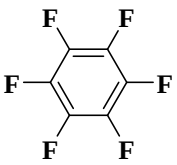
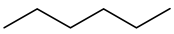
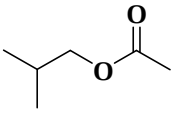
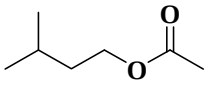
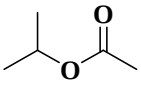
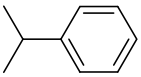
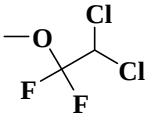
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
12	95-50-1	3.71	3.35	3.28	3.43	145.969	-0.030	
13[a]	107-06-2	1.60	1.83	1.83	1.48	97.969	-0.038	
14	78-87-5	1.99	2.23	2.25	1.98	111.985	-0.041	
15[a]	367-11-3	2.62	2.45	2.39	2.37	114.028	-0.033	
16[a]	372-38-3	2.93	2.69	2.59		132.019	-0.020	
17	108-67-8	3.49	3.84	3.63	3.42	120.094	-0.035	
18	541-73-1	3.84	3.45	3.28	3.53	145.969	-0.017	
19	540-36-3	2.58	2.49	2.39	2.13	114.028	-0.028	
20[a]	107-04-0	2.07	1.72	1.92		141.918	-0.038	
21	71-36-3	0.02	0.40	0.84	0.88	74.073	-0.089	
22	109-69-3	2.78	2.76	2.56	2.64	92.039	-0.033	
23	543-59-9	3.48	3.26	3.05	2.73	106.055	-0.033	
24	540-54-5	2.22	2.27	2.07	2.04	78.024	-0.032	
25[a]	111-27-3	1.36	1.39	1.82	2.03	102.104	-0.089	
26	107-98-2	-1.53	-1.19	-0.49		90.068	-0.084	
27	108-03-2	0.97	0.60	0.95	0.87	89.048	-0.070	

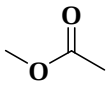
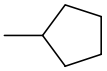
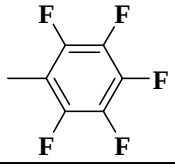
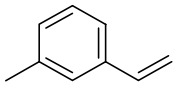
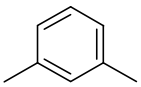
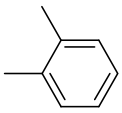
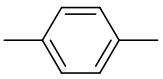
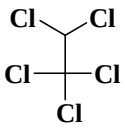
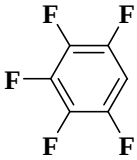
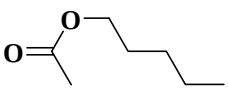
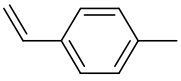
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
28[a]	71-41-0	0.54	0.89	1.33	1.51	88.089	-0.089	
29[a]	71-23-8	-0.48	-0.10	0.35	0.25	60.058	-0.088	
30	540-84-1	4.64	4.65	4.09		114.141	-0.005	
31	306-83-2	1.81	2.15	2.17		151.941	-0.014	
32[a]	75-83-2	3.79	3.73	3.18	3.82	86.110	-0.005	
33	565-75-3	5.05	4.61	4.05		114.141	-0.005	
34	111-76-2	-0.21	-0.11	0.57	0.83	118.099	-0.085	
35[a]	75-29-6	2.03	2.17	2.00	1.90	78.024	-0.033	
36	110-80-5	-1.27	-0.46	-0.42	-0.32	90.068	-0.003	
37[a]	420-26-8	1.38	1.72	1.68		62.053	-0.052	
38	110-43-0	1.81	1.27	1.73	1.98	114.104	-0.083	
39[a]	591-78-6	1.19	0.78	1.24	1.38	100.089	-0.082	
40	109-59-1	-1.16	-0.71	0.00	0.05	104.084	-0.086	
41	109-86-4	-1.67	-1.67	-0.91	-0.77	76.052	-0.092	
42[a]	78-83-1	-0.06	0.34	0.77	0.76	74.073	-0.085	
43	75-65-0	-0.73	0.27	0.73	0.35	74.073	-0.088	
44[a]	107-83-5	3.99	3.77	3.21		86.110	-0.005	

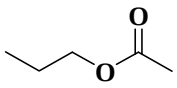
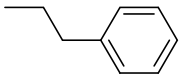
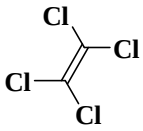
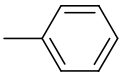
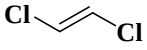
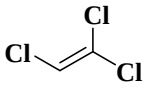
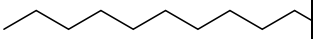
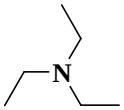
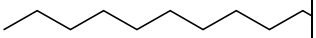
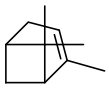
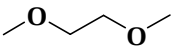
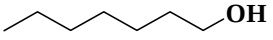
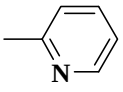
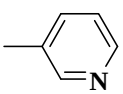
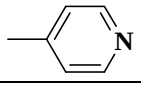
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
45	79-46-9	0.61	0.50	0.87	0.93	89.048	-0.071	
46	107-87-9	0.65	0.29	0.75	0.91	86.073	-0.082	
47[a]	67-63-0	-0.82	-0.18	0.28	0.05	60.058	-0.088	
48	123-51-3	0.41	0.82	1.26	1.16	88.089	-0.088	
49[a]	589-34-4	4.61	4.28	3.71		100.125	-0.005	
50	96-14-0	4.07	3.77	3.21	3.60	86.110	-0.005	
51	96-22-0	0.56	0.28	0.75	0.99	86.073	-0.082	
52	108-10-1	1.05	0.71	1.16	1.31	100.089	-0.080	
53	67-64-1	-0.32	-0.72	-0.24	-0.24	58.042	-0.082	
54	300-57-2	2.96	3.62	3.39	3.23	118.078	-0.030	
55[a]	71-43-2	2.12	2.20	1.99	2.13	78.047	-0.029	
56	74-97-5	1.49	1.35	1.43	1.41	127.903	-0.022	
57	78-93-3	0.18	-0.22	0.26	0.29	72.058	-0.083	
58[a]	106-97-8	3.03	2.86	2.31	2.89	58.078	-0.005	
59	123-86-4	1.59	1.33	1.85	1.78	116.084	-0.092	
60	56-23-5	3.18	2.53	2.44	2.83	151.875	-0.006	
61	76-14-2	3.00	2.83	2.78	2.82	169.931	-0.007	

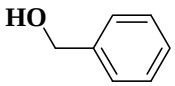
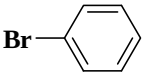
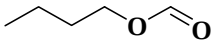
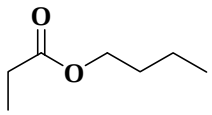
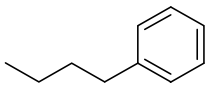
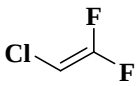
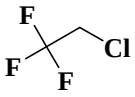
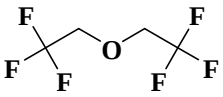
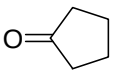
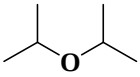
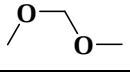
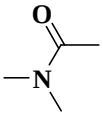
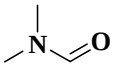
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
62	377-36-6	2.50	1.98	2.28		202.003	-0.021	
63	680-00-2	1.49	1.44	1.61		152.006	-0.022	
64	359-35-3	0.92	0.86	0.94		102.009	-0.028	
65	75-37-6	0.91	1.16	1.13	0.75	66.028	-0.041	
66	151-67-7	2.28	2.03	2.26	2.30	195.890	-0.015	
67	811-97-2	1.03	1.72	1.68		102.009	-0.028	
68	406-90-6	1.26	0.99	1.33		126.029	-0.053	
69[a]	75-73-0	1.12	1.41	1.19	1.18	87.994	-0.005	
70[a]	462-39-5	0.66	1.74	1.70		80.044	-0.043	
71[a]	13838-16-9[b]	2.03	1.76	2.06	2.10	183.971	-0.027	
72	26675-46-7	1.99	1.05	1.51	2.06	183.971	-0.036	
73	57041-67-5	1.88	0.80	1.20		168.001	-0.032	

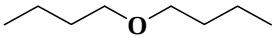
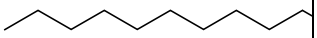
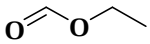
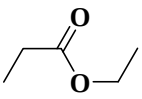
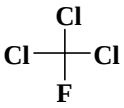
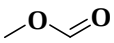
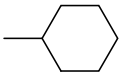
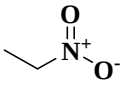
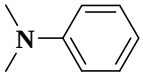
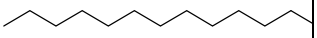
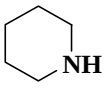
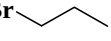
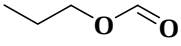
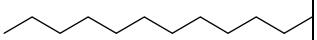
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
74[a]	28523-86-6[b]	1.87	1.21	1.75		200.007	-0.040	
75[a]	108-90-7	2.73	2.83	2.64	2.84	112.008	-0.023	
76[a]	124-48-1[b]	2.12	1.34	1.70	2.16	205.813	-0.014	
77	75-00-3	1.58	1.76	1.58	1.43	64.008	-0.032	
78	67-66-3	2.02	1.57	1.52	1.97	117.914	-0.014	
79	156-59-2	1.59	2.11	1.98	1.86	95.953	-0.027	
80	291-64-5	4.82	4.25	3.67	4.00	98.110	-0.004	
81[a]	110-82-7	4.05	3.75	3.18	3.44	84.094	-0.004	
82[a]	287-92-3	3.50	3.23	2.68	3.00	70.078	-0.005	
83	75-19-4	1.73	2.07	1.70	1.72	42.047	-0.025	
84	124-18-5	6.39	5.86	5.25	5.01	142.172	-0.005	
85	74-95-3	1.76	1.24	1.52	1.70	171.852	-0.021	
86[a]	75-09-2	1.28	1.46	1.34	1.25	83.953	-0.023	
87	60-29-7	0.79	0.66	1.05	0.89	74.073	-0.087	
88	75-10-5	0.53	0.78	0.71	0.20	52.012	-0.036	
89	109-93-3	1.69	1.66	1.68		70.042	-0.055	
90	74-84-0	1.73	1.85	1.32	1.81	30.047	-0.004	—

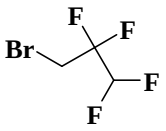
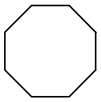
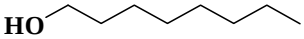
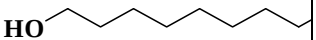
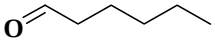
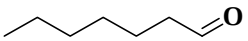
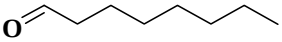
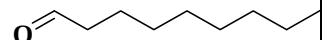
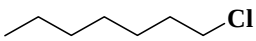
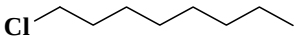
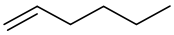
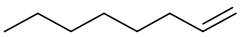
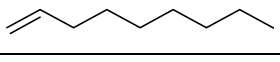
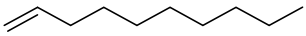
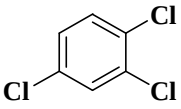
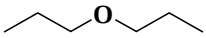
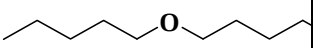
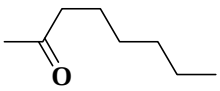
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
91	64-17-5	-1.14	-0.60	-0.14	-0.31	46.042	-0.088	
92[a]	74-85-1	0.84	1.58	1.27	1.13	28.031	-0.032	
93[a]	141-78-6	0.46	0.31	0.86	0.73	88.052	-0.094	
94	637-92-3	1.37	1.54	1.92		102.104	-0.085	
95	919-94-8	1.93	2.04	2.41		116.120	-0.085	
96	100-41-4	3.14	3.25	3.03	3.15	106.078	-0.031	
97	462-06-6	2.41	2.31	2.19	2.27	96.038	-0.032	
98[a]	353-36-6	0.62	1.32	1.26		48.038	-0.051	
99[a]	593-70-4	0.77	1.09	1.03	0.51	67.983	-0.033	
100	142-82-5	4.71	4.36	3.78	4.66	100.125	-0.004	
101	392-56-3	2.45	3.21	3.20	2.55	185.990	-0.011	
102	110-54-3	4.11	3.86	3.29	3.90	86.110	-0.005	
103[a]	110-19-0	1.60	1.33	1.77	1.78	116.084	-0.081	
104	123-92-2	2.11	1.83	2.26	2.25	130.099	-0.081	
105	108-21-4	1.02	0.72	1.28		102.068	-0.095	
106	98-82-8	3.52	3.67	3.45	3.66	120.094	-0.031	
107	76-38-0	2.11	1.68	2.02	2.21	163.961	-0.044	
108[a]	74-82-8	0.75	1.30	0.78	1.09	16.031	-0.004	CH_4

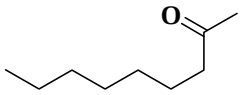
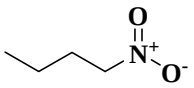
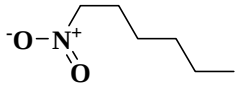
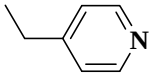
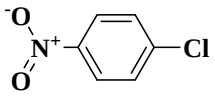
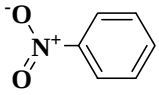
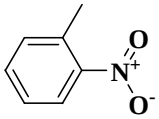
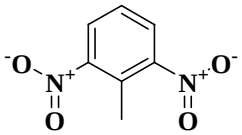
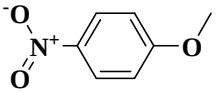
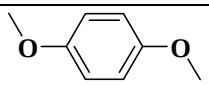
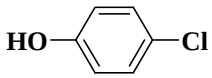
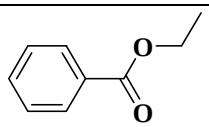
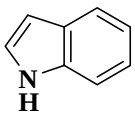
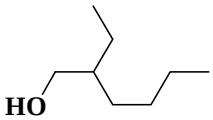
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
109	67-56-1	-1.95	-1.11	-0.63	-0.77	32.026	-0.090	—OH
110	79-20-9	-0.02	-0.08	0.37	0.18	74.037	-0.080	
111	74-87-3	0.80	1.27	1.09	0.91	49.992	-0.031	—Cl
112	96-37-7	4.00	3.65	3.10	3.37	84.094	-0.005	
113	771-56-2	3.27	3.55	3.54		182.015	-0.020	
114	100-80-1	3.23	3.65	3.44		118.078	-0.032	
115[a]	108-38-3	3.16	3.30	3.09	3.20	106.078	-0.034	
116	111-84-2	5.82	5.36	4.76	5.65	128.157	-0.004	
117	95-47-6	3.12	3.30	3.09	3.12	106.078	-0.034	
118[a]	106-42-3	3.16	3.30	3.09	3.15	106.078	-0.033	
119[a]	76-01-7	2.93	2.99	3.11	3.22	199.852	-0.016	
120	363-72-4	2.31	3.01	2.99	2.53	168.000	-0.017	
121	109-66-0	3.49	3.36	2.80	3.39	72.094	-0.005	
122	628-63-7	2.11	1.82	2.34	2.30	130.099	-0.094	
123[a]	622-97-9	3.21	3.65	3.44		118.078	-0.033	
124	74-98-6	2.35	2.35	1.81	2.36	44.063	-0.005	

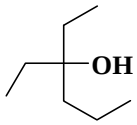
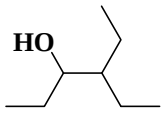
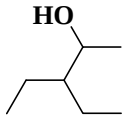
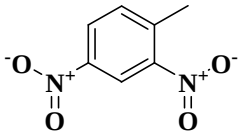
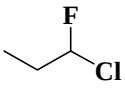
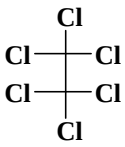
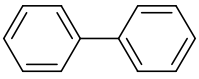
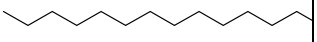
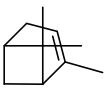
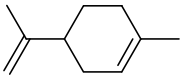
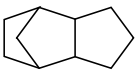
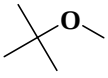
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
125	109-60-4	1.02	0.82	1.36	1.24	102.068	-0.094	
126	103-65-1	3.65	3.74	3.52	3.69	120.094	-0.032	
127	127-18-4	3.57	3.07	2.97	3.40	163.875	-0.009	
128	108-88-3	2.67	2.74	2.54	2.73	92.063	-0.031	
129	156-60-5	2.06	2.22	1.98	2.09	95.953	-0.014	
130	79-01-6	2.80	2.59	2.47	2.42	129.914	-0.017	
131	629-50-5	8.16	7.37	6.73		184.219	-0.004	
132[a]	121-44-8[b]	1.04	0.95	1.51	1.45	101.120	-0.099	
133	1120-21-4	7.03	6.36	5.74		156.188	-0.004	
134[a]	7785-26-4	4.58	4.48	4.27	4.48	136.125	-0.039	
135[a]	110-71-4[b]	-0.33	-0.81	-0.21	-0.21	90.068	-0.077	
136[a]	123-91-1[b]	-0.24	-0.95	-0.32	-0.27	88.052	-0.079	
137	111-70-6	1.84	1.90	2.31	2.62	116.120	-0.088	
138	109-06-8	0.61	0.77	1.35	1.11	93.058	-0.104	
139[a]	108-99-6[b]	0.84	0.76	1.35	1.20	93.058	-0.105	
140	108-89-4	0.82	0.75	1.35	1.22	93.058	-0.107	

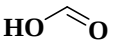
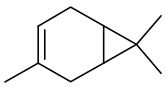
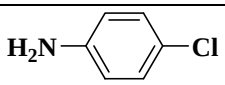
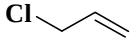
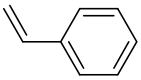
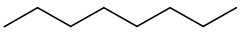
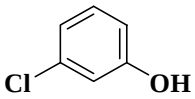
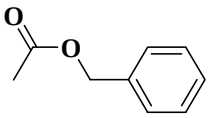
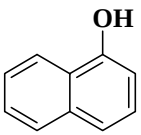
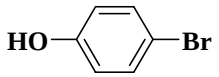
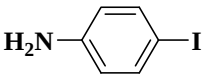
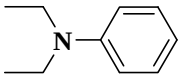
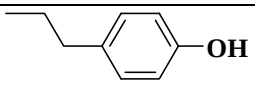
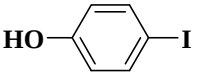
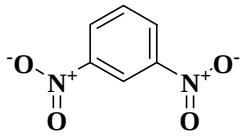
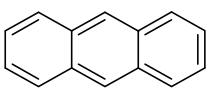
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
141[a]	100-51-6	0.12	0.60	1.08	1.10	108.058	-0.077	
142	108-86-1	3.27	2.89	2.88	2.99	155.957	-0.023	
143	592-84-7	1.46	0.83	1.30		102.068	-0.084	
144	590-01-2	2.35	1.92	2.34		130.099	-0.081	
145	104-51-8	4.13	4.24	4.01	4.38	134.110	-0.031	
146	359-10-4	1.63	1.74	1.60		97.973	-0.016	
147	75-88-7	1.34	2.06	1.99		117.980	-0.021	
148	333-36-8	1.92	1.40	1.88		182.017	-0.047	
149	110-83-8	3.33	3.13	2.96	2.86	82.078	-0.051	
150	120-92-3	0.39	0.16	0.63	0.38	84.058	-0.081	
151	75-45-6	0.72	0.95	0.89	1.08	85.973	-0.019	
152	108-20-3	1.29	1.47	1.88	1.52	102.104	-0.088	
153	109-87-5	0.18	-0.75	-0.19	0.00	76.052	-0.081	
154	115-10-6	0.13	-0.33	0.07	0.10	46.042	-0.084	
155[a]	127-19-5[b]	-1.25	-1.31	-0.49	-0.77	87.068	-0.100	
156[a]	68-12-2[b]	-1.57	-1.72	-0.93	-1.01	73.053	-0.097	

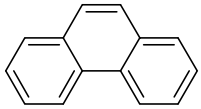
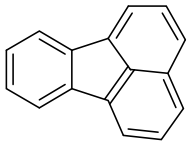
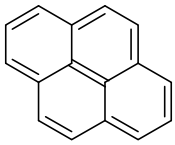
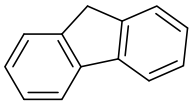
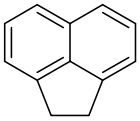
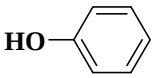
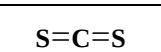
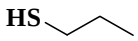
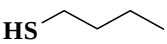
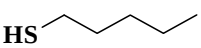
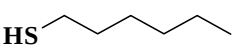
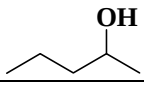
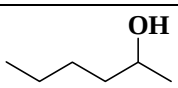
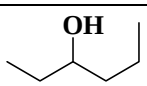
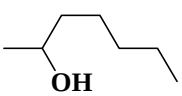
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
157	142-96-1	3.14	2.69	3.01	3.21	130.136	-0.083	
158	112-40-3	7.59	6.86	6.23	6.10	170.203	-0.005	
159[a]	109-94-4	0.16	-0.16	0.32	0.23	74.037	-0.083	
160	105-37-3	1.13	0.92	1.36	1.21	102.068	-0.081	
161	75-03-6	1.85	1.95	2.08	2.00	155.940	-0.024	
162	75-69-4	2.28	2.23	2.13	2.53	135.905	-0.009	
163[a]	107-31-3	-0.48	-0.65	-0.17	0.03	60.021	-0.081	
164	108-87-2	4.54	4.15	3.59	3.61	98.110	-0.004	
165	79-24-3	0.45	0.08	0.45	0.18	75.032	-0.071	
166	75-52-5	-0.02	-0.41	-0.04	-0.35	61.016	-0.069	
167[a]	121-69-7	2.29	2.09	2.17	2.31	121.089	-0.041	
168[a]	629-62-9[b]	9.31	8.37	7.71		212.250	-0.005	
169	110-89-4	1.01	0.56	1.19	0.84	85.089	-0.112	
170	106-94-5	2.47	2.17	2.16	2.10	121.973	-0.029	
171	110-74-7	0.87	0.34	0.81	0.83	88.052	-0.083	
172	110-86-1	0.15	0.21	0.80	0.65	79.042	-0.103	
173	629-59-4[b]	8.74	7.87	7.22	7.20	198.235	-0.005	
174[a]	109-99-9	0.62	0.53	0.94	0.46	72.058	-0.088	

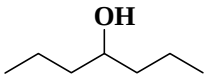
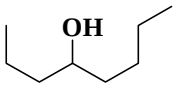
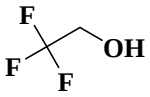
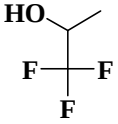
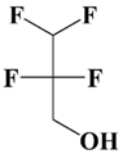
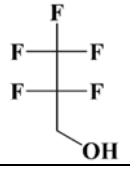
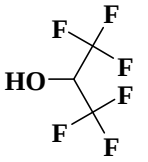
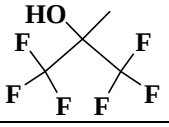
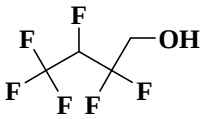
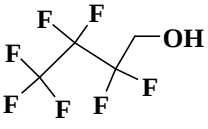
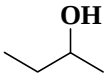
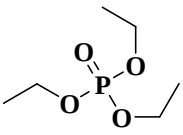
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
175	679-84-5	2.91	2.14	2.44		193.935	-0.028	
176	292-64-8	5.34	4.75	4.16	4.45	112.125	-0.004	
177[a]	111-87-5	2.46	2.40	2.81	3.00	130.136	-0.089	
178	143-08-8	3.01	2.90	3.30	3.77	144.151	-0.089	
179	66-25-1	1.92	1.47	1.80	1.78	100.089	-0.077	
180[a]	111-71-7	2.46	1.97	2.29		114.104	-0.077	
181	124-13-0	3.01	2.47	2.78		128.120	-0.078	
182	124-19-6	3.42	2.97	3.27		142.136	-0.077	
183[a]	629-06-1	4.37	4.26	4.03	4.15	134.086	-0.033	
184[a]	111-85-3	4.95	4.76	4.52		148.102	-0.033	
185	592-41-6	3.51	3.46	3.15	3.39	84.094	-0.035	
186	592-76-7	4.04	3.96	3.64	3.99	98.110	-0.035	
187	111-66-0	4.60	4.46	4.13	4.57	112.125	-0.035	
188	124-11-8	5.15	4.96	4.62	5.15	126.141	-0.035	
189[a]	872-05-9[b]	5.64	5.47	5.12	5.70	140.157	-0.035	
190	120-82-1	4.17	3.99	3.93	4.02	179.930	-0.023	
191	111-43-3	2.06	1.69	2.03	2.03	102.104	-0.082	
192	693-65-2	4.16	3.70	4.00		158.167	-0.083	
193	111-13-7	2.31	1.80	2.22	2.37	128.120	-0.080	

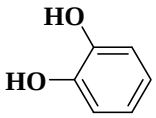
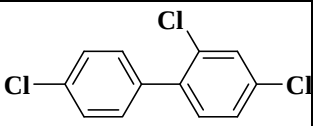
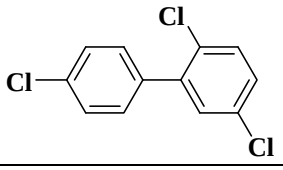
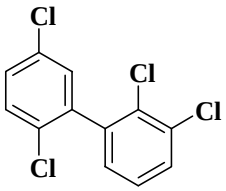
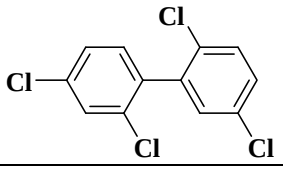
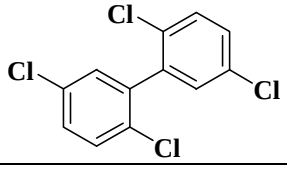
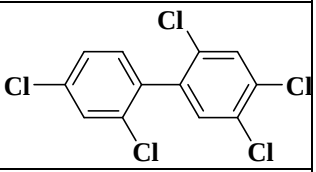
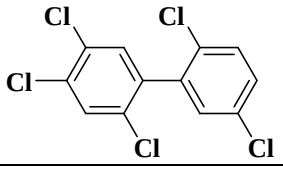
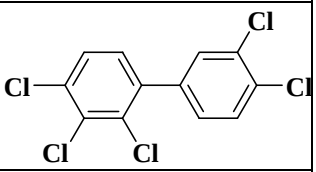
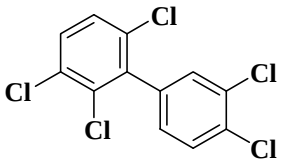
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
194	821-55-6	2.79	2.30	2.71	3.14	142.136	-0.080	
195[a]	627-05-4	1.53	1.09	1.44	1.47	103.063	-0.071	
196	646-14-0	2.58	2.10	2.42	2.70	131.095	-0.070	
197	536-75-4	1.14	1.25	1.84	1.65	107.074	-0.106	
198	100-00-5	2.38	2.06	2.46	2.39	156.993	-0.064	
199	98-95-3	1.92	1.44	1.81	1.85	123.032	-0.069	
200[a]	88-72-2	2.40	2.00	2.36	2.30	137.048	-0.070	
201[a]	606-20-2	1.94	1.68	2.18	2.10	182.033	-0.056	
202[a]	100-17-4	2.32	1.34	1.89	2.03	153.043	-0.074	
203[a]	150-78-7	2.12	1.78	2.15	2.04	138.068	-0.066	
204[a]	106-48-9	1.51	1.93	2.16	2.39	128.003	-0.056	
205	93-89-0	2.59	1.84	2.32	2.64	150.068	-0.075	
206	120-72-9	1.99	1.98	2.05	2.14	117.058	-0.040	
207	104-76-7	2.04	2.33	2.73		130.136	-0.087	

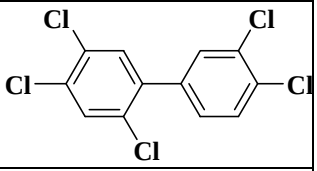
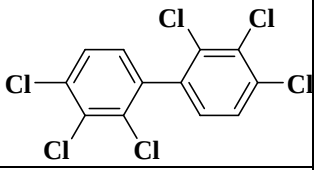
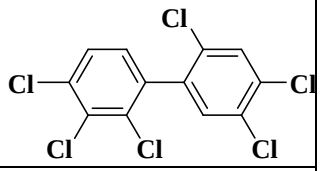
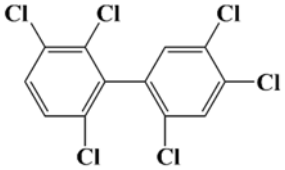
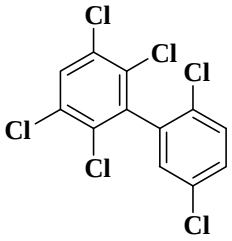
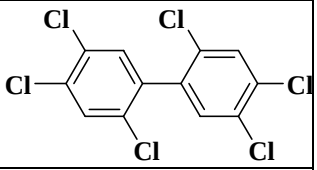
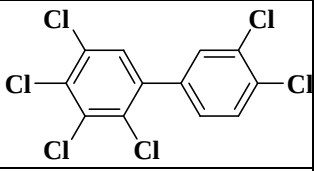
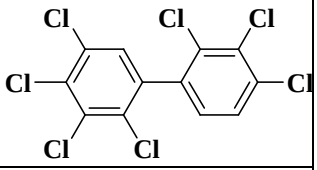
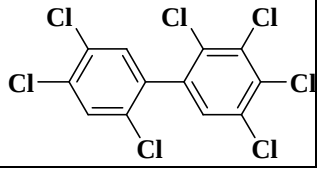
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
208[a]	597-76-2	1.70	2.26	2.69		130.136	-0.089	
209	19780-44-0	1.92	2.24	2.66		130.136	-0.087	
210	597-49-9	1.13	1.79	2.20		116.120	-0.086	
211	121-14-2	2.34	1.65	2.18	1.98	182.033	-0.059	
212[a]	430-55-7	0.98	1.98	1.94		96.014	-0.037	
213	67-72-1	3.71	3.95	4.03	4.14	233.813	-0.009	
214[a]	92-52-4	4.14	3.89	3.76	4.01	154.078	-0.027	
215	544-76-3[b]	9.88	8.87	8.20		226.266	-0.005	
216	75-26-3	2.28	2.07	2.08	2.14	121.973	-0.030	
217	127-91-3	4.11	4.58	4.35	4.16	136.125	-0.038	
218	5989-27-5	4.17	5.15	4.83	4.57	136.125	-0.036	
219[a]	593-53-3	0.00	0.83	0.77	0.51	34.022	-0.049	
220	2825-83-4	4.62	3.92	3.59		136.125	-0.009	
221[a]	1634-04-4	0.89	1.03	1.43	0.94	88.089	-0.086	
222	75-01-4	1.58	1.90	1.62		61.992	-0.022	
223	67-68-5	-2.66	-2.21	-1.22	-1.35	78.014	-0.113	

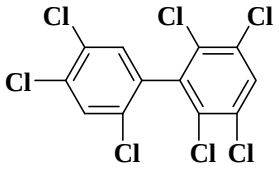
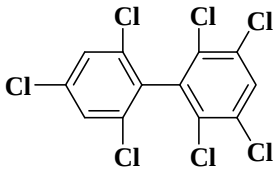
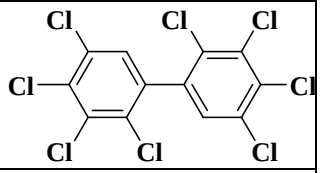
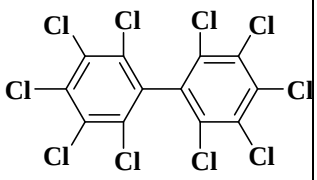
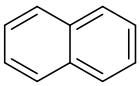
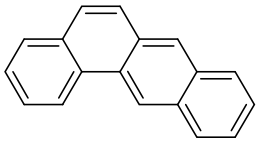
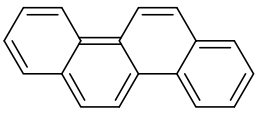
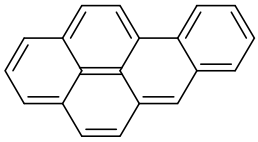
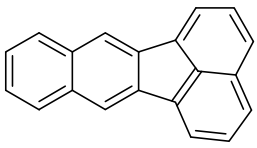
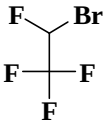
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
224[a]	64-18-6	-1.69	-0.84	-0.46	-0.54	46.005	-0.072	
225	13466-78-9	4.71	4.89	4.61	4.38	136.125	-0.036	
226	593-60-2	1.34	1.57	1.52	1.57	105.942	-0.021	
227	106-47-8	1.62	1.35	1.72	1.83	127.019	-0.064	
228	107-05-1	1.84	2.09	1.93		76.008	-0.034	
229	100-42-5	2.68	3.10	2.89	2.95	104.063	-0.031	
230	111-65-9	5.27	4.86	4.27	5.18	114.141	-0.005	
231[a]	108-43-0	1.66	1.93	2.16	2.50	128.003	-0.055	
232[a]	140-11-4	1.70	1.46	2.08	1.96	150.068	-0.088	
233	90-15-3	2.19	2.48	2.69	2.85	144.058	-0.054	
234	106-41-2	1.61	2.00	2.40	2.59	171.952	-0.054	
235	540-37-4	2.19	1.54	2.24	2.34	218.950	-0.059	
236	91-66-7	3.17	3.03	3.15	3.31	149.120	-0.049	
237	645-56-7	2.19	2.83	3.04	3.20	136.089	-0.065	
238[a]	540-38-5[b]	2.29	2.08	2.68	2.91	219.934	-0.054	
239	99-65-0	1.42	1.11	1.63	1.49	168.017	-0.056	
240	120-12-7	4.83	4.46	4.35	4.45	178.078	-0.027	

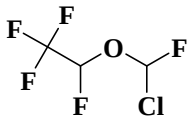
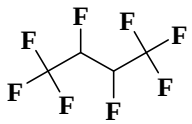
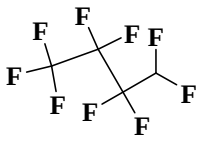
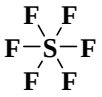
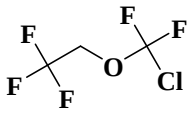
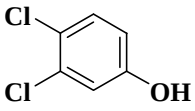
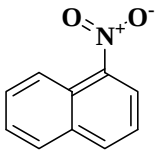
No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
241[a]	85-01-8	4.80	4.46	4.35	4.46	178.078	-0.027	
242	206-44-0	5.18	5.00	4.93	5.16	202.078	-0.028	
243[a]	129-00-0	5.26	5.02	4.93	4.88	202.078	-0.026	
244	86-73-7	4.39	4.11	4.02	4.18	166.078	-0.029	
245	83-32-9	3.97	4.31	4.15	3.92	154.078	-0.031	
246	108-95-2	-0.16		1.51	1.46	94.042	-0.063	
247[a]	75-15-0	2.46	2.35	1.94	1.94	75.944	-0.003	
248	74-86-2	-0.63	0.68	0.50	0.37	26.016	-0.034	
249	50-00-0	-0.41	0.22	0.35	0.35	30.011	-0.067	
250	107-03-9	1.93	1.76	1.76	1.81	76.035	-0.050	
251[a]	109-79-5	2.53	2.26	2.25	2.28	90.050	-0.051	
252	110-66-7	3.28	2.76	2.74		104.066	-0.051	
253	111-31-9	4.02	3.26	3.23		118.082	-0.051	
254	6032-29-7	0.30	0.83	1.26	1.19	88.089	-0.087	
255	626-93-7	0.91	1.33	1.75	1.76	102.104	-0.087	
256	623-37-0	0.48	1.33	1.75	1.65	102.104	-0.087	
257	543-49-7	1.52	1.80	2.24	2.31	116.120	-0.090	

No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
258	589-55-9	1.67	1.83	2.24	2.22	116.120	-0.086	
259	589-62-8	2.42	2.35	2.73	2.68	130.136	-0.084	
260	75-89-8	-0.55	-0.22	0.27	0.41	100.014	-0.067	
261	374-01-6	-0.05	0.17	0.69	0.71	114.029	-0.070	
262	76-37-9	-0.10	0.00	0.63		132.020	-0.071	
263[a]	422-05-9	0.34	0.66	1.24	1.23	150.010	-0.066	
264	920-66-1	0.76	0.54	1.11	1.66	168.001	-0.051	
265	1515-14-6	1.10	0.96	1.56		182.017	-0.056	
266[a]	382-31-0[b]	0.66	0.89	1.60		182.017	-0.070	
267	375-01-9	1.17	1.19	1.91	1.94	200.007	-0.066	
268	78-92-2	-0.28	0.33	0.77	0.61	74.073	-0.087	
269	78-40-0	0.22	-0.23	0.87	0.80	182.071	-0.103	

No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
270	120-80-9	0.79	0.51	1.03	0.88	110.037	-0.079	
271	7012-37-5	5.83	5.66	5.69	5.62	255.961	-0.022	
272	16606-02-3	5.83	5.66	5.69	5.69	255.961	-0.023	
273	41464-39-5	6.01	6.22	6.34	5.81	289.922	-0.026	
274[a]	41464-40-8[b]	6.03	6.27	6.34	6.22	289.922	-0.020	
275	35693-99-3	6.04	6.27	6.34	6.09	289.922	-0.020	
276	38380-01-7	6.52	6.83	6.98	7.21	323.883	-0.022	
277	37680-73-2	6.52	6.83	6.98	6.80	323.883	-0.022	
278[a]	32598-14-4[b]	6.82	6.80	6.98	6.79	323.883	-0.025	
279	38380-03-9	6.53	6.78	6.98	6.22	323.883	-0.027	

No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
280	31508-00-6	6.81	6.81	6.98	7.12	323.883	-0.024	
281	38380-07-3	6.97	7.41	7.62	7.31	357.844	-0.021	
282[a]	35065-28-2[b]	7.00	7.41	7.62	7.44	357.844	-0.020	
283	38380-04-0	6.83	7.40	7.62	7.28	357.844	-0.022	
284[a]	52663-63-5[b]	6.77	7.42	7.62		357.844	-0.020	
285	35065-27-1	7.03	7.42	7.62	7.75	357.844	-0.019	
286[a]	38380-08-4[b]	7.34	7.39	7.62	7.60	357.844	-0.023	
287[a]	35065-30-6[b]	7.45	8.01	8.27		391.805	-0.019	
288	35065-29-3[b]	7.49	8.02	8.27		391.805	-0.018	

No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
289	52663-68-0[b]	7.27	7.98	8.27		391.805	-0.023	
290	74487-85-7[b]	7.03	8.02	8.27		391.805	-0.018	
291[a]	35694-08-7[b]	8.01	8.61	8.91	8.68	425.766	-0.015	
292	2051-24-3	8.26		10.20	8.27	493.689	-0.013	
293[a]	91-20-3	3.61	5.57	3.17	3.30	128.063	-0.027	
294[a]	56-55-3	6.26	5.57	5.52	5.76	228.094	-0.026	
295	218-01-9	6.25	6.14	5.52	5.81	228.094	-0.026	
296	50-32-8	6.79	6.13	6.11	6.13	252.094	-0.026	
297	207-08-9	6.84	1.45	6.11	6.11	252.094	-0.027	
298[a]	124-72-1[b]	1.80	3.33	1.95		239.840	-0.015	

No.	CAS	log $K_{lip/w}$		log K_{ow}	*Exp*	M_w (a.u.)	$V_{s,min}$ (eV)	Structures
		Exp.	Pred.					
299	56885-28-0	2.15		0.96		183.971	-0.027	
300[a]	75995-72-1	2.44	2.68	2.87		202.003	-0.019	
301[a]	375-17-7[b]	2.82	2.63	2.89		219.993	-0.016	
302	2551-62-4	1.85	1.40	1.64	1.68	145.962	-0.034	
303[a]	33018-78-9	2.73	1.96	2.25		183.971	-0.030	
304	95-77-2	2.42	2.94	2.80	3.33	161.964	-0.002	
305	86-57-7	3.45	2.56	2.99	3.13	173.048	-0.069	

a: The chemicals are used in test set.

b: The h_i value of the compound is larger than the h^* value

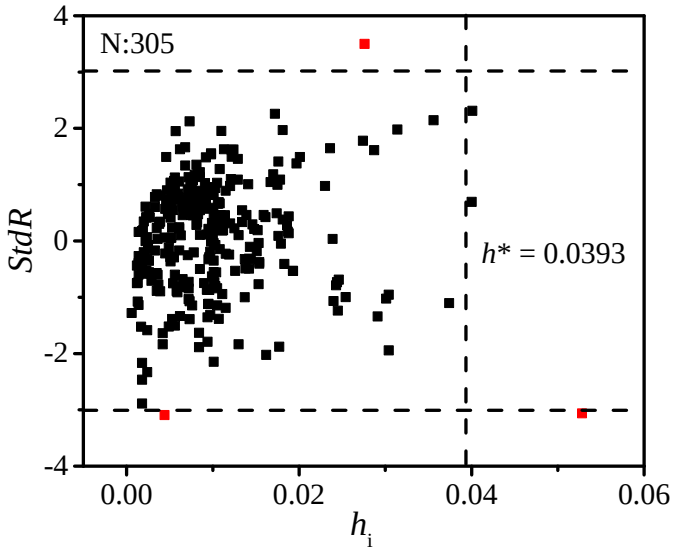


Fig. S1. Williams plot for Model (1)

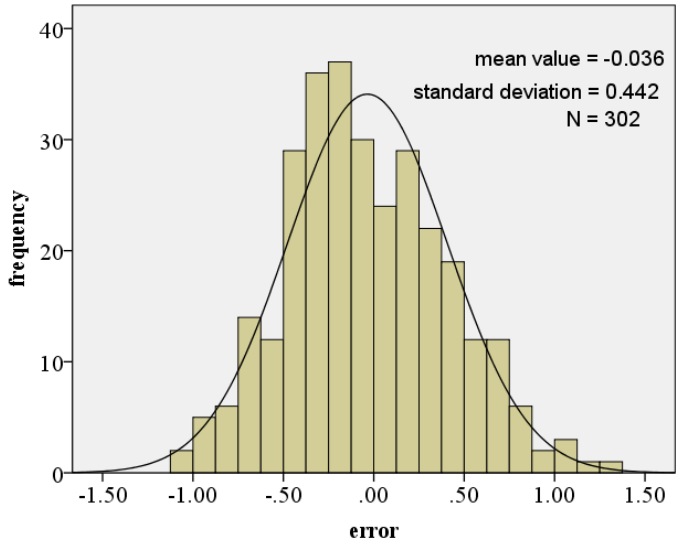


Fig. S2. Normal distribution plot for Model (2)

If the predictive log K_{ow} values used in model (2) were replaced by experimental log K_{ow} values, a new model was yielded:

$$\log K_{lip/w} = 1.115\log K_{ow} - 0.003M_w + 6.654V_{s,min} + 0.307 \quad \text{(S1)}$$

For the model (S1), R^2 = 0.979 and *RMSE* = 0.452.