

Supporting Information for

Extrapolative prediction of propagation rate coefficient in free-radical polymerization based on $k_p(T, M)$ -QSPR model

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Table S1. Dataset for monomers, temperature, experimental and calculated $\ln k_p$ values

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
1	BMA	253.15	0.003950	72.50	4.28	4.43	'training'
2	BMA	263.15	0.003800	116.00	4.75	4.82	'training'
3	BMA	273.15	0.003661	185.00	5.22	5.18	'training'
4	BMA	279.25	0.003581	188.33	5.24	5.39	'training'
5	BMA	283.15	0.003532	251.50	5.53	5.52	'training'
6	BMA	291.05	0.003436	273.86	5.61	5.77	'training'
7	BMA	291.85	0.003426	304.00	5.72	5.80	'training'
8	BMA	293.15	0.003411	350.50	5.86	5.84	'training'
9	BMA	301.65	0.003315	368.00	5.91	6.09	'training'
10	BMA	303.15	0.003299	455.63	6.12	6.13	'training'
11	BMA	311.75	0.003208	509.00	6.23	6.37	'training'
12	BMA	320.55	0.003120	680.00	6.52	6.59	'training'
13	BMA	323.15	0.003095	772.54	6.65	6.66	'training'
14	BMA	333.15	0.003002	1018.50	6.93	6.90	'training'
15	BMA	343.15	0.002914	1364.75	7.22	7.13	'training'
16	BMA	363.15	0.002754	1938.31	7.57	7.55	'training'
17	BzA	248.35	0.004027	4596.50	8.43	8.46	'training'
18	BzA	248.55	0.004023	4464.40	8.40	8.46	'training'
19	BzA	253.25	0.003949	5333.30	8.58	8.61	'training'
20	BzA	253.35	0.003947	5385.70	8.59	8.61	'training'
21	BzA	256.45	0.003899	6076.30	8.71	8.70	'training'
22	BzA	256.65	0.003896	6113.10	8.72	8.71	'training'
23	BzA	260.05	0.003845	6830.20	8.83	8.81	'training'
24	BzA	260.35	0.003841	6872.20	8.84	8.82	'training'
25	BzA	263.95	0.003789	7614.70	8.94	8.92	'training'
26	BzA	264.05	0.003787	7899.60	8.97	8.92	'training'
27	BzA	269.95	0.003704	9173.50	9.12	9.08	'training'
28	BzA	270.05	0.003703	9068.90	9.11	9.08	'training'
29	BzA	274.15	0.003648	10188.20	9.23	9.19	'training'
30	BzA	277.85	0.003599	11160.00	9.32	9.29	'training'
31	BzA	281.85	0.003548	12300.55	9.42	9.38	'training'
32	CHMA	283.15	0.003532	383.00	5.95	5.95	'training'
33	CHMA	294.15	0.003400	477.50	6.17	6.28	'training'
34	CHMA	303.15	0.003299	691.75	6.54	6.54	'training'
35	CHMA	313.15	0.003193	922.75	6.83	6.80	'training'
36	CHMA	323.15	0.003095	1201.08	7.09	7.05	'training'
37	CHMA	333.15	0.003002	1604.50	7.38	7.29	'training'
38	CHMA	343.15	0.002914	1936.25	7.57	7.51	'training'
39	CHMA	353.15	0.002832	2533.00	7.84	7.72	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
40	CHMA	363.15	0.002754	3091.77	8.04	7.92	'training'
41	CHMA	364.15	0.002746	3146.00	8.05	7.94	'training'
42	DEAEMA	273.15	0.003661	233.50	5.45	5.50	'training'
43	DEAEMA	283.15	0.003532	338.50	5.82	5.83	'training'
44	DEAEMA	292.85	0.003415	475.00	6.16	6.13	'training'
45	DEAEMA	292.95	0.003414	464.00	6.14	6.13	'training'
46	DEAEMA	293.05	0.003412	468.00	6.15	6.14	'training'
47	DEAEMA	303.15	0.003299	626.50	6.44	6.43	'training'
48	DEAEMA	313.15	0.003193	812.67	6.70	6.70	'training'
49	DEAEMA	323.05	0.003095	1010.50	6.92	6.94	'training'
50	DEAEMA	333.05	0.003003	1340.00	7.20	7.18	'training'
51	DEAEMA	333.35	0.003000	1306.00	7.17	7.19	'training'
52	DEAEMA	343.35	0.002912	1599.00	7.38	7.41	'training'
53	DEAEMA	353.05	0.002832	1964.00	7.58	7.62	'training'
54	DEAEMA	353.15	0.002832	1792.00	7.49	7.62	'training'
55	DEAEMA	363.25	0.002753	2261.00	7.72	7.82	'training'
56	DEAEMA	363.35	0.002752	2626.00	7.87	7.82	'training'
57	DMA	282.15	0.003544	333.00	5.81	5.65	'training'
58	DMA	282.25	0.003543	275.00	5.62	5.65	'training'
59	DMA	283.15	0.003532	352.80	5.87	5.68	'training'
60	DMA	283.35	0.003529	354.00	5.87	5.69	'training'
61	DMA	283.65	0.003525	356.00	5.87	5.70	'training'
62	DMA	293.45	0.003408	402.00	6.00	6.00	'training'
63	DMA	293.75	0.003404	472.00	6.16	6.01	'training'
64	DMA	293.85	0.003403	389.00	5.96	6.01	'training'
65	DMA	298.15	0.003354	536.67	6.29	6.14	'training'
66	DMA	303.15	0.003299	595.78	6.39	6.28	'training'
67	DMA	313.15	0.003193	763.67	6.64	6.55	'training'
68	DMA	313.25	0.003192	744.00	6.61	6.55	'training'
69	DMA	313.35	0.003191	771.00	6.65	6.55	'training'
70	DMA	323.15	0.003095	990.54	6.90	6.80	'training'
71	DMA	323.65	0.003090	1125.00	7.03	6.81	'training'
72	DMA	332.35	0.003009	1267.00	7.14	7.02	'training'
73	DMA	332.85	0.003004	1108.00	7.01	7.03	'training'
74	DMA	332.95	0.003003	1238.00	7.12	7.03	'training'
75	DMA	333.15	0.003002	1207.33	7.10	7.04	'training'
76	DMA	333.45	0.002999	1157.50	7.05	7.05	'training'
77	DMA	343.15	0.002914	1598.67	7.38	7.26	'training'
78	DMA	363.15	0.002754	2400.65	7.78	7.67	'training'
79	DMA ^{PM} AE	273.15	0.003661	206.25	5.33	5.33	'training'
80	DMA ^{PM} AE	283.15	0.003532	307.00	5.73	5.66	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
81	DMAPMAE	283.85	0.003523	239.00	5.48	5.68	'training'
82	DMAPMAE	292.65	0.003417	368.00	5.91	5.96	'training'
83	DMAPMAE	303.35	0.003297	483.25	6.18	6.27	'training'
84	DMAPMAE	313.25	0.003192	624.50	6.44	6.54	'training'
85	DMAPMAE	313.35	0.003191	646.50	6.47	6.54	'training'
86	DMAPMAE	323.15	0.003095	873.75	6.77	6.79	'training'
87	DMAPMAE	333.15	0.003002	1005.00	6.91	7.03	'training'
88	DMAPMAE	343.15	0.002914	1382.67	7.23	7.26	'training'
89	DMAPMAE	353.15	0.002832	1581.00	7.37	7.47	'training'
90	DMAPMAE	363.15	0.002754	1763.00	7.47	7.68	'training'
91	EA	248.15	0.004030	3303.40	8.10	8.05	'training'
92	EA	248.25	0.004028	3254.40	8.09	8.06	'training'
93	EA	257.55	0.003883	4570.40	8.43	8.38	'training'
94	EA	265.15	0.003771	5838.70	8.67	8.63	'training'
95	EA	265.35	0.003769	5819.10	8.67	8.64	'training'
96	EA	273.95	0.003650	7747.20	8.96	8.90	'training'
97	EA	274.05	0.003649	7716.30	8.95	8.91	'training'
98	EA	280.95	0.003559	9466.95	9.16	9.11	'training'
99	EA	288.15	0.003470	11618.90	9.36	9.31	'training'
100	EA	288.25	0.003469	11598.50	9.36	9.31	'training'
101	EA	295.45	0.003385	14017.70	9.55	9.50	'training'
102	EA	303.65	0.003293	16974.80	9.74	9.70	'training'
103	EA	310.35	0.003222	19894.50	9.90	9.86	'training'
104	EA	310.55	0.003220	19755.30	9.89	9.87	'training'
105	EEA	278.25	0.003594	15620.00	9.66	9.61	'training'
106	EEA	278.35	0.003593	15800.00	9.67	9.61	'training'
107	EEA	286.95	0.003485	19220.00	9.86	9.81	'training'
108	EEA	287.45	0.003479	19460.00	9.88	9.82	'training'
109	EEA	298.45	0.003351	23990.00	10.09	10.06	'training'
110	EEA	299.05	0.003344	24010.00	10.09	10.07	'training'
111	EEA	303.05	0.003300	26450.00	10.18	10.15	'training'
112	EEA	312.55	0.003199	31040.00	10.34	10.33	'training'
113	EEA	313.55	0.003189	31440.00	10.36	10.35	'training'
114	EEA	323.45	0.003092	36060.00	10.49	10.53	'training'
115	EEA	324.65	0.003080	37790.00	10.54	10.55	'training'
116	EEA	333.55	0.002998	42780.00	10.66	10.70	'training'
117	EEA	334.25	0.002992	42810.00	10.66	10.71	'training'
118	EEA	343.75	0.002909	49570.00	10.81	10.87	'training'
119	EEA	344.95	0.002899	50770.00	10.84	10.88	'training'
120	EEA	354.05	0.002824	52510.00	10.87	11.02	'training'
121	EEA	355.65	0.002812	56260.00	10.94	11.04	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
122	EHA	283.25	0.003530	10440.00	9.25	9.22	'training'
123	EHA	283.35	0.003529	11500.00	9.35	9.22	'training'
124	EHA	293.15	0.003411	14490.00	9.58	9.48	'training'
125	EHA	293.85	0.003403	15050.00	9.62	9.50	'training'
126	EHA	302.85	0.003302	17280.00	9.76	9.72	'training'
127	EHA	302.95	0.003301	18190.00	9.81	9.72	'training'
128	EHA	313.95	0.003185	21820.00	9.99	9.97	'training'
129	EHA	314.05	0.003184	21550.00	9.98	9.97	'training'
130	EHA	323.95	0.003087	24780.00	10.12	10.18	'training'
131	EHA	333.95	0.002994	30860.00	10.34	10.38	'training'
132	EHA	334.05	0.002994	33060.00	10.41	10.39	'training'
133	EHA	344.35	0.002904	34425.00	10.45	10.58	'training'
134	EHA	354.35	0.002822	34250.00	10.44	10.76	'training'
135	EHA	354.65	0.002820	39990.00	10.60	10.76	'training'
136	GMA	293.15	0.003411	494.00	6.20	6.20	'training'
137	GMA	303.15	0.003299	693.14	6.54	6.49	'training'
138	GMA	312.15	0.003204	961.00	6.87	6.73	'training'
139	GMA	313.15	0.003193	1018.00	6.93	6.75	'training'
140	GMA	323.15	0.003095	1151.00	7.05	7.00	'training'
141	GMA	334.15	0.002993	1857.50	7.53	7.26	'training'
142	GMA	343.15	0.002914	1941.00	7.57	7.46	'training'
143	GMA	353.15	0.002832	2370.00	7.77	7.66	'training'
144	GMA	363.15	0.002754	3132.70	8.05	7.86	'training'
145	HA	248.95	0.004017	3742.80	8.23	8.31	'training'
146	HA	249.05	0.004015	3723.00	8.22	8.31	'training'
147	HA	252.25	0.003964	4110.30	8.32	8.42	'training'
148	HA	252.35	0.003963	4110.70	8.32	8.42	'training'
149	HA	257.35	0.003886	5004.30	8.52	8.59	'training'
150	HA	257.65	0.003881	4951.40	8.51	8.60	'training'
151	HA	262.55	0.003809	5906.80	8.68	8.75	'training'
152	HA	262.65	0.003807	5907.40	8.68	8.75	'training'
153	HA	265.65	0.003764	6597.90	8.79	8.85	'training'
154	HA	265.85	0.003762	6599.20	8.79	8.85	'training'
155	HA	268.85	0.003720	7188.15	8.88	8.94	'training'
156	HA	273.85	0.003652	8412.60	9.04	9.09	'training'
157	HA	273.95	0.003650	8413.50	9.04	9.09	'training'
158	HA	277.35	0.003606	9206.85	9.13	9.19	'training'
159	HA	280.85	0.003561	10245.00	9.23	9.28	'training'
160	HA	280.95	0.003559	10298.20	9.24	9.28	'training'
161	HA	281.95	0.003547	10520.40	9.26	9.31	'training'
162	HA	288.85	0.003462	12588.90	9.44	9.49	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
163	HEA	293.15	0.003411	13608.50	9.52	9.61	'training'
164	HEA	300.15	0.003332	16172.00	9.69	9.75	'training'
165	HEA	303.15	0.003299	17132.00	9.75	9.80	'training'
166	HEA	313.15	0.003193	21567.50	9.98	9.98	'training'
167	HEA	323.15	0.003095	26365.75	10.18	10.15	'training'
168	HEA	333.15	0.003002	31901.00	10.37	10.31	'training'
169	HPMA	303.15	0.003299	905.00	6.81	6.77	'training'
170	HPMA	323.15	0.003095	1490.25	7.31	7.25	'training'
171	HPMA	343.15	0.002914	2435.25	7.80	7.67	'training'
172	HPMA	363.15	0.002754	3512.73	8.16	8.05	'training'
173	HPMA	383.15	0.002610	5097.75	8.54	8.39	'training'
174	MA	245.15	0.004079	3300.00	8.10	7.97	'training'
175	MA	246.75	0.004053	2992.00	8.00	8.02	'training'
176	MA	247.35	0.004043	3166.00	8.06	8.04	'training'
177	MA	247.65	0.004038	3359.00	8.12	8.05	'training'
178	MA	248.15	0.004030	3329.67	8.11	8.07	'training'
179	MA	248.55	0.004023	3684.00	8.21	8.08	'training'
180	MA	248.95	0.004017	3553.00	8.18	8.10	'training'
181	MA	253.85	0.003939	3790.00	8.24	8.26	'training'
182	MA	254.05	0.003936	3740.00	8.23	8.27	'training'
183	MA	254.65	0.003927	3680.00	8.21	8.29	'training'
184	MA	255.25	0.003918	3860.00	8.26	8.31	'training'
185	MA	255.65	0.003912	3920.00	8.27	8.32	'training'
186	MA	256.05	0.003905	3870.00	8.26	8.33	'training'
187	MA	256.55	0.003898	3930.00	8.28	8.35	'training'
188	MA	256.85	0.003893	4060.00	8.31	8.36	'training'
189	MA	256.95	0.003892	4120.00	8.32	8.36	'training'
190	MA	257.15	0.003889	3930.00	8.28	8.37	'training'
191	MA	257.35	0.003886	4135.00	8.33	8.38	'training'
192	MA	257.45	0.003884	4643.00	8.44	8.38	'training'
193	MA	257.55	0.003883	4567.00	8.43	8.38	'training'
194	MA	258.15	0.003874	5300.00	8.58	8.40	'training'
195	MA	261.85	0.003819	5272.86	8.57	8.52	'training'
196	MA	265.15	0.003771	5792.50	8.66	8.62	'training'
197	MA	270.25	0.003700	6560.00	8.79	8.77	'training'
198	MA	270.45	0.003698	6570.00	8.79	8.77	'training'
199	MA	270.65	0.003695	6680.00	8.81	8.78	'training'
200	MA	271.25	0.003687	6790.00	8.82	8.80	'training'
201	MA	272.65	0.003668	6790.00	8.82	8.84	'training'
202	MA	272.85	0.003665	6170.00	8.73	8.84	'training'
203	MA	273.15	0.003661	7395.13	8.91	8.85	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
204	MA	273.25	0.003660	7325.00	8.90	8.85	'training'
205	MA	274.05	0.003649	7606.00	8.94	8.88	'training'
206	MA	275.05	0.003636	6170.00	8.73	8.91	'training'
207	MA	275.35	0.003632	6370.00	8.76	8.91	'training'
208	MA	276.95	0.003611	6435.00	8.77	8.96	'training'
209	MA	277.15	0.003608	6530.00	8.78	8.96	'training'
210	MA	277.35	0.003606	5990.00	8.70	8.97	'training'
211	MA	280.95	0.003559	9303.50	9.14	9.07	'training'
212	MA	284.45	0.003516	9401.00	9.15	9.16	'training'
213	MA	285.05	0.003508	10320.00	9.24	9.18	'training'
214	MA	285.55	0.003502	9740.00	9.18	9.19	'training'
215	MA	288.15	0.003470	11397.00	9.34	9.26	'training'
216	MA	292.95	0.003414	12294.50	9.42	9.38	'training'
217	MA	293.15	0.003411	11431.70	9.34	9.38	'training'
218	MA	293.55	0.003407	12826.00	9.46	9.39	'training'
219	MA	294.95	0.003390	13727.00	9.53	9.43	'training'
220	MA	295.45	0.003385	13808.00	9.53	9.44	'training'
221	MA	298.15	0.003354	13775.00	9.53	9.50	'training'
222	MA	302.85	0.003302	15851.00	9.67	9.61	'training'
223	MA	302.95	0.003301	16461.00	9.71	9.61	'training'
224	MA	303.05	0.003300	16317.00	9.70	9.62	'training'
225	MA	303.95	0.003290	13944.00	9.54	9.64	'training'
226	MA	305.15	0.003277	14900.00	9.61	9.67	'training'
227	MA	308.85	0.003238	16796.00	9.73	9.75	'training'
228	MA	309.65	0.003229	19376.00	9.87	9.77	'training'
229	MA	310.35	0.003222	19578.00	9.88	9.78	'training'
230	MA	313.15	0.003193	17621.14	9.78	9.84	'training'
231	MA	313.45	0.003190	21279.50	9.97	9.85	'training'
232	MA	323.35	0.003093	26041.00	10.17	10.06	'training'
233	MA	323.55	0.003091	26297.00	10.18	10.06	'training'
234	MA	333.15	0.003002	24725.00	10.12	10.25	'training'
235	MA	333.65	0.002997	31654.00	10.36	10.26	'training'
236	MA	333.75	0.002996	31965.00	10.37	10.26	'training'
237	MMA	272.15	0.003674	129.33	4.86	5.00	'training'
238	MMA	278.15	0.003595	151.00	5.02	5.20	'training'
239	MMA	283.15	0.003532	210.75	5.35	5.36	'training'
240	MMA	293.15	0.003411	274.00	5.61	5.67	'training'
241	MMA	298.15	0.003354	318.58	5.76	5.81	'training'
242	MMA	303.15	0.003299	388.55	5.96	5.95	'training'
243	MMA	313.15	0.003193	520.60	6.25	6.22	'training'
244	MMA	323.15	0.003095	630.50	6.45	6.47	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
245	MMA	333.15	0.003002	858.25	6.75	6.71	'training'
246	MMA	343.15	0.002914	1058.00	6.96	6.93	'training'
247	MMA	353.15	0.002832	1307.25	7.18	7.14	'training'
248	MMA	363.15	0.002754	1531.33	7.33	7.33	'training'
249	MOMA	272.95	0.003664	279.67	5.63	5.57	'training'
250	MOMA	273.05	0.003662	255.00	5.54	5.57	'training'
251	MOMA	283.45	0.003528	364.00	5.90	5.91	'training'
252	MOMA	283.55	0.003527	388.50	5.96	5.91	'training'
253	MOMA	283.65	0.003525	394.00	5.98	5.92	'training'
254	MOMA	293.15	0.003411	463.00	6.14	6.20	'training'
255	MOMA	293.35	0.003409	510.00	6.23	6.21	'training'
256	MOMA	293.65	0.003405	501.00	6.22	6.22	'training'
257	MOMA	303.95	0.003290	584.50	6.37	6.51	'training'
258	MOMA	304.05	0.003289	633.00	6.45	6.51	'training'
259	MOMA	304.15	0.003288	638.00	6.46	6.51	'training'
260	MOMA	313.25	0.003192	761.50	6.64	6.75	'training'
261	MOMA	322.95	0.003096	1080.50	6.99	6.99	'training'
262	MOMA	323.25	0.003094	1047.00	6.95	7.00	'training'
263	MOMA	333.25	0.003001	1315.00	7.18	7.23	'training'
264	MOMA	333.35	0.003000	1325.67	7.19	7.23	'training'
265	MOMA	343.35	0.002912	1523.00	7.33	7.45	'training'
266	MOMA	343.45	0.002912	1562.00	7.35	7.45	'training'
267	MOMA	353.85	0.002826	1735.50	7.46	7.67	'training'
268	MOMA	353.95	0.002825	1824.00	7.51	7.67	'training'
269	MOMA	354.05	0.002824	1741.00	7.46	7.67	'training'
270	MOMA	363.85	0.002748	2213.00	7.70	7.86	'training'
271	MOMA	363.95	0.002748	2438.33	7.80	7.86	'training'
272	NEAEMA	282.95	0.003534	318.00	5.76	5.84	'training'
273	NEAEMA	283.15	0.003532	338.00	5.82	5.85	'training'
274	NEAEMA	293.45	0.003408	470.00	6.15	6.15	'training'
275	NEAEMA	294.15	0.003400	437.00	6.08	6.17	'training'
276	NEAEMA	302.95	0.003301	609.50	6.41	6.42	'training'
277	NEAEMA	313.05	0.003194	771.00	6.65	6.68	'training'
278	NEAEMA	313.15	0.003193	832.00	6.72	6.69	'training'
279	NEAEMA	322.85	0.003097	985.00	6.89	6.93	'training'
280	NEAEMA	332.95	0.003003	1220.50	7.11	7.16	'training'
281	NEAEMA	343.15	0.002914	1585.00	7.37	7.38	'training'
282	NEAEMA	353.55	0.002828	1581.00	7.37	7.59	'training'
283	NEAEMA	353.65	0.002828	1912.00	7.56	7.60	'training'
284	NEAEMA	362.65	0.002757	2247.50	7.72	7.77	'training'
285	PHA	265.85	0.003762	6222.50	8.74	8.65	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
286	PHA	273.25	0.003660	7439.00	8.91	8.87	'training'
287	PHA	273.95	0.003650	7578.00	8.93	8.89	'training'
288	PHA	283.45	0.003528	10689.50	9.28	9.16	'training'
289	PHA	292.25	0.003422	12694.00	9.45	9.39	'training'
290	PHA	292.75	0.003416	13462.00	9.51	9.40	'training'
291	PHA	303.35	0.003297	15502.00	9.65	9.67	'training'
292	PHA	303.45	0.003295	15782.00	9.67	9.67	'training'
293	PHA	308.45	0.003242	17365.50	9.76	9.79	'training'
294	PHA	313.35	0.003191	18958.00	9.85	9.90	'training'
295	PHA	318.45	0.003140	20594.00	9.93	10.01	'training'
296	PHA	323.25	0.003094	22094.00	10.00	10.11	'training'
297	PHA	323.35	0.003093	25322.00	10.14	10.11	'training'
298	PHA	328.25	0.003046	26464.00	10.18	10.22	'training'
299	PHA	328.45	0.003045	26704.00	10.19	10.22	'training'
300	PHA	333.55	0.002998	28927.00	10.27	10.32	'training'
301	PHMA	264.35	0.003783	167.00	5.12	4.94	'training'
302	PHMA	264.65	0.003779	133.00	4.89	4.96	'training'
303	PHMA	273.05	0.003662	210.00	5.35	5.26	'training'
304	PHMA	273.15	0.003661	182.00	5.20	5.26	'training'
305	PHMA	282.55	0.003539	281.00	5.64	5.58	'training'
306	PHMA	283.05	0.003533	247.00	5.51	5.60	'training'
307	PHMA	292.55	0.003418	373.00	5.92	5.90	'training'
308	PHMA	292.95	0.003414	336.00	5.82	5.91	'training'
309	PHMA	303.15	0.003299	469.00	6.15	6.21	'training'
310	PHMA	303.25	0.003298	622.00	6.43	6.22	'training'
311	PHMA	312.75	0.003197	587.00	6.38	6.48	'training'
312	PHMA	313.45	0.003190	707.00	6.56	6.50	'training'
313	PHMA	323.35	0.003093	803.00	6.69	6.76	'training'
314	PHMA	323.45	0.003092	949.00	6.86	6.76	'training'
315	PHMA	333.25	0.003001	1182.00	7.07	7.00	'training'
316	PHMA	333.35	0.003000	993.00	6.90	7.00	'training'
317	PHMA	343.05	0.002915	1341.00	7.20	7.22	'training'
318	PHMA	343.65	0.002910	1524.00	7.33	7.24	'training'
319	PHMA	353.45	0.002829	1863.00	7.53	7.45	'training'
320	PHMA	353.85	0.002826	1634.00	7.40	7.46	'training'
321	PipEMA	273.15	0.003661	234.50	5.46	5.47	'training'
322	PipEMA	282.85	0.003535	321.00	5.77	5.79	'training'
323	PipEMA	283.05	0.003533	333.33	5.81	5.80	'training'
324	PipEMA	292.85	0.003415	444.00	6.10	6.10	'training'
325	PipEMA	293.35	0.003409	454.00	6.12	6.11	'training'
326	PipEMA	293.85	0.003403	465.00	6.14	6.13	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
327	PipEMA	303.35	0.003297	575.00	6.35	6.40	'training'
328	PipEMA	303.45	0.003295	611.00	6.42	6.40	'training'
329	PipEMA	313.15	0.003193	718.00	6.58	6.66	'training'
330	PipEMA	313.25	0.003192	790.00	6.67	6.67	'training'
331	PipEMA	323.25	0.003094	1077.00	6.98	6.92	'training'
332	PipEMA	323.35	0.003093	1081.50	6.99	6.92	'training'
333	PipEMA	333.45	0.002999	1313.00	7.18	7.16	'training'
334	PipEMA	333.55	0.002998	1399.00	7.24	7.16	'training'
335	PipEMA	343.35	0.002912	1659.67	7.41	7.38	'training'
336	PipEMA	343.45	0.002912	1750.00	7.47	7.38	'training'
337	PipEMA	353.35	0.002830	1888.00	7.54	7.59	'training'
338	PipEMA	353.45	0.002829	2015.50	7.61	7.59	'training'
339	PipEMA	363.55	0.002751	2294.00	7.74	7.80	'training'
340	PipEMA	363.65	0.002750	2387.50	7.78	7.80	'training'
341	STY	261.35	0.003826	13.50	2.60	2.65	'training'
342	STY	261.45	0.003825	13.50	2.60	2.66	'training'
343	STY	261.95	0.003818	14.20	2.65	2.69	'training'
344	STY	262.25	0.003813	14.62	2.68	2.70	'training'
345	STY	270.85	0.003692	23.65	3.16	3.17	'training'
346	STY	271.25	0.003687	24.50	3.20	3.20	'training'
347	STY	271.85	0.003678	24.60	3.20	3.23	'training'
348	STY	281.65	0.003551	43.55	3.77	3.72	'training'
349	STY	281.85	0.003548	43.80	3.78	3.73	'training'
350	STY	293.75	0.003404	75.50	4.32	4.29	'training'
351	STY	294.15	0.003400	75.90	4.33	4.31	'training'
352	STY	294.45	0.003396	71.90	4.28	4.32	'training'
353	STY	298.15	0.003354	82.52	4.41	4.49	'training'
354	STY	302.85	0.003302	112.00	4.72	4.69	'training'
355	STY	302.95	0.003301	113.00	4.73	4.69	'training'
356	STY	303.15	0.003299	111.50	4.71	4.70	'training'
357	STY	304.45	0.003285	114.00	4.74	4.75	'training'
358	STY	308.15	0.003245	120.00	4.79	4.91	'training'
359	STY	311.95	0.003206	172.00	5.15	5.06	'training'
360	STY	312.55	0.003199	168.00	5.12	5.08	'training'
361	STY	312.65	0.003198	170.00	5.14	5.09	'training'
362	STY	318.15	0.003143	168.00	5.12	5.30	'training'
363	STY	322.05	0.003105	240.00	5.48	5.45	'training'
364	STY	322.15	0.003104	248.00	5.51	5.45	'training'
365	STY	322.95	0.003096	229.00	5.43	5.48	'training'
366	STY	323.15	0.003095	252.00	5.53	5.49	'training'
367	STY	328.15	0.003047	249.00	5.52	5.67	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
368	STY	331.45	0.003017	343.00	5.84	5.79	'training'
369	STY	331.55	0.003016	343.00	5.84	5.80	'training'
370	STY	332.25	0.003010	344.00	5.84	5.82	'training'
371	STY	332.45	0.003008	341.00	5.83	5.83	'training'
372	STY	332.85	0.003004	342.00	5.83	5.84	'training'
373	STY	340.65	0.002936	477.00	6.17	6.11	'training'
374	STY	341.55	0.002928	469.00	6.15	6.14	'training'
375	STY	341.75	0.002926	473.00	6.16	6.15	'training'
376	STY	343.15	0.002914	492.00	6.20	6.19	'training'
377	STY	344.75	0.002901	550.00	6.31	6.24	'training'
378	STY	348.65	0.002868	622.00	6.43	6.37	'training'
379	STY	348.75	0.002867	600.00	6.40	6.37	'training'
380	STY	351.25	0.002847	612.00	6.42	6.45	'training'
381	STY	359.45	0.002782	884.00	6.78	6.70	'training'
382	STY	363.15	0.002754	865.00	6.76	6.81	'training'
383	STY	364.75	0.002742	889.00	6.79	6.86	'training'
384	STY	365.75	0.002734	1002.00	6.91	6.89	'training'
385	VAc	282.55	0.003539	1960.00	7.58	7.65	'training'
386	VAc	283.15	0.003532	2364.71	7.77	7.66	'training'
387	VAc	283.25	0.003530	2500.00	7.82	7.67	'training'
388	VAc	284.05	0.003521	2250.00	7.72	7.69	'training'
389	VAc	287.25	0.003481	2367.00	7.77	7.79	'training'
390	VAc	287.75	0.003475	2460.00	7.81	7.81	'training'
391	VAc	288.15	0.003470	2496.00	7.82	7.82	'training'
392	VAc	288.85	0.003462	2697.00	7.90	7.84	'training'
393	VAc	288.95	0.003461	2657.00	7.88	7.84	'training'
394	VAc	289.35	0.003456	2551.00	7.84	7.85	'training'
395	VAc	293.15	0.003411	2917.50	7.98	7.97	'training'
396	VAc	298.15	0.003354	3549.00	8.17	8.11	'training'
397	VAc	298.35	0.003352	3519.00	8.17	8.12	'training'
398	VAc	299.85	0.003335	3539.00	8.17	8.16	'training'
399	VAc	300.05	0.003333	3633.50	8.20	8.16	'training'
400	VAc	300.95	0.003323	3853.00	8.26	8.19	'training'
401	VAc	301.15	0.003321	3868.00	8.26	8.19	'training'
402	VAc	301.35	0.003318	3802.50	8.24	8.20	'training'
403	VAc	301.85	0.003313	3916.00	8.27	8.21	'training'
404	VAc	302.05	0.003311	4058.00	8.31	8.22	'training'
405	VAc	302.55	0.003305	3777.50	8.24	8.23	'training'
406	VAc	303.15	0.003299	3814.58	8.25	8.25	'training'
407	VAc	313.15	0.003193	5293.43	8.57	8.51	'training'
408	VAc	315.35	0.003171	5074.00	8.53	8.57	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
409	VAc	315.45	0.003170	5015.00	8.52	8.57	'training'
410	VAc	316.45	0.003160	5196.00	8.56	8.60	'training'
411	VAc	317.35	0.003151	5596.00	8.63	8.62	'training'
412	VAc	317.95	0.003145	5550.00	8.62	8.64	'training'
413	VAc	318.05	0.003144	5510.00	8.61	8.64	'training'
414	VAc	318.15	0.003143	5691.00	8.65	8.64	'training'
415	VAc	318.45	0.003140	5845.00	8.67	8.65	'training'
416	VAc	323.15	0.003095	6770.42	8.82	8.76	'training'
417	VAc	327.55	0.003053	6110.00	8.72	8.87	'training'
418	VAc	328.15	0.003047	7223.00	8.89	8.88	'training'
419	VAc	328.65	0.003043	7430.00	8.91	8.89	'training'
420	VAc	330.45	0.003026	6514.50	8.78	8.93	'training'
421	VAc	331.95	0.003013	6262.00	8.74	8.97	'training'
422	VAc	332.05	0.003012	6157.00	8.73	8.97	'training'
423	VAc	332.25	0.003010	7962.00	8.98	8.98	'training'
424	VAc	332.75	0.003005	8013.00	8.99	8.99	'training'
425	VAc	333.15	0.003002	8761.29	9.08	9.00	'training'
426	VAc	333.95	0.002994	7916.00	8.98	9.01	'training'
427	VAc	334.35	0.002991	7878.00	8.97	9.02	'training'
428	VAc	338.15	0.002957	9207.80	9.13	9.11	'training'
429	iBMA	283.15	0.003532	219.00	5.39	5.45	'training'
430	iBMA	303.15	0.003299	443.50	6.09	6.07	'training'
431	iBMA	323.15	0.003095	722.00	6.58	6.61	'training'
432	iBMA	343.15	0.002914	1213.00	7.10	7.08	'training'
433	iBMA	363.15	0.002754	1853.00	7.52	7.51	'training'
434	iBoMA	273.15	0.003661	235.00	5.46	5.48	'training'
435	iBoMA	283.15	0.003532	322.00	5.77	5.81	'training'
436	iBoMA	296.65	0.003371	589.00	6.38	6.22	'training'
437	iBoMA	303.15	0.003299	617.60	6.43	6.41	'training'
438	iBoMA	313.15	0.003193	900.00	6.80	6.68	'training'
439	iBoMA	323.15	0.003095	1012.50	6.92	6.93	'training'
440	iBoMA	324.15	0.003085	1209.00	7.10	6.96	'training'
441	iBoMA	333.15	0.003002	1645.50	7.41	7.17	'training'
442	iBoMA	343.15	0.002914	1766.00	7.48	7.40	'training'
443	iBoMA	363.15	0.002754	2584.80	7.86	7.81	'training'
444	iBoMA	364.15	0.002746	3192.00	8.07	7.83	'training'
445	iDMA	283.15	0.003532	321.00	5.77	5.81	'training'
446	iDMA	303.15	0.003299	576.00	6.36	6.39	'training'
447	iDMA	323.15	0.003095	941.50	6.85	6.90	'training'
448	iDMA	343.15	0.002914	1565.50	7.36	7.35	'training'
449	iDMA	363.15	0.002754	2199.00	7.70	7.75	'training'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
450	tBMA	295.15	0.003388	301.00	5.71	5.84	'training'
451	tBMA	303.15	0.003299	379.50	5.94	6.07	'training'
452	tBMA	313.15	0.003193	502.60	6.22	6.33	'training'
453	tBMA	323.15	0.003095	648.00	6.47	6.58	'training'
454	tBMA	333.15	0.003002	842.00	6.74	6.82	'training'
455	BA	208.15	0.004804	859.14	6.76	6.58	'test'
456	BA	211.15	0.004736	702.00	6.55	6.73	'test'
457	BA	216.15	0.004626	1184.00	7.08	6.96	'test'
458	BA	217.15	0.004605	1350.00	7.21	7.01	'test'
459	BA	219.15	0.004563	1070.00	6.98	7.10	'test'
460	BA	225.15	0.004441	1638.33	7.40	7.36	'test'
461	BA	226.15	0.004422	1601.00	7.38	7.40	'test'
462	BA	227.15	0.004402	1739.17	7.46	7.44	'test'
463	BA	232.15	0.004308	1881.60	7.54	7.65	'test'
464	BA	237.45	0.004211	2910.00	7.98	7.85	'test'
465	BA	237.55	0.004210	2865.00	7.96	7.86	'test'
466	BA	242.15	0.004130	2768.00	7.93	8.03	'test'
467	BA	253.95	0.003938	4073.40	8.31	8.44	'test'
468	BA	261.85	0.003819	6520.00	8.78	8.69	'test'
469	BA	262.65	0.003807	5574.00	8.63	8.72	'test'
470	BA	262.95	0.003803	6720.00	8.81	8.73	'test'
471	BA	263.05	0.003802	6520.00	8.78	8.73	'test'
472	BA	263.15	0.003800	6590.00	8.79	8.73	'test'
473	BA	263.35	0.003797	5793.83	8.66	8.74	'test'
474	BA	265.25	0.003770	5940.00	8.69	8.80	'test'
475	BA	265.65	0.003764	6030.00	8.70	8.81	'test'
476	BA	265.75	0.003763	5690.00	8.65	8.81	'test'
477	BA	265.95	0.003760	5920.00	8.69	8.82	'test'
478	BA	272.45	0.003670	7232.33	8.89	9.01	'test'
479	BA	273.15	0.003661	7670.00	8.95	9.03	'test'
480	BA	273.25	0.003660	8117.50	9.00	9.04	'test'
481	BA	278.15	0.003595	11237.67	9.33	9.17	'test'
482	BA	283.15	0.003532	12512.64	9.43	9.31	'test'
483	BA	283.75	0.003524	11600.00	9.36	9.33	'test'
484	BA	284.05	0.003521	10800.00	9.29	9.33	'test'
485	BA	287.95	0.003473	12300.00	9.42	9.44	'test'
486	BA	288.15	0.003470	12744.57	9.45	9.44	'test'
487	BA	293.15	0.003411	14854.11	9.61	9.57	'test'
488	BzMA	279.25	0.003581	393.00	5.97	5.97	'test'
489	BzMA	291.05	0.003436	558.67	6.33	6.33	'test'
490	BzMA	294.15	0.003400	563.50	6.33	6.42	'test'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
491	BzMA	295.15	0.003388	555.50	6.32	6.45	'test'
492	BzMA	300.85	0.003324	783.33	6.66	6.60	'test'
493	BzMA	310.75	0.003218	1071.17	6.98	6.87	'test'
494	BzMA	313.15	0.003193	935.50	6.84	6.93	'test'
495	BzMA	320.55	0.003120	1391.17	7.24	7.11	'test'
496	BzMA	323.15	0.003095	1340.00	7.20	7.17	'test'
497	BzMA	333.15	0.003002	1643.25	7.40	7.40	'test'
498	BzMA	343.15	0.002914	2068.50	7.63	7.62	'test'
499	BzMA	353.15	0.002832	2455.00	7.81	7.82	'test'
500	BzMA	363.15	0.002754	3000.50	8.01	8.02	'test'
501	DMAEMA	273.15	0.003661	286.75	5.66	5.56	'test'
502	DMAEMA	282.95	0.003534	406.00	6.01	5.88	'test'
503	DMAEMA	283.15	0.003532	413.00	6.02	5.89	'test'
504	DMAEMA	283.25	0.003530	402.00	6.00	5.89	'test'
505	DMAEMA	284.05	0.003521	416.00	6.03	5.92	'test'
506	DMAEMA	293.05	0.003412	560.00	6.33	6.19	'test'
507	DMAEMA	293.25	0.003410	562.00	6.33	6.20	'test'
508	DMAEMA	303.35	0.003297	715.50	6.57	6.49	'test'
509	DMAEMA	313.15	0.003193	911.00	6.81	6.75	'test'
510	DMAEMA	323.15	0.003095	1207.50	7.10	7.00	'test'
511	DMAEMA	333.05	0.003003	1525.00	7.33	7.23	'test'
512	DMAEMA	333.25	0.003001	1464.00	7.29	7.24	'test'
513	DMAEMA	333.35	0.003000	1462.00	7.29	7.24	'test'
514	DMAEMA	343.15	0.002914	1805.67	7.50	7.46	'test'
515	DMAEMA	353.05	0.002832	2204.00	7.70	7.67	'test'
516	DMAEMA	353.15	0.002832	2390.50	7.78	7.67	'test'
517	DMAEMA	363.05	0.002754	2732.00	7.91	7.86	'test'
518	EHMA	283.15	0.003532	321.50	5.77	5.52	'test'
519	EHMA	303.15	0.003299	582.50	6.37	6.13	'test'
520	EHMA	323.15	0.003095	912.50	6.82	6.66	'test'
521	EHMA	343.15	0.002914	1503.50	7.32	7.14	'test'
522	EHMA	363.15	0.002754	2165.00	7.68	7.56	'test'
523	EMA	279.25	0.003581	154.50	5.04	5.14	'test'
524	EMA	283.15	0.003532	218.80	5.39	5.27	'test'
525	EMA	291.05	0.003436	224.33	5.41	5.53	'test'
526	EMA	293.15	0.003411	329.50	5.80	5.59	'test'
527	EMA	300.85	0.003324	321.17	5.77	5.83	'test'
528	EMA	303.15	0.003299	391.50	5.97	5.89	'test'
529	EMA	310.75	0.003218	434.17	6.07	6.11	'test'
530	EMA	313.15	0.003193	586.00	6.37	6.18	'test'
531	EMA	320.85	0.003117	567.83	6.34	6.38	'test'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction
532	EMA	323.15	0.003095	702.00	6.55	6.44	'test'
533	EMA	333.15	0.003002	931.67	6.84	6.69	'test'
534	EMA	343.15	0.002914	1169.50	7.06	6.92	'test'
535	EMA	353.15	0.002832	1538.50	7.34	7.14	'test'
536	EMA	363.15	0.002754	1733.29	7.46	7.35	'test'
537	HEMA	268.75	0.003721	513.00	6.24	6.52	'test'
538	HEMA	269.55	0.003710	510.00	6.23	6.54	'test'
539	HEMA	282.35	0.003542	725.00	6.59	6.90	'test'
540	HEMA	295.15	0.003388	1162.83	7.06	7.22	'test'
541	HEMA	302.15	0.003310	1482.00	7.30	7.39	'test'
542	HEMA	303.15	0.003299	1293.00	7.16	7.41	'test'
543	HEMA	304.15	0.003288	1365.00	7.22	7.44	'test'
544	HEMA	313.15	0.003193	1993.75	7.60	7.64	'test'
545	HEMA	323.15	0.003095	2411.75	7.79	7.85	'test'
546	HEMA	333.15	0.003002	3374.00	8.12	8.04	'test'
547	HEMA	343.15	0.002914	4157.00	8.33	8.23	'test'
548	HEMA	344.15	0.002906	3917.00	8.27	8.25	'test'
549	tBA	264.95	0.003774	6730.00	8.81	8.56	'test'
550	tBA	265.05	0.003773	6810.00	8.83	8.57	'test'
551	tBA	278.05	0.003596	9530.00	9.16	8.94	'test'
552	tBA	279.15	0.003582	9920.00	9.20	8.97	'test'
553	tBA	286.85	0.003486	12300.00	9.42	9.18	'test'
554	tBA	303.25	0.003298	18060.00	9.80	9.58	'test'
555	tBA	304.45	0.003285	18560.00	9.83	9.60	'test'
556	tBA	311.95	0.003206	22630.00	10.03	9.77	'test'
557	tBA	323.35	0.003093	28090.00	10.24	10.01	'test'
558	tBA	324.55	0.003081	28880.00	10.27	10.04	'test'
559	tBA	333.55	0.002998	34580.00	10.45	10.21	'test'
560	tBA	333.65	0.002997	33700.00	10.43	10.21	'test'
561	tBA	343.65	0.002910	44350.00	10.70	10.40	'test'
562	tBA	343.85	0.002908	44645.00	10.71	10.40	'test'
563	tBA	343.95	0.002907	43465.00	10.68	10.41	'test'
564	tBA	344.05	0.002907	42010.00	10.65	10.41	'test'
565	tBA	354.95	0.002817	50675.00	10.83	10.60	'test'
566	C17A	298.15	0.003354	22026.47	10.00	10.82	prediction'
567	C17A	323.15	0.003095	34891.55	10.46	11.29	prediction'
568	C17A	348.15	0.002872	51534.15	10.85	11.70	prediction'
569	C17A	373.15	0.002680	72402.78	11.19	12.05	prediction'
570	C21A	298.15	0.003354	16983.54	9.74	9.91	prediction'
571	C21A	323.15	0.003095	25591.10	10.15	10.46	prediction'
572	C21A	348.15	0.002872	36315.50	10.50	10.93	prediction'

No.	Monomers	T	1/T	Experimental k_p	Experimental $\ln k_p$	Calculated $\ln k_p$ (MLR)	training/test/ prediction'
573	C21A	373.15	0.002680	49020.80	10.80	11.33	prediction'
574	HCPA	298.15	0.003354	22247.84	10.01	9.08	prediction'
575	HCPA	323.15	0.003095	34544.37	10.45	9.59	prediction'
576	HCPA	348.15	0.002872	50513.71	10.83	10.03	prediction'
577	HCPA	373.15	0.002680	70262.96	11.16	10.41	prediction'
578	PhCEA	298.15	0.003354	37421.47	10.53	8.87	prediction'
579	PhCEA	323.15	0.003095	58688.55	10.98	9.35	prediction'
580	PhCEA	348.15	0.002872	85819.37	11.36	9.75	prediction'
581	PhCEA	373.15	0.002680	119372.01	11.69	10.10	prediction'
582	AN	298.15	0.003354	3604.72	8.19	6.15	prediction'
583	AN	323.15	0.003095	5825.50	8.67	6.98	prediction'
584	AN	348.15	0.002872	8777.97	9.08	7.69	prediction'
585	AN	373.15	0.002680	12456.53	9.43	8.30	prediction'
586	iBoA	298.15	0.003354	9798.65	9.19	9.77	prediction'
587	iBoA	323.15	0.003095	15835.35	9.67	10.33	prediction'
588	iBoA	348.15	0.002872	23860.99	10.08	10.81	prediction'
589	iBoA	373.15	0.002680	34200.65	10.44	11.23	prediction'
590	INA-A	298.15	0.003354	17154.23	9.75	9.72	prediction'
591	INA-A	323.15	0.003095	28566.79	10.26	10.29	prediction'
592	INA-A	348.15	0.002872	44355.86	10.70	10.77	prediction'
593	INA-A	373.15	0.002680	65512.75	11.09	11.19	prediction'
594	HCEA	298.15	0.003354	30946.03	10.34	9.11	prediction'
595	HCEA	323.15	0.003095	46630.03	10.75	9.61	prediction'
596	HCEA	348.15	0.002872	66836.19	11.11	10.04	prediction'
597	HCEA	373.15	0.002680	91126.14	11.42	10.41	prediction'
598	PhCPA	298.15	0.003354	15994.50	9.68	8.36	prediction'
599	PhCPA	323.15	0.003095	24834.77	10.12	8.92	prediction'
600	PhCPA	348.15	0.002872	36315.50	10.50	9.40	prediction'
601	PhCPA	373.15	0.002680	50513.71	10.83	9.82	prediction'
602	PnMA	298.15	0.003354	407.48	6.01	6.18	prediction'
603	PnMA	323.15	0.003095	854.06	6.75	6.85	prediction'
604	PnMA	348.15	0.002872	1603.59	7.38	7.43	prediction'
605	PnMA	373.15	0.002680	2807.36	7.94	7.93	prediction'
606	BuDE	298.15	0.003354	45.15	3.81	4.17	prediction'
607	BuDE	323.15	0.003095	135.64	4.91	5.18	prediction'
608	BuDE	348.15	0.002872	354.25	5.87	6.04	prediction'
609	BuDE	373.15	0.002680	812.41	6.70	6.79	prediction'
610	NVF	298.15	0.003354	2465.13	7.81	7.05	prediction'
611	NVF	323.15	0.003095	4491.76	8.41	7.71	prediction'
612	NVF	348.15	0.002872	7555.27	8.93	8.26	prediction'
613	NVF	373.15	0.002680	11968.10	9.39	8.75	prediction'

Detailed procedure for calculating norm descriptors

The properties are shown as follows:

Electronegativity (E), number of valence electrons (oue), total natural population by Natural Population Analysis (NPA_tnp), atomic charge by Natural Population Analysis (NPA_ac), and electrostatic properties (elp).

The step matrices, distance matrices and its derived distance matrices are shown as:

$$MS_A = [a_{ij}] \quad a_{ij} = \begin{cases} 1/s_{ij} & s_{ij} = 1 \\ 0 & \text{others} \end{cases} \quad (S1)$$

$$MS_{ABC} = [a_{ij}] \quad a_{ij} = \begin{cases} 1/s_{ij} & s_{ij} = 1, 2 \text{ or } 3 \\ 0 & \text{others} \end{cases} \quad (S2)$$

$$MD = [1/d_{ij}^e] \quad s_{ij} \neq 0 \quad (S3)$$

$$MD_A = [a_{ij}] \quad a_{ij} = \begin{cases} 1/d_{ij} & s_{ij} = 1 \\ 0 & \text{others} \end{cases} \quad (S4)$$

$$MD_{AB} = [a_{ij}] \quad a_{ij} = \begin{cases} 1/s_{ij} \times d_{ij} & s_{ij} = 1 \text{ or } 2 \\ 0 & \text{others} \end{cases} \quad (S5)$$

$$MD_{ABC} = [a_{ij}] \quad a_{ij} = \begin{cases} 1/s_{ij} \times d_{ij} & s_{ij} = 1, 2 \text{ or } 3 \\ 0 & \text{others} \end{cases} \quad (S6)$$

where s_{ij} is the step between atom i and atom j , d_{ij} is the Euclidean space distance between atom i and atom j .

The norm descriptors are calculated through the following equations:

$$\|M\|_1 = \max(\sum_i |m_{ij}|) \quad (S7)$$

$$\|M\|_2 = \sqrt{\max(\sum_i m_{ij}^2)} \quad (S8)$$

$$\|M\|_3 = \sqrt{\max(\lambda_i(M^H \times M))} \quad (S9)$$

$$\|M\|_4 = \frac{1}{n} \left(\sum_i \sum_j |m_{ij}| \right) \quad (S10)$$

where m_{ij} is the element in matrix M , λ_i is the matrix eigenvalue, the M^H is the Hermite matrix of M .

Table S2. The atomic distribution matrices (MA_a), norm descriptors (NI_a)

a	MA_a	NI_a	α_i/β_i
1	$MA_1 = NPA_ac \times NPA_ac^T \times MD_A$	$NI_1 = \ MA_1\ _2$	278.8065
2	$MA_2 = NPA_tnp - NPA_tnp^T \times MD_A$	$NI_2 = \ MA_2\ _1$	0.2350
3	$MA_3 = NPA_ac \times NPA_ac^T \times MD_{AB}$	$NI_3 = \ MA_3\ _2$	-281.0402
4	$MA_4 = elp - elp^T \times MD_{ABC}$	$NI_4 = \ MA_4\ _2$	-0.1698
5	$MA_5 = E \times E^T \times MS_A$	$NI_5 = \ MA_5\ _1$	-769.6389
6	$MA_6 = E - E^T \times MS_A$	$NI_6 = \ MA_6\ _3$	5.8069×10^4
7	$MA_7 = eou \times eou^T \times MS_{ABC}$	$NI_7 = \ MA_7\ _1$	84.5578
8	$MA_8 = NPA_ac - NPA_ac^T \times MD_A$	$NI_8 = \ MA_8\ _4$	-5.1908×10^3
9	$MA_9 = NPA_ac \times NPA_ac^T \times MD_{AB}$	$NI_9 = \ MA_9\ _1$	5.4726×10^4
10	$MA_{10} = NPA_ac - NPA_ac^T \times MD_{AB}$	$NI_{10} = \ MA_{10}\ _1$	-3.8720×10^4
11	$MA_{11} = NPA_tnp \times NPA_tnp^T \times MD_{AB}$	$NI_{11} = \ MA_{11}\ _4$	-61.7566
12	$MA_{12} = elp - elp^T \times MD$	$NI_{12} = \ MA_{12}\ _2$	-369.5886

*Notably, the meanings of “ $\times$ ” and “ $-$ ” used are illustrated by the following example:

$$P = [p_{ij}], M = [m_{ij}], P \times M = [p_{ij} \times m_{ij}] \text{ and } P - P^T = [p_i - p_j]$$

The definition of statistical parameters (R^2 , $RMSE$, MAE , eqs S1–S3) is shown as:

$$R^2 = 1 - \frac{\sum_{i=1}^n (\ln k_{i,\text{exp}} - \ln k_{i,\text{cal}})^2}{\sum_{i=1}^n (\ln k_{i,\text{exp}} - \overline{\ln k_{i,\text{exp}}})^2} \quad (\text{S11})$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (\ln k_{i,\text{exp}} - \ln k_{i,\text{cal}})^2} \quad (\text{S12})$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |\ln k_{i,\text{exp}} - \ln k_{i,\text{cal}}| \quad (\text{S13})$$

where n is the sample size, $\ln k_{i,\text{exp}}$ is the experimental $\ln k_p$ and $\ln k_{i,\text{cal}}$ is the calculated $\ln k_p$. $\overline{\ln k_{i,\text{exp}}}$ is the average experimental $\ln k_p$. $\overline{\ln k_{i,\text{tr}}}$ is the mean experimental $\ln k_p$ for training set. $\overline{\ln k_{i,\text{test}}}$ is the mean experimental $\ln k_p$ for test set.

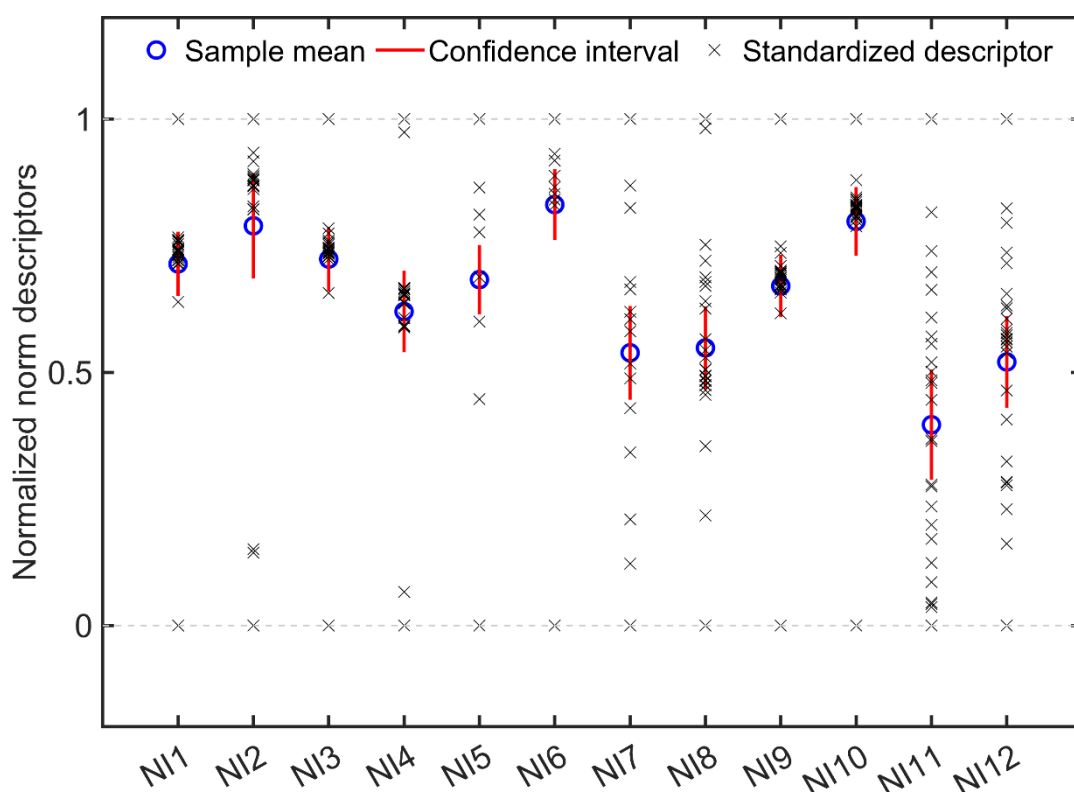


Figure S1. Sample mean, Confidence interval of sample mean, and distribution of normalized norm descriptors

Table S3. Variance and associated confidence interval of descriptors

Descriptors	Variance	Variance confidence interval	Descriptors	Variance	Variance confidence interval
NI_1	0.0246	[0.0151, 0.0468]	NI_7	0.0524	[0.0322, 0.0999]
NI_2	0.0665	[0.0409, 0.1267]	NI_8	0.0412	[0.0254, 0.0786]
NI_3	0.0248	[0.0153, 0.0473]	NI_9	0.0232	[0.0143, 0.0442]
NI_4	0.0395	[0.0243, 0.0753]	NI_{10}	0.0280	[0.0172, 0.0534]
NI_5	0.0288	[0.0177, 0.0549]	NI_{11}	0.0727	[0.0447, 0.1384]
NI_6	0.0300	[0.0184, 0.0571]	NI_{12}	0.0503	[0.0310, 0.0959]