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SUPPLEMENTARY MATERIAL TO

Quantitative structure–property relationship studies for the prediction of the vapor pressure of volatile organic compounds

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TABLE S-I. The data set and the corresponding experimental and predicted values of log (*p*/Pa) for the training and validation sets

ID	Name	log (p_v/Pa) (Exp)	log (p_v/Pa) (Pred)	*X0sol*	*SpPosA_H2*	*GATS2e*	*Hy*	*Hat* (h_{ii})	$e_{istd.}$
1	1,1,2-Trichloroethane	3.48	3.3841	5.784	0.541	1.078	–0.359	0.105	–0.4647
2	Iodomethane	4.72	4.7638	3.5	0.5	0.97	–0.315	0.101	0.211
3	Iodoethane	4.12	4.631	4.207	0.515	1.071	–0.528	0.072	2.3469
4	1-Bromobutane	3.72	3.63	5.121	0.57	0.95	–0.719	0.03	–0.3867
5	Hexan-2-one	2.71	3.1166	5.699	0.56	0.534	–0.802	0.118	2.014
6	2-Methylheptane	3.41	3.662	6.406	0.576	1.317	–0.946	0.108	1.2283
7	2,3,4-Trimethylpentane	3.53	3.6423	6.732	0.548	1.128	–0.946	0.145	0.5827
8	1,1-Dichloroethane	4.47	4.1496	4.577	0.5	0.74	–0.431	0.1	–1.5394
9	Ethylcyclohexane	3.12	3.264	5.82	0.633	1.348	–0.946	0.136	0.7362
10	1-Propoxypropane	3.95	4.1052	5.536	0.588	1.641	–0.802	0.163	0.8319
11	1,2-Dichloroethene	4.63	4.188	4.414	0.55	1.25	–0.431	0.054	–1.9698
12	2-Bromopropane	4.42	4.4842	4.577	0.5	0.801	–0.646	0.12	0.3188
13	3,3-Dimethylpentane	4.02	3.9226	5.914	0.55	1.076	–0.936	0.073	–0.4478
14	Toluene	3.42	3.2118	5.113	0.632	1.016	–0.936	0.132	–1.0569
15	1,4-Xylene	3.12	2.9552	5.983	0.61	0.893	–0.946	0.085	–0.7732
16	Ethylbenzène	3.12	2.9638	5.82	0.633	1.084	–0.946	0.118	–0.7736
17	1,2-Xylene	2.42	2.9182	5.983	0.613	0.893	–0.946	0.09	2.3562
18	Ethanol	3.87	3.8322	2.707	0.515	1.026	0.638	0.261	–0.2442
19	Methylcyclopentane	4.25	4.2475	4.406	0.599	1.299	–0.921	0.109	–0.0122
20	2-Methyl-2-propanol	3.7	3.6991	4.5	0.482	0.728	0.132	0.173	–0.0051
21	2-Propylenenitrile	4.15	4.0264	3.414	0.55	0.47	–0.646	0.23	–0.751
22	Pent-1-ene	4.96	4.7238	4.121	0.57	1.313	–0.898	0.111	–1.1554
23	Dichloromethane	4.75	4.7186	3.707	0.515	1.232	–0.264	0.094	–0.1493

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TABLE S-I. Continued

ID	Name	log (p_v/Pa) (Exp)	log (p_v/Pa) (Pred)	*X0sol*	*SpPosA_H2*	*GATS2e*	*Hy*	*Hat* (h_{ii})	$e_{istd.}$
24	Butyronitrile	3.12	3.4784	4.121	0.57	0.412	–0.719	0.211	2.099
25	Propan-1-ol	3.41	3.384	3.414	0.55	0.956	0.323	0.182	–0.144
26	Butan-1-ol	2.82	3.0135	4.121	0.57	0.926	0.132	0.158	1.0282
27	2-Methylpropan-1-ol	3.12	3.2801	4.284	0.541	0.912	0.132	0.118	0.7935
28	1,2-Dichlorobenzene	2.13	1.8814	6.983	0.613	0.642	–0.71	0.232	–1.5148
29	2,2,4-Trimethylpentane	3.79	3.7334	6.784	0.53	1.034	–0.946	0.185	–0.3156
30	Pentan-2-one	3.31	3.4448	4.992	0.556	0.531	–0.767	0.115	0.6638
31	2,4-Dimethylpentane	4.1	4.1299	5.862	0.545	1.183	–0.936	0.089	0.141
32	(1-Methylethyl)benzene	2.82	2.6799	6.69	0.619	1.026	–0.954	0.124	–0.7011
33	Propan-2-ol	3.75	3.8153	3.577	0.5	0.859	0.323	0.15	0.3419
34	1-Chloropropane	4.66	4.324	3.914	0.55	0.934	–0.646	0.069	–1.5356
35	2,2-Dimethylbutane	4.63	4.4817	5.207	0.523	1.005	–0.921	0.104	–0.717
36	pentamethylene	4.63	4.907	3.536	0.585	1.4	–0.898	0.195	1.5733
37	2-Methyl-2-butene	4.72	4.6084	4.284	0.541	0.963	–0.898	0.097	–0.5337
38	propyl formate	4.02	3.5854	4.828	0.57	0.906	–0.614	0.034	–1.8789
39	Diethyl ether	4.87	4.9728	4.121	0.57	1.726	–0.719	0.211	0.6022
40*	Dibromomethane	3.76	4.3039	4.707	0.515	1.272	–0.264	0.107	2.3622
41*	1,3-Dichlorobenzene	2.12	1.8198	6.983	0.618	0.642	–0.71	0.237	–1.4105
42*	3-Pentanone	3.33	3.3708	4.992	0.562	0.531	–0.767	0.113	0.1776
43*	Ethyl acetate	4.12	3.5608	4.992	0.556	0.799	–0.614	0.04	–2.342
44*	2-Butanone	4.11	3.8998	4.284	0.541	0.534	–0.719	0.136	–0.9284
45*	Hexane	4.29	4.5053	4.828	0.57	1.382	–0.921	0.085	0.9237
46*	Pentane	4.85	4.7773	4.121	0.57	1.36	–0.898	0.116	–0.3174
47*	1,2-Dichloropropane	3.83	3.7066	5.284	0.541	0.964	–0.539	0.042	–0.5175
48*	Heptane	3.76	3.9942	5.536	0.588	1.398	–0.936	0.082	1.0032
49*	1,2-dichloroethane	4.03	4.0937	4.414	0.55	1.167	–0.431	0.041	0.2668
50*	1-Bromopropane	4.12	4.1189	4.414	0.55	0.956	–0.646	0.039	–0.0048
51*	Ethyl acetate	2.42	2.8565	5.983	0.618	0.893	–0.946	0.098	1.886

*Test compounds