



SUPPLEMENTARY MATERIAL TO
**QSPR study of supercooled liquid vapour pressures of
polybrominated diphenyl ethers using the molecular distance–
edge vector index**

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J. Serb. Chem. Soc. 80 (4) (2015) 499–508

TABLE S-I. MDEV indexes of the investigated PBDEs

No.	PBDE	M_{11}	M_{12}
1	2-BDE	0	1.0625
2	3-BDE	0	1.04
3	2,4-BDE	0.0625	2.0903
4	2,4'-BDE	0.0156	2.0903
5	2,6-BDE	0.0625	2.125
6	3,4-BDE	0.1111	2.0678
7	3,4'-BDE	0.0123	2.0678
8	4,4'-BDE	0.01	2.0556
9	2,4,6-BDE	0.1875	3.1528
10	2,4',6-BDE	0.0938	3.1528
11	3,3',4-BDE	0.1391	3.1078
12	3,4,4'-BDE	0.1335	3.0956
13	2,2',4,4'-BDE	0.194	4.1806
14	2,3',4,4'-BDE	0.232	4.1581
15	2,3',4,6-BDE	0.2407	4.1928
16	2,4,4',6-BDE	0.2288	4.1806
17	3,3',4,4'-BDE	0.2725	4.1356
18	2,2',3,3',4-BDE	0.508	5.2328
19	2,2',4,4',5-BDE	0.3779	5.2206
20	2,3',4,4',6-BDE	0.393	5.2206
21	2,2',4,4',5,5'-BDE	0.5774	6.2606
22	2,3,3',4,4',5,6-BDE	1.0359	7.3006

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TABLE S-II. Results of the leave-one-out cross validation

No.	PBDE	Experimental $\log p_L$	Predicted $\log p_L$		Relative error, %	
			MLR	ANN	MLR	ANN
1	2-BDE	-0.79	-1.01	-0.96	27.85	21.52
2	3-BDE	-0.89	-0.95	-0.93	6.74	4.49
3	2,4-BDE	-1.77	-1.81	-1.79	2.26	1.13
4	2,4'-BDE	-1.86	-1.82	-1.85	-2.15	-0.54
5	2,6-BDE	-1.56	-1.86	-1.85	19.23	18.59
6	3,4-BDE	-1.92	-1.76	-1.78	-8.33	-7.29
7	3,4'-BDE	-1.88	-1.80	-1.81	-4.26	-3.72
8	4,4'-BDE	-2.01	-1.77	-1.80	-11.94	-10.45
9	2,4,6-BDE	-2.34	-2.69	-2.68	14.96	14.53
10	2,4',6-BDE	-2.65	-2.70	-2.69	1.89	1.51
11	3,3',4-BDE	-2.86	-2.63	-2.65	-8.04	-7.34
12	3,4,4'-BDE	-2.99	-2.62	-2.64	-12.37	-11.71
13	2,2',4,4'-BDE	-3.5	-3.54	-3.55	1.14	1.43
14	2,3',4,4'-BDE	-3.62	-3.50	-3.50	-3.31	-3.31
15	2,3',4,6-BDE	-3.4	-3.55	-3.55	4.41	4.41
16	2,4,4',6-BDE	-3.31	-3.55	-3.54	7.25	6.95
17	3,3',4,4'-BDE	-3.81	-3.46	-3.47	-9.19	-8.92
18	2,2',3,3',4-BDE	-4.19	-4.35	-4.34	3.82	3.58
19	2,2',4,4',5-BDE	-4.17	-4.39	-4.37	5.28	4.80
20	2,3',4,4',6-BDE	-4.52	-4.34	-4.35	-3.98	-3.76
21	2,2',4,4',5,5'-BDE	-5.07	-5.21	-5.19	2.76	2.37
22	2,3,3',4,4',5,6-BDE	-6.04	-5.54	-5.58	-8.28	-7.62

TABLE S-III. Results of the k -fold cross validation

Fold	PBDE	Experimental $\log p_L$	Predicted $\log p_L$		Relative error, %	
			MLR	ANN	MLR	ANN
1	2-BDE	-0.79	-0.95	-0.89	20.25	12.66
	3,4-BDE	-1.92	-1.77	-1.72	-7.81	-10.42
	3,3',4-BDE	-2.86	-2.65	-2.64	-7.34	-7.69
	2,4,4',6-BDE	-3.31	-3.53	-3.54	6.65	6.95
2	3-BDE	-0.89	-0.92	-0.90	3.37	1.12
	3,4'-BDE	-1.88	-1.76	-1.79	-6.38	-4.79
	3,4,4'-BDE	-2.99	-2.59	-2.61	-13.38	-12.71
3	3,3,4,4'-BDE	-3.81	-3.43	-3.43	-9.97	-9.97
	2,4-BDE	-1.77	-1.80	-1.79	1.69	1.13
	4,4'-BDE	-2.01	-1.78	-1.78	-11.44	-11.44
4	2,2',4,4'-BDE	-3.50	-3.54	-3.56	1.14	1.71
	2,2',3,3',4-BDE	-4.19	-4.36	-4.35	4.06	3.82
	2,4'-BDE	-1.86	-1.84	-1.82	-1.08	-2.15
	2,4,6-BDE	-2.34	-2.69	-2.68	14.96	14.53
	2,3',4,4'-BDE	-3.62	-3.53	-3.53	-2.49	-2.49
	2,2',4,4',5-BDE	-4.17	-4.39	-4.40	5.28	5.52

TABLE S-III. Continued

Fold	PBDE	Experimental log p_L	Predicted log p_L		Relative error, %	
			MLR	ANN	MLR	ANN
5	2,6-BDE	-1.56	-1.87	-1.85	19.87	18.59
	2,4',6-BDE	-2.65	-2.72	-2.70	2.64	1.89
	2,3',4,6-BDE	-3.40	-3.54	-3.54	4.12	4.12
	2,3',4,4',6-BDE	-4.52	-4.35	-4.36	-3.76	-3.54
6	3,4-BDE	-1.92	-1.74	-1.79	-9.38	-6.77
	3,3',4-BDE	-2.86	-2.65	-2.67	-7.34	-6.64
	2,4,4',6-BDE	-3.31	-3.55	-3.56	7.25	7.55
	2,2',4,4',5,5'-BDE	-5.07	-5.24	-5.23	3.35	3.16
7	3,4'-BDE	-1.88	-1.80	-1.81	-4.26	-3.72
	3,4,4'-BDE	-2.99	-2.61	-2.62	-12.71	-12.37
	3,3,4,4'-BDE	-3.81	-3.42	-3.42	-10.24	-10.24
	2,3,3',4,4',5,6-BDE	-6.04	-5.57	-5.57	-7.78	-7.78