QSPR Flash Point Prediction of Solvents Using Topological Indices for Application in Computer Aided Molecular Design.
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This revision corrects an unfortunate mistake in compiling data for experimental flash point values for hydrocarbons published in Table 4 (pages 7381−7384). The ensuing changes to the text of the publication are on the following pages: page 7378 in the Abstract "The neural network model showed higher accuracy (training set, r = **0.939**, R^2 = **0.883**)"; page 7380 in the Methodology section "(range of flash points = **513.15 K** − **157.15 K** = **356 K**, standard deviation = **64.81 K**)"; and page 7385 in the Results and Discussion "Upon using the entire data set for multiple linear regression analysis, poor accuracy was obtained (R^2 = **0.479**, r = **0.692**)", "The average absolute deviation is **20.819 K**, the average absolute relative deviation is **6.57%,** and the average bias is −0.21% for the data set using MLR", "A 16:**6**:1 network (consisting of 16 input nodes as given in Table 2, one output node, and one hidden layer with **6** nodes)", "The average absolute relative deviation is **5.35%**, the average absolute deviation is **16.08 K**, and the average percent bias is **−0.22%** for the complete data set using ANN".

The ensuing changes for figures in the publication are Figures 3−5 (on page 7379), Figure 6 (on page 7380), and Figure 7 (on page 7385).

The ensuing changes for tables in the publication are Tables 1 and 3 (on page 7380) and Table 4 (on pages 7381−7384).

The authors gratefully acknowledge Mr. Max Bernhardt and Dr. Andreas Klamt (Universität Regensburg, Germany), who found the issues with the reported flash point values and kindly brought these problems to our attention.

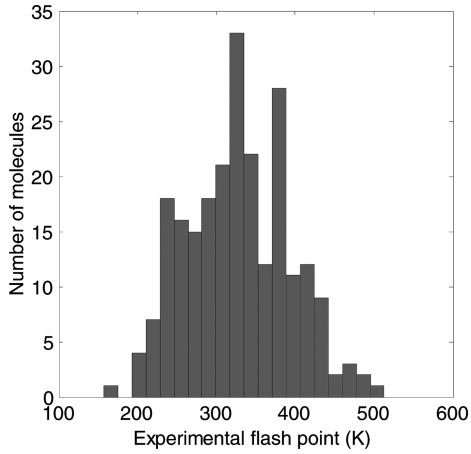

Figure 3. Distribution of flash point values in data set (n = 236).

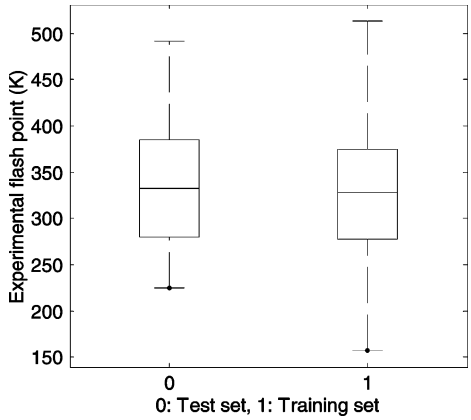

Figure 4. Box plots of test set and training set.

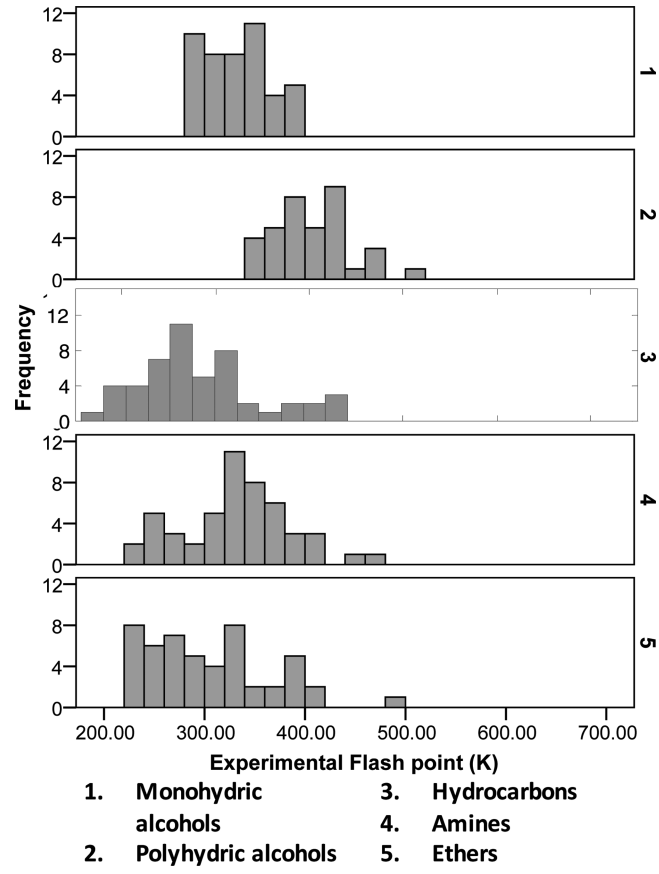

Figure 5. Distribution of flash point values for each class.

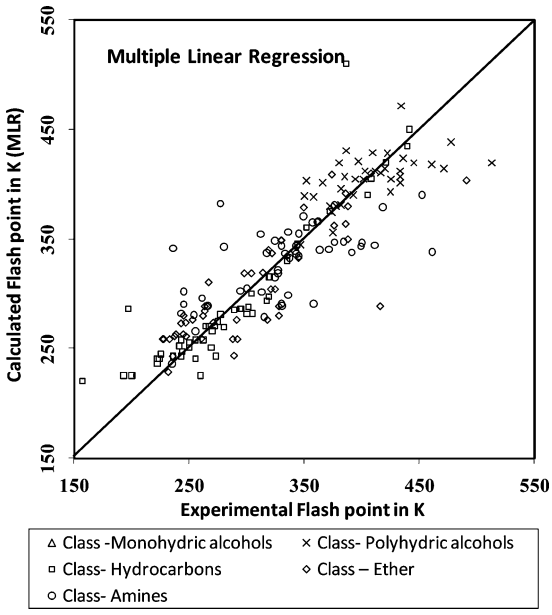

Figure 6. Plot of calculated versus experimental values of flash point using MLR (graph depicts correlations from Table 1 for all classes).

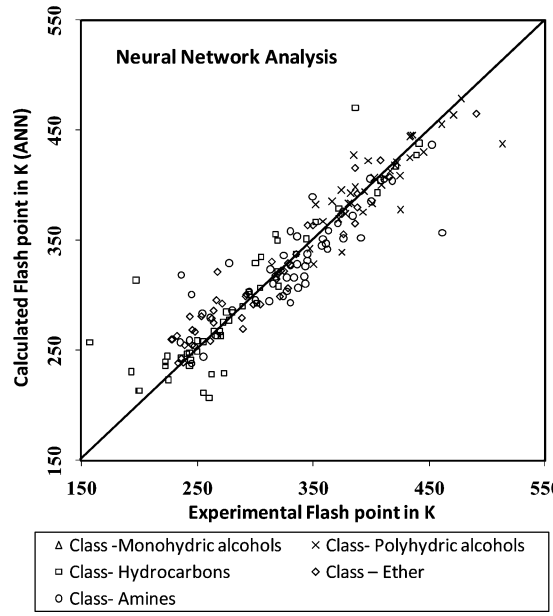

Figure 7. Plot of calculated versus experimental values of flash point using ANN.

Table 1. Results of Multiple Linear Regression on Different Classes of Solvents for Flash Point Prediction[a]

		training set				test set	
class of solvents	equation	r	R^2	R^2(CV)	F	r	R^2
monohydric alcohols	$T_f = 9.248(SC:2) - 34.953(^3\chi_{cluster}) + 286.053$	0.925	0.855	0.613	109.06	0.933	0.870
polyhydric alcohols	$T_f = 13.064(^2\kappa) - 8.665(^3\kappa) + 385.328$	0.608	0.370		7.62	0.500	0.251
hydrocarbons	$\boldsymbol{T_f = 29.929(^1\chi) - 105.054}$	**0.881**	**0.776**	**0.696**	**132.15**	**0.792**	**0.628**
amines	$T_f = 50.264(^1\chi) - 31.887(^2\chi_v) + 210.783$	0.691	0.477	0.22	16.89	0.396	0.157
ethers	$T_f = 30.045(^1\chi) + 186.184$	0.825	0.680	0.600	80.75	0.875	0.770

[a] R^2 = coefficient of determination; r = correlation coefficient; R^2(CV) = R^2 for the cross validation set, F = Fisher test statistic; SC:2 = subgraph counts (second order): path; $^3\chi_{cluster}$ = chi(3): cluster; $^n\kappa$ = kappa-n; $^n\chi$ = chi(n); $^2\chi_v$ = chi(2) (valence modified).

Table 3. Results of Neural Network Analysis for Flash Point Prediction (n = 236, Network Configuration =16:6:1)

	r	R^2	R^2(CV)
training set	**0.940**	**0.883**	**0.638**
test set	**0.878**	**0.772**	**0.664**

Table 4. Solvent Data Set with Experimental and Predicted (MLR and ANN) Flash Point

no.	iupac/cas name	T_f(exptl) (K)	T_f(predicted) (K)	
			MLR	ANN
	Class: Monohydric Alcohols			
1	methanol	283.706	286.053	**285.091**
2	ethanol	286.483	295.302	**281.885**
3	propan-1-ol	298.15	304.55	**274.462**
4	butan-2-ol	295.372	308.776	**301.044**
5	2-methylpropan-1-ol	303.15	308.776	**291.057**
6	2-methylpropan-2-ol	284.261	271.635	**258.303**
7	pentan-2-ol	313.706	318.024	**308.542**
8	2-methylbutan-2-ol	294.261	296.24	**288.576**
9	hexan-1-ol	347.039	332.294	**321.632**
10	2-ethylbutan-1-ol	331.483	334.407	**325.531**
11	octan-2-ol	358.15	345.769	**347.779**
12	nonan-1-ol	353.15	360.038	**357.757**
13	decan-1-ol	377.594	369.287	**371.028**
14	phenylmethanol	373.706	362.152	**354.812**
15	4-hydroxy-4-methylpentan-2-one	325.372	309.714	**348.755**
16	2-furylmethanol	356.483	352.904	**350.476**
17	2-methylpropanoic acid (3-hydroxy-2,2,4-trimethylpentyl) ester	393.15	396.931	**378.539**
18	1-chloropropan-2-ol	324.15	308.776	**307.247**
19	1,4-dibromobutan-2-ol	386.15	331.452	**385.71**
20	heptan-2-ol	332.15	336.521	**333.879**
21	heptan-1-ol	346.15	341.542	**332.95**
22	hexan-2-ol	314.15	327.272	**321.81**
23	1-methoxypropan-2-ol	306.15	318.024	**333.533**
24	octan-1-ol	354.15	350.79	**346.454**
25	(2r)-2,4-dihydroxy-*N*-(3-hydroxypropyl)-3,3-dimethylbutanamide	386.15	392.489	**472.342**
26	pentan-3-ol	313.15	322.204	**305.993**
27	oct-1-en-3-ol	341.15	349.948	**367.998**
28	2,2,2-trifluoroethanol	302.15	296.24	**306.357**
29	2,3,4-trimethylpentan-1-ol	333.15	351.918	**330.423**
30	4-methylpentan-2-ol	314.15	322.251	**316.174**
31	2-methylbutan-2-ol	293.15	296.24	**288.576**
32	3,3-dimethylbutan-1-ol	302.15	305.488	**311.749**
33	2-ethylbutan-1-ol	330.15	334.407	**325.531**
34	2-ethylhexan-1-ol	350.15	352.904	**347.905**
35	2,2,4-trimethylpentan-1-ol	333.15	331.32	**325.312**
36	3-methylheptan-3-ol	327.15	336.342	**307.242**
37	tetradecan-1-ol	418.15	406.279	**416.163**
38	5-methylheptan-3-ol	327.15	349.106	**332.281**
39	8-methylnonan-1-ol	377.15	364.265	**369.771**
40	tridecan-1-ol	389.15	397.031	**404.323**
41	propan-2-ol[a]	284.817	293.617	**278.532**
42	butan-1-ol[a]	309.817	313.798	**297.732**
43	pentan-1-ol[a]	330.372	323.046	**308.322**
44	3-methylbutan-1-ol[a]	324.817	318.024	**317.046**
45	cyclohexanol[a]	340.928	349.948	**311.449**
46	octan-1-ol[a]	363.706	350.79	**346.454**
47	prop-2-en-1-ol[a]	295.372	304.55	**326.194**
48	2-tetrahydrofuranylmethanol[a]	347.039	352.904	**352.845**
49	(1*R*)-1-(2-furyl)ethanol[a]	383.15	361.058	**378.618**
50	5-methylheptan-1-ol[a]		349.948	**408.592**
	Class: Polyhydric Alcohols			
51	ethylene glycol	392.594	389.86	**375.36**
52	2-(2-hydroxyethoxy)ethanol	411.483	411.722	**407.13**
53	2-[2-(2-hydroxyethoxy)ethoxy]ethanol	435.928	423.681	**445.617**
54	2-[2-[2-(2-hydroxyethoxy)ethoxy]ethoxy]ethanol	477.594	438.116	**478.926**
55	propane-1,2-diol	377.594	380.062	**373.765**
56	3-(3-hydroxypropoxy)propan-1-ol	397.039	420.52	**422.148**
57	2-[2-(2-hydroxypropoxy)propoxy]propan-1-ol	416.483	409.9	**412.671**
58	glycerol	433.15	401.138	**424.783**
59	butane-1,3-diol	382.039	380.919	**392.755**
60	butane-1,4-diol	394.261	404.435	**394.196**
61	pentane-1,5-diol	402.594	411.722	**406.614**
62	propane-1,1-diol	372.15	380.062	**369.324**
63	propane-1,3-diol	352.15	402.925	**382.459**
64	butane-1,2-diol	366.15	401.138	**385.339**
65	butane-2,3-diol	358.15	388.364	**366.991**
66	(*E*)-but-2-ene-1,4-diol	401.15	404.435	**383.484**
67	but-2-yne-1,4-diol	425.15	404.435	**377.609**
68	hexane-1,6-diol	420.15	414.388	**417.903**
69	hexane-2,5-diol	374.15	374.379	**395.676**
70	2,2-diethylpropane-1,3-diol	380.15	419.21	**383.197**

Table 4. Continued

no.	iupac/cas name	T_f(exptl) (K)	T_f(predicted) (K)	
			MLR	ANN
71	2,5-dimethylhex-3-yne-2,5-diol	347.05	344.495	**342.359**
72	benzoic acid [4-[(oxo-phenylmethoxy)methyl]cyclohexyl]methyl ester	434.15	471.191	**445.312**
73	[4-(hydroxymethyl)phenyl]methanol	460.95	417.78	**455.097**
74	2-butyl-2-ethylpropane-1,3-diol	386.15	430.521	**398.383**
75	3,6-dimethyloct-4-yne-3,6-diol	382.15	395.317	**383.748**
76	2-ethyl-2-(hydroxymethyl)propane-1,3-diol	445.15	419.21	**430**
77	2,2-bis(hydroxymethyl)propane-1,3-diol	513.15	419.21	**437.612**
78	(2*R*,3*R*,4*R*,5*S*)-hexane-1,2,3,4,5,6-hexol	422.05	428.185	**420.714**
79	2-(hydroxymethyl)-2-methylpropane-1,3-diol	433.15	406.717	**444.377**
80	2,2-dimethylpropane-1,3-diol[a]	424.817	392.84	**408.592**
81	2-methylpentane-2,4-diol[a]	374.817	355.86	**339.105**
82	(2*S*)-butane-1,2,4-triol[a]	385.15	406.488	**427.459**
83	2,3-dimethylbutane-2,3-diol[a]	350.15	388.935	**328.351**
84	2-ethylhexane-1,3-diol[a]	409.15	428.496	**400.474**
85	2-(2-hydroxyethylthio)ethanol[a]	433.15	411.722	**424.956**
86	hexane-1,2,6-triol[a]	471.15	414.417	**463.775**
	Class: Hydrocarbons			
87	pentane	**224.15**	**240.353**	**244.722**
88	hexane	**250.15**	**255.318**	**258.673**
89	heptanes	**272.15**	**270.283**	**275.413**
90	octane	**289.15**	**285.248**	**289.989**
91	nonane	**304.15**	**300.212**	**306.757**
92	decane	**319.15**	**315.177**	**321.133**
93	dodecane	**344.15**	**345.107**	**351.052**
94	cyclohexane	**255.15**	**257.885**	**257.711**
95	cyclohexene	**243.15**	**257.885**	**247.574**
96	benzene	**262.15**	**257.885**	**228.335**
97	methylbenzene	**280.15**	**269.673**	**284.393**
98	1,2-dimethylbenzene	**305.15**	**281.965**	**334.563**
99	1,4-dimethylbenzene	**300.15**	**281.461**	**328.904**
100	1,3,5-trimethylbenzene	**317.15**	**293.249**	**355.192**
101	isopropylbenzene	**319.15**	**296.93**	**349.884**
102	tridecane	**352.15**	**360.072**	**366.468**
103	tetradecane	**372.15**	**375.037**	**378.976**
104	hexadecane	**408.15**	**404.967**	**404.401**
105	heptadecane	**421.15**	**419.932**	**417.163**
106	nonadecane	**441.15**	**449.862**	**438.092**
107	isopentane	**222.15**	**236.038**	**235.877**
108	isohexane	**250.15**	**251.003**	**248.665**
109	3-methylpentane	**241.15**	**252.141**	**247.182**
110	2,3-dimethylbutane	**244.15**	**247.192**	**241.401**
111	buta-1,3-diene	**197.05**	**285.775**	**313.615**
112	but-2-ene	**199.85**	**225.388**	**213.151**
113	(z)-but-2-ene	**200.15**	**225.388**	**213.151**
114	but-1-ene	**193.15**	**225.388**	**230.56**
115	2-methylprop-1-ene	**157.15**	**219.936**	**257.358**
116	(*Z*)-pent-2-ene	**255.15**	**240.353**	**211.277**
117	pent-1-ene	**222.15**	**240.353**	**239.464**
118	dec-1-ene	**320.15**	**315.177**	**307.973**
119	hept-1-ene	**264.15**	**270.283**	**267.451**
120	cyclooctane	**301.15**	**287.815**	**292.725**
121	cyclopenta-1,3-diene	273.15	**242.92**	**229.461**
122	cyclopentane	236.15	**242.92**	**242.668**
123	cyclopentene	243.15	**242.92**	**235.476**
124	2-methylheptane	277.15	**280.933**	**277.254**
125	4-vinylcyclohexene	294.15	**285.775**	**302.944**
126	4-methylpent-1-yne	269.15	**251.003**	**267.136**
127	ethylbenzene[a]	**295.15**	**285.775**	**300.509**
128	undecane[a]	**335.15**	**330.142**	**337.442**
129	pentadecane[a]	**405.15**	**390.002**	**393.184**
130	octadecane[a]	**439.15**	**434.897**	**426.962**
131	tricosane[a]	**386.15**	**509.721**	**470.086**
132	2,2-dimethylbutane[a]	**225.15**	**244.736**	**223.052**
133	2-methylhexane[a]	**270.15**	**265.968**	**263.382**
134	but-2-yne[a]	**260.15**	**225.388**	**206.812**
135	2,4,4-trimethylpent-1-ene[a]	267.15	**270.351**	**262.589**
136	2,3,4-trimethylpent-2-ene[a]	275.15	**274.449**	**284.713**
	Class: Ether			
137	methoxymethane	232.039	228.675	**262.678**
138	ethoxyethane	233.15	258.72	**237.91**
139	2-methoxy-2-methylpropane	238.706	263.12	**254.253**
140	2-isopropoxypropane	245.372	280.103	**268.041**

Table 4. Continued

no.	iupac/cas name	T_f(exptl) (K)	T_f(predicted) (K)	
			MLR	ANN
141	1-butoxybutane	304.261	318.811	**291.177**
142	1-pentoxypentane	330.372	348.856	**327.25**
143	1-ethenoxybutane	263.706	288.765	**274.498**
144	2-methyloxirane	235.928	243.085	**242.002**
145	2-ethyloxirane	260.928	259.25	**258.008**
146	1,4-dioxane	291.483	276.32	**298.632**
147	(2,2-dimethyl-1,3-dioxolan-4-yl)methanol	267.039	310.541	**320.874**
148	2-methylfuran	243.15	273.131	**280.25**
149	tetrahydrofuran	247.594	261.298	**266.445**
150	tetrahydropyran	253.15	276.32	**280.536**
151	methoxybenzene	324.817	304.318	**321.482**
152	1,2-bis(2-methoxyethoxy)ethane	386.15	363.879	**364.855**
153	2-(phenoxymethyl)oxirane	388.15	349.916	**379.468**
154	2-methoxy-2-methylbutane	262.15	279.965	**278.489**
155	2-(2-hydroxyethoxy)ethanol	416.15	288.765	**407.13**
156	ethoxyethylene	228.15	258.72	**259.356**
157	allyloxybenzene	335.15	334.363	**336.911**
158	2-methoxy-2-methylpropane	245.15	263.12	**254.253**
159	phenylmethoxymethylbenzene	408.15	410.007	**422.252**
160	1-chloro-2-(2-chloroethoxy)ethane	328.15	288.765	**328.89**
161	1-chloro-2-methoxyethane	288.15	258.72	**278.95**
162	1-[2-(2-butoxyethoxy)ethoxy]butane	374.15	408.947	**373.549**
163	3-allyloxyprop-1-ene	266.15	288.765	**295.111**
164	1-chloro-4-(phenoxy)benzene	386.15	391.794	**415.391**
165	1-isopentyloxy-3-methylbutane	319.15	340.193	**318.73**
166	2-(allyloxymethyl)oxirane	321.15	304.318	**298.392**
167	chloro-(chloromethoxy)methane	292.15	258.72	**300.365**
168	2-(butoxymethyl)oxirane	314.15	319.341	**330.12**
169	1-chloro-1-(1-chloroethoxy)ethane	328.15	280.103	**305.909**
170	1-butoxybutane	298.15	318.811	**291.177**
171	1,2-dimethoxybenzene	345.15	332.822	**363.198**
172	1,2-dimethoxyethane	271.15	273.743	**292.028**
173	(3*S*,3a*R*,6*R*,6a*R*)-3,6-dimethoxy-2,3,3a,5,6,6a-hexahydrofuro[3,2-b]furan	376.15	362.361	**355.042**
174	phenoxybenzene	388.15	379.961	**391.754**
175	1,3,5-trioxane	318.15	276.32	**314.384**
176	ethoxyethylene	227.15	258.72	**259.356**
177	1-hexoxyhexane[a]	349.817	378.901	**363.131**
178	ethoxyethylene[a]	227.594	258.72	**259.356**
179	1-ethenoxy-2-methylpropane[a]	263.706	284.434	**285.693**
180	furan[a]	237.594	261.297	**238.432**
181	phenoxybenzene[a]	388.15	379.961	**391.754**
182	4-(4-aminophenoxy)aniline[a]	491.15	403.628	**464.648**
183	chloro-methoxymethane[a]	289.15	243.697	**268.983**
184	4,7,7-trimethyl-8-oxabicyclo[2.2.2]octane[a]	322.15	336.993	**322.116**
185	1-pentoxypentane[a]	330.15	348.856	**327.25**
186	1-ethenoxypropane[a]	247.15	273.743	**253.605**
	Class: Amines			
187	acetamide	315.15	278.371	**310.272**
188	1-(2-pyridyl)ethanone	349.15	370.67	**389.519**
189	2-(bis(2-hydroxyethyl)amino)ethanol	452.15	390.196	**436.342**
190	prop-2-en-1-amine	245.15	290.279	**300.604**
191	6-methyl-2-pyridinamine	376.15	346.839	**351.516**
192	2-(2-aminoethoxy)ethanol	400.15	346.534	**385.27**
193	2-pyridinamine	236.15	341.367	**318.273**
194	aniline	343.15	336.39	**310.158**
195	phenylmethanamine	345.15	354.535	**337.317**
196	3-bromopyridine	324.15	314.827	**298.997**
197	butan-2-amine	254.15	280.705	**283.293**
198	2-methylpropan-2-amine	235.15	235.866	**257.271**
199	3-chloroaniline	391.15	337.668	**352.07**
200	2-chloroaniline	371.15	340.514	**365.247**
201	2-chloropyridine	337.15	332.276	**306.731**
202	2,4,6-trimethylpyridine	330.15	343.568	**358.223**
203	2-pyridinecarbonitrile	362.15	366.108	**341.904**
204	3-pyridinecarbonitrile	357.15	365.256	**344.993**
205	4-pyridinecarbonitrile	361.15	365.441	**347.087**
206	1-cyclohexyl-2-pyrrolidinone	418.15	379.197	**404.158**
207	cyclohexanamine	300.15	304.905	**295.267**
208	*N*-pentylpentan-1-amine	277.15	382.028	**329.366**
209	2,6-ditert-butylpyridine	345.15	334.552	**331.44**
210	ethane-1,2-diamine	330.35	288.59	**327.026**
211	*N*-cyclohexylcyclohexanamine	376.15	380.74	**376.24**
212	*N*,*N*-diethylacetamide	343.15	343.773	**326.557**

Table 4. Continued

no.	iupac/cas name	T_f(exptl) (K)	T_f(predicted) (K)	
			MLR	ANN
213	*N*-ethylethanamine	245.15	301.613	**237.992**
214	2-diethylaminoethanol	324.65	348.285	**336.194**
215	diethylcyanamide	342.15	338.401	**316.907**
216	*N*-(2-aminoethyl)ethane-1,2-diamine	363.15	340.071	**358.463**
217	*N*,*N*-diethylformamide	333.15	336.669	**316.305**
218	1-(2-hydroxypropylamino)propan-2-ol	399.15	343.034	**405.999**
219	n-isopropylpropan-2-amine	266.15	288.95	**263.146**
220	*N*-methylmethanamine	255.15	265.924	**244.246**
221	*N*,*N*-dimethylaniline	336.15	356.04	**353.182**
222	2-dimethylaminoethanol	313.15	301.33	**323.81**
223	*N*,*N*-dimethylformamide	330.15	290.798	**293.096**
224	3,5-dimethylpiperidine	294.65	302.183	**303.333**
225	heptan-2-amine	327.15	321.424	**316.324**
226	heptan-1-amine	317.15	337.285	**316.826**
227	3-methyl-2-pyridinamine[a]	384.15	347.631	**371.888**
228	propan-1-amine[a]	243.15	281.851	**259.021**
229	2-bromopyridine[a]	327.15	318.717	**303.486**
230	butan-1-amine[a]	261.15	295.71	**279.44**
231	4-chloroaniline[a]	461.15	337.778	**356.749**
232	*N*-allylprop-2-en-1-amine[a]	280.15	342.997	**286.198**
233	*N*-butylbutan-1-amine[a]	312.15	354.311	**294.626**
234	2-(2-hydroxyethylamino)ethanol[a]	411.15	344.221	**405.273**
235	*N*,*N*-dimethylacetamide[a]	336.15	298.548	**328.412**
236	2-aminoethanol[a]	358.15	290.664	**351.183**

[a] The solvents belonging to the test set for MLR calculations.

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