

# Supplementary Material

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### **Semiempirical Topological Index: A Novel Molecular Descriptor for Quantitative Structure–Retention Relationship Studies**

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**Table 1.** Values of experimental retention indices ( $RI_{exp}$ ), values of calculated retention indices ( $RI_{calc}$ ) using Eqs. 2 and 3,  $\Delta RI$  ( $RI_{exp} - RI_{calc}$ ) and values of calculated semi-empirical topological index ( $I_{ET}$ ) for alkanes, alkenes, esters, ketones, aldehydes and alcohols.

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
<b>Branched alkanes</b>							
1	01C*	100	68.26	31.74	–	–	1.0000
2	02C	200	191.98	8.02	198.87	1.14	2.0000
3	03C	300	292.00	8.00	298.68	1.32	2.8084
4	04C	400	392.01	7.99	398.50	1.50	3.6168
5	02,02Me03C*	412.6	449.37	–36.77	–	–	4.0804
6	02Me04C	475.4	478.72	–3.32	485.04	–9.64	4.3177
7	05C	500	492.04	7.96	498.33	1.67	4.4253
8	02,02Me04C	537.6	549.38	–11.78	555.56	–17.96	4.8888
9	02,03Me04C	568.1	565.44	2.66	571.59	–3.49	5.0186
10	02Me05C	569.8	578.74	–8.94	584.86	–15.06	5.1261
11	03Me05C	584.6	578.75	5.85	584.88	–0.28	5.1262
12	06C	600	592.06	7.94	598.16	1.84	5.2338
13	02,02Me05C*	626.3	649.39	–23.09	–	–	5.6972
14	02,04Me05C*	630.1	665.45	–35.35	–	–	5.8270
15	02,02,03Me04C	641.1	636.09	5.01	642.11	–1.01	5.5897
16	03,03Me05C	660.2	649.41	10.79	655.39	4.81	5.6973
17	02Me06C	666.8	678.76	–11.96	684.69	–17.89	5.9346
18	02,03Me05C	672.5	665.45	7.05	671.41	1.09	5.8270
19	03Me06C	676.5	678.76	–2.26	684.69	–8.19	5.9346
20	03Et05C	686.6	678.76	7.84	684.69	1.91	5.9346
21	02,02,04Me05C*	690.9	736.11	–45.21	–	–	6.3981
22	07C	700	692.09	7.91	697.99	2.01	6.0423
23	02,02,Me06C*	719.9	749.42	–29.52	–	–	6.5057
24	02,02,03Me05C	738.6	736.11	2.49	741.92	–3.32	6.3981
25	02,03Me06C	760.8	765.47	–4.67	771.22	–10.42	6.6354
26	02,03,03Me05C*	761.4	736.11	25.29	–	–	6.3981
27	03Et02Me05C	762.4	765.48	–3.08	771.24	–8.84	6.6355
28	02Me07C	765	778.79	–13.79	784.52	–19.52	6.7431
29	04Me07C	767.4	778.78	–11.38	784.51	–17.11	6.7430
30	03,04Me06C	771.6	765.47	6.13	771.22	0.38	6.6354
31	03Me07C	772.6	778.79	–6.19	784.52	–11.92	6.7431
32	02,02,04,04Me05C*	774.6	806.76	–32.16	–	–	6.9692
33	03,03Me06C*	775.7	749.42	26.28	–	–	6.5057
34	02,02,04Me06C*	777.3	836.13	–58.83	–	–	7.2066
35	02,02,05Me06C*	790.7	836.12	–45.42	–	–	7.2065
36	08C	800	792.11	7.89	797.82	2.18	6.8508
37	02,04,04Me06C*	809.7	852.18	–42.48	–	–	7.3363
38	02,03,05Me06C*	813.2	852.18	–38.98	–	–	7.3363
39	02,02Me07C*	816.2	849.45	–33.25	–	–	7.3142
40	02,02,05,05Me06C*	820.1	906.78	–86.68	–	–	7.7776
41	02,04Me07C*	821.2	865.49	–44.29	–	–	7.4439
42	02,02,03,04Me05C	821.9	822.82	–0.92	828.47	–6.57	7.099
43	02,02,03Me06C	823.3	836.12	–12.82	841.74	–18.44	7.2065
44	02,02Me03Et05C	824.4	836.13	–11.73	841.75	–17.35	7.2066
45	04Et02Me06C*	824.9	865.49	–40.59	–	–	7.4439
46	02,06Me07C*	827.5	865.49	–37.99	–	–	7.4439
47	04,04Me07C*	828.6	849.43	–20.83	–	–	7.3141
48	02,05Me07C*	833.7	865.50	–31.80	–	–	7.4440
49	03,05Me07C*	834.4	865.50	–31.10	–	–	7.4440
50	03,03Me07C	837.5	849.45	–11.95	855.04	–17.54	7.3142
51	02,04Me03Et05C	838.4	852.18	–13.78	857.77	–19.37	7.3363

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
52	02,03,03Me06C	841.7	836.12	5.58	841.74	-0.04	7.2065
53	03Et02Me06C*	844.4	865.49	-21.09	-	-	7.4439
54	02,03,04Me06C	849.7	852.18	-2.48	857.77	-8.07	7.3363
55	03,03,04Me06C	855.1	836.12	18.98	841.74	13.36	7.2065
56	02,03Me07C	855.5	865.49	-9.99	871.05	-15.55	7.4439
57	03Et04Me06C	855.6	865.49	-9.89	871.05	-15.45	7.4439
58	02,02,03,03Me05C*	855.8	806.76	49.04	-	-	6.9692
59	03Et03Me06C	856	849.43	6.57	855.03	0.97	7.3141
60	03,04Me07C	858	865.48	-7.48	871.04	-13.04	7.4438
61	04Et07C*	858.2	878.79	-20.59	-	-	7.5514
62	02,03,03,04Me05C*	861.1	822.82	38.28	-	-	7.0990
63	04Me08C	863.3	878.80	-15.50	884.34	-21.04	7.5515
64	02Me08C	864.8	878.82	-14.02	884.35	-19.55	7.5516
65	03Et07C	867.4	878.80	-11.40	884.34	-16.94	7.5515
66	02,04,06Me07C*	870.1	952.21	-82.11	-	-	8.1448
67	03Me08C	870.8	878.82	-8.02	884.35	-13.55	7.5516
68	02,02,04,05Me06C*	872.1	922.83	-50.73	-	-	7.9074
69	02,02,06Me07C*	873	936.15	-63.15	-	-	8.0150
70	02,02,03,05Me06C*	873.3	922.83	-49.53	-	-	7.9074
71	02,03Me03Et05C*	875	836.13	38.87	-	-	7.2066
72	02,02,04Me07C*	875.7	936.15	-60.45	-	-	8.0150
73	02,02,05Me07C*	878.1	936.15	-58.05	-	-	8.0150
74	03,03Et05C*	880.2	849.45	30.75	-	-	7.3142
75	02,02Me04Et06C*	881.3	936.15	-54.85	-	-	8.0150
76	02,02,04,04Me06C	888.6	906.79	-18.19	912.27	-23.67	7.7777
77	02,04,04Me07C*	889.4	936.15	-46.75	-	-	8.0150
78	02,05Me03Et06C*	891.4	952.21	-60.81	-	-	8.1448
79	02,05,05Me07C*	891.7	936.15	-44.45	-	-	8.0150
80	09C	900	892.14	7.86	897.65	2.35	7.6593
81	02,02Me03Et06C*	902.1	936.15	-34.05	-	-	8.0150
82	02,03,03,05Me06C	903.3	922.83	-19.53	928.29	-24.99	7.9074
83	03Et02,02,04Me05C	903.9	922.83	-18.93	928.29	-24.39	7.9074
84	02,04,05Me07C*	906.7	952.19	-45.49	-	-	8.1447
85	04Et02Me07C*	907.4	965.51	-58.11	-	-	8.2523
86	03,03,05Me07C*	907.7	936.15	-28.45	-	-	8.0150
87	02,02,03,04Me06C	908.8	922.83	-14.03	928.29	-19.49	7.9074
88	02,03,05Me07C*	912.9	952.21	-39.31	-	-	8.1448
89	02,02,03Me07C*	914.4	936.15	-21.75	-	-	8.0150
90	02,02Me08C*	914.9	949.47	-34.57	-	-	8.1227
91	02,04Me03Isoprop05C*	915.1	938.89	-23.79	-	-	8.0372
92	03Isoprop02Me06C*	915.5	952.19	-36.69	-	-	8.1447
93	02,04Me08C*	915.8	965.52	-49.72	-	-	8.2524
94	04,04Me08C*	918	963.81	-45.81	-	-	8.2386
95	02,03,06Me07C*	919	952.19	-33.19	-	-	8.1447
96	02,04Me04Et06C	920.7	936.15	-15.45	941.57	-20.87	8.0150
97	02,02,03,04,04Me05C*	921.7	893.48	28.22	-	-	7.6701
98	03,05Me08C*	921.8	965.52	-43.72	-	-	8.2524
99	02,05Me08C*	921.8	965.51	-43.71	-	-	8.2523
100	02,03,04,05Me06C	923.1	938.89	-15.79	944.31	-21.21	8.0372
101	05Et02Me07C*	924.8	965.51	-40.71	-	-	8.2523
102	04Isoprop07C*	925	965.51	-40.51	-	-	8.2523
103	02,07Me08C*	928.5	965.52	-37.02	-	-	8.2524
104	02,02,03,03Me06C*	928.8	906.78	22.02	-	-	7.7776
105	03,06Me08C*	929	965.52	-36.52	-	-	8.2524
106	02,04Me03Et06C*	929.8	952.19	-22.39	-	-	8.1447
107	02,06Me08C*	931.5	965.52	-34.02	-	-	8.2524

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{\text{exp}}$	$RI_{\text{calc}}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{\text{calc}}$ (Eq. 3)	$\Delta RI$ (Eq. 3)	$I_{\text{ET}}$
108	02,03,03Me07C	931.7	936.15	-4.45	941.57	-9.87	8.0150
109	03,03Me08C	932	949.47	-17.47	954.87	-22.87	8.1227
110	03,04,04Me07C	932.2	936.13	-3.93	941.56	-9.36	8.0149
111	02,03,04Me07C	933.4	952.19	-18.79	957.59	-24.19	8.1447
112	02,03,04,04Me06C	935	922.83	12.17	928.29	6.71	7.9074
113	04Et03Me07C*	935.7	965.51	-29.81	-	-	8.2523
114	03,04Me08C*	936	965.51	-29.51	-	-	8.2523
115	03,03,04Me07C	936.6	936.13	0.47	941.56	-4.96	8.0149
116	04Et04Me07C	937.6	949.45	-11.85	954.85	-17.25	8.1225
117	03,03Me04Et06C	937.8	936.15	1.65	941.57	-3.77	8.0150
118	03Et04Me07C*	940.5	965.51	-25.01	-	-	8.2523
119	03Et02Me07C*	941	965.52	-24.52	-	-	8.2524
120	04,05Me08C*	943.1	965.49	-22.39	-	-	8.2522
121	03,04,05Me07C	945	952.19	-7.19	957.59	-12.59	8.1447
122	03,04Et06C	945.8	965.52	-19.72	970.89	-25.09	8.2524
123	02,03,03,04Me06C*	949.1	922.83	26.27	-	-	7.9074
124	02,03Me04Et06C	949.4	952.21	-2.81	957.60	-8.20	8.1448
125	04Et08C*	951.5	978.82	-27.32	-	-	8.3599
126	02,03Me08C	952.1	965.52	-13.42	970.89	-18.79	8.2524
127	02Et02Me07C	953	956.65	-3.65	962.03	-9.03	8.1807
128	02,02,03,03,04Me05C*	953.4	893.48	59.92	-	-	7.6701
129	03,03Et06C	954.1	949.46	4.64	954.86	-0.76	8.1226
130	05Me09C*	957.4	978.83	-21.43	-	-	8.3600
131	04Me09C	960	978.83	-18.83	984.17	-24.17	8.3600
132	03Et08C	964	978.83	-14.83	984.17	-20.17	8.3600
133	03,04Me03Et06C*	964.6	936.15	28.45	-	-	8.0150
134	03Et02,02,03Me05C*	965.7	906.79	58.91	-	-	7.7777
135	03Et02,03,04Me05C*	969.4	922.83	46.57	-	-	7.9074
136	03,03,04,04Me06C*	983.7	906.78	76.92	-	-	7.7776
137	10C	1000	992.17	7.83	997.48	2.52	8.4678
138	11C	1100	1092.19	7.81	1097.31	2.69	9.2763
139	06Me11C*	1151.8	1178.88	-27.08	-	-	9.9770
140	04Me11C*	1158.6	1178.88	-20.28	-	-	9.9770
141	12C	1200	1192.22	7.78	1197.14	2.86	10.0848
142	05,07Me11C*	1190.4	1265.58	-75.18	-	-	10.6778
143	04,06Me11C*	1193	1265.58	-72.58	-	-	10.6778
144	03,05Me11C*	1207.2	1265.60	-58.40	-	-	10.6779
145	02,04Me11C*	1208.2	1265.60	-57.40	-	-	10.6779
146	02,05Me11C*	1210.4	1265.58	-55.18	-	-	10.6778
147	02,06Me11C*	1210.4	1265.58	-55.18	-	-	10.6778
148	02,07Me11C*	1215.8	1265.58	-49.78	-	-	10.6778
149	05,06Me11C*	1223.4	1265.57	-42.17	-	-	10.6777
150	04,05Me11C*	1230.4	1265.57	-35.17	-	-	10.6777
151	02,09Me11C*	1232.6	1265.60	-33.00	-	-	10.6779
152	03,04Me11C	1247	1265.58	-18.58	1270.36	-23.36	10.6778
153	02,03Me11C	1251.4	1265.60	-14.20	1270.38	-18.98	10.6779
<b>Methyl-branched alkanes</b>							
154	02Me09C	966.5	959.17	7.33	964.55	1.95	8.2011
155	03Me09C	973	959.76	13.24	965.14	7.86	8.2059
156	02Me11C	1166.5	1159.22	7.28	1164.21	2.29	9.8181
157	03Me11C	1172.5	1160.96	11.54	1165.94	6.56	9.8321
158	02Me13C	1366.5	1359.28	7.22	1363.87	2.63	11.4351
159	03Me13C	1373	1362.15	10.85	1366.74	6.26	11.4583
160	02Me15C	1566.5	1559.33	7.17	1563.53	2.97	13.0521
161	03Me15C	1573.7	1563.35	10.35	1567.54	6.16	13.0846
162	02Me17C	1765.8	1759.38	6.42	1763.19	2.61	14.6691

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
163	03Me17C	1774	1764.54	9.46	1768.34	5.66	14.7108
164	02Me19C	1966	1959.43	6.57	1962.85	3.15	16.2861
165	03Me19C	1974.3	1965.73	8.57	1969.14	5.16	16.3370
166	10Me19C	1943	1936.16	6.84	1939.63	3.37	16.0980
167	02Me21C	2166	2159.49	6.51	2162.51	3.49	17.9031
168	03Me21C	2174.5	2166.92	7.58	2169.93	4.57	17.9632
169	11Me21C	2141	2134.66	6.34	2137.73	3.27	17.7024
170	02Me23C	2364	2359.54	4.46	2362.17	1.83	19.5201
171	03Me23C	2374.5	2368.11	6.39	2370.73	3.77	19.5894
172	12Me23C	2337	2333.27	3.73	2335.96	1.04	19.3078
173	02Me25C	2563	2559.57	3.43	2561.81	1.19	21.1369
174	03Me25C	2574.4	2569.30	5.10	2571.53	2.87	21.2156
175	13Me25C	2534.5	2531.98	2.52	2534.27	0.23	20.9139
176	02Me27C	2763	2759.62	3.38	2761.47	1.53	22.7539
177	03Me27C	2774.4	2770.47	3.93	2772.30	2.10	22.8416
178	14Me27C	2733	2730.79	2.21	2732.70	0.30	22.5209
179	02Me29C	2962.2	2959.67	2.53	2961.13	1.07	24.3709
180	03Me29C	2974	2971.67	2.33	2973.11	0.89	24.4679
181	15Me29C	2931.5	2929.68	1.82	2931.20	0.30	24.1285
182	02Me31C	3161.5	3159.71	1.79	3160.78	0.72	25.9878
183	03Me31C	3174.1	3172.86	1.24	3173.90	0.20	26.0941
184	04Me31C	3157.5	3150.57	6.93	3151.65	5.85	25.9139
185	05Me31C	3150	3147.30	2.70	3148.39	1.61	25.8875
186	06Me31C	3143.2	3144.54	-1.34	3145.64	-2.44	25.8652
187	07Me31C	3140	3142.16	-2.16	3143.26	-3.26	25.8459
188	13Me31C	3130.8	3132.13	-1.33	3133.26	-2.46	25.7649
189	16Me31C	3129.8	3128.66	1.14	3129.79	0.01	25.7368
190	02Me33C	3362	3359.76	2.24	3360.44	1.56	27.6048
191	03Me33C	3374.5	3374.05	0.45	3374.70	-0.20	27.7203
192	04Me33C	3357.5	3350.62	6.88	3351.31	6.19	27.5309
193	05Me33C	3350	3347.35	2.65	3348.05	1.95	27.5045
194	06Me33C	3343.7	3344.60	-0.90	3345.30	-1.60	27.4822
195	13Me33C	3328.5	3332.19	-3.69	3332.92	-4.42	27.3819
196	17Me33C	3328.5	3327.68	0.82	3328.42	0.08	27.3455
197	02Me35C	3562	3559.82	2.18	3560.10	1.90	29.2218
198	03Me35C	3574.3	3575.24	-0.94	3575.50	-1.20	29.3465
199	18Me35C	3527.3	3526.76	0.54	3527.11	0.19	28.9546
200	08,12Me22C	2267	2272.86	-5.86	2275.67	-8.67	18.8195
201	03,09Me23C	2410	2404.25	5.75	2406.80	3.20	19.8815
202	05,09Me24C	2485	2483.08	1.92	2485.48	-0.48	20.5187
203	03,11Me25C	2609	2603.45	5.55	2605.61	3.39	21.4916
204	03,15Me25C	2605	2600.01	4.99	2602.17	2.83	21.4638
205	05,11Me25C	2582	2581.12	0.88	2583.32	-1.32	21.3111
206	05,17Me25C	2585	2576.21	8.79	2578.42	6.58	21.2714
207	07,11Me25C	2577	2575.96	1.04	2578.17	-1.17	21.2694
208	02,06Me26C	2704	2699.03	4.97	2701.00	3.00	22.2642
209	04,08Me26C	2695	2687.49	7.51	2689.48	5.52	22.1709
210	05,11Me26C	2682	2681.16	0.84	2683.16	-1.16	22.1197
211	06,10Me26C	2678	2679.36	-1.36	2681.37	-3.37	22.1052
212	07,11Me26C	2675	2676.00	-1.00	2678.01	-3.01	22.0780
213	03,07Me27C	2809	2808.91	0.09	2810.66	-1.66	23.1523
214	03,15Me27C	2805	2801.21	3.79	2802.98	2.02	23.0901
215	05,11Me27C	2782	2781.18	0.82	2782.99	-0.99	22.9282
216	05,17Me27C	2786	2776.26	9.74	2778.08	7.92	22.8884
217	07,13Me27C	2774	2774.23	-0.23	2776.05	-2.05	22.8720
218	09,19Me27C	2765	2765.73	-0.73	2767.57	-2.57	22.8033

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{\text{exp}}$	$RI_{\text{calc}}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{\text{calc}}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
219	02,06Me28C	2905	2899.09	5.91	2900.66	4.34	23.8812
220	02,10Me28C	2899	2894.58	4.42	2896.17	2.83	23.8448
221	04,10Me28C	2895	2885.44	9.56	2887.04	7.96	23.7709
222	05,15Me28C	2882	2877.78	4.22	2879.40	2.60	23.7090
223	07,13Me28C	2873	2874.26	-1.26	2875.88	-2.88	23.6805
224	03,07Me29C	3008	3010.10	-2.10	3011.46	-3.46	24.7785
225	03,13Me29C	3004	3004.04	-0.04	3005.41	-1.41	24.7295
226	05,13Me29C	2982	2979.44	2.56	2980.86	1.14	24.5307
227	05,19Me29C	2983	2974.94	8.06	2976.37	6.63	24.4943
228	07,17Me29C	2973	2971.16	1.84	2972.60	0.40	24.4638
229	02,06Me30C	3105	3099.14	5.86	3100.32	4.68	25.4982
230	02,10Me30C	3099	3094.64	4.36	3095.83	3.17	25.4618
231	02,12Me30C	3095	3092.75	2.25	3093.95	1.05	25.4466
232	03,07Me30C	3108	3110.69	-2.69	3111.86	-3.86	25.5916
233	04,10Me30C	3094	3085.49	8.51	3086.70	7.30	25.3879
234	06,10Me30C	3075	3079.47	-4.47	3080.69	-5.69	25.3392
235	03,07Me31C	3209	3211.29	-2.29	3212.26	-3.26	26.4047
236	03,13Me31C	3203.5	3205.23	-1.73	3206.20	-2.70	26.3557
237	03,15Me31C	3209	3203.59	5.41	3204.57	4.43	26.3425
238	05,13Me31C	3180.5	3179.49	1.01	3180.52	-0.02	26.1477
239	05,17Me31C	3182	3176.36	5.64	3177.40	4.60	26.1224
240	07,11Me31C	3170.2	3176.13	-5.93	3177.16	-6.96	26.1205
241	11,21Me31C	3162.9	3161.29	1.61	3162.36	0.54	26.0006
242	02,08Me32C	3297	3296.80	0.20	3297.60	-0.60	27.0959
243	04,08Me32C	3292	3287.65	4.35	3288.46	3.54	27.0219
244	06,10Me32C	3273.5	3279.52	-6.02	3280.35	-6.85	26.9562
245	08,12Me32C	3266	3273.12	-7.12	3273.97	-7.97	26.9045
246	09,21Me32C	3262	3264.59	-2.59	3265.45	-3.45	26.8355
247	14,18Me32C	3257.5	3259.28	-1.78	3260.15	-2.65	26.7926
248	03,09Me33C	3403	3410.23	-7.23	3410.80	-7.80	28.0127
249	03,15Me33C	3409	3404.78	4.22	3405.37	3.63	27.9687
250	05,17Me33C	3380	3376.42	3.58	3377.06	2.94	27.7394
251	05,19Me33C	3382	3375.04	6.96	3375.69	6.31	27.7283
252	07,17Me33C	3370	3371.27	-1.27	3371.92	-1.92	27.6978
253	11,23Me33C	3362.4	3360.15	2.25	3360.82	1.58	27.6079
254	02,10Me34C	3494	3494.74	-0.74	3495.15	-1.15	28.6958
255	04,16Me34C	3489	3480.44	8.56	3480.88	8.12	28.5802
256	06,10Me34C	3473.8	3479.57	-5.77	3480.01	-6.21	28.5732
257	08,12Me34C	3465	3473.18	-8.18	3473.63	-8.63	28.5215
258	12,22Me34C	3461.4	3459.33	2.07	3459.81	1.59	28.4096
259	13,17Me34C	3455	3461.27	-6.27	3461.75	-6.75	28.4253
260	03,07Me35C	3609.5	3613.67	-4.17	3613.85	-4.35	29.6571
261	03,15Me35C	3601	3605.98	-4.98	3606.17	-5.17	29.5949
262	05,09Me35C	3580	3583.38	-3.38	3583.62	-3.62	29.4123
263	05,19Me35C	3580.5	3575.10	5.40	3575.35	5.15	29.3453
264	07,17Me35C	3569.7	3571.32	-1.62	3571.58	-1.88	29.3148
265	09,21Me35C	3561	3564.67	-3.67	3564.94	-3.94	29.2610
266	02,12Me36C	3695	3692.91	2.09	3692.93	2.07	30.2976
267	05,17Me36C	3680	3676.50	3.50	3676.55	3.45	30.1649
268	13,23Me36C	3661	3657.47	3.53	3657.56	3.44	30.0111
269	03,15Me37C	3801	3807.17	-6.17	3806.96	-5.96	31.2211
270	05,09Me37C	3779	3783.44	-4.44	3783.28	-4.28	31.0293
271	05,17Me37C	3780	3776.52	3.48	3776.38	3.62	30.9734
272	13,23Me37C	3759	3757.49	1.51	3757.39	1.61	30.8196
273	05,17Me38C	3878	3876.52	1.48	3876.18	1.82	31.7817
274	04,08,12Me24C	2520	2509.96	10.04	2512.30	7.70	20.7359

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
275	05,09,13Me25C	2610	2605.13	4.87	2607.29	2.71	21.5052
276	04,08,12Me26C	2719	2710.01	8.99	2711.96	7.04	22.3529
277	03,07,11Me27C	2838	2832.06	5.94	2833.76	4.24	23.3394
278	04,08,2Me28C	2918	2910.04	7.96	2911.59	6.41	23.9697
279	03,07,11Me29C	3037	3033.25	3.75	3034.56	2.44	24.9656
280	05,13,17Me29C	3007	2999.62	7.38	3001.00	6.00	24.6938
281	06,14,18Me30C	3100	3095.61	4.39	3096.81	3.19	25.4697
282	03,07,11Me31C	3236.5	3234.44	2.06	3235.36	1.14	26.5918
283	05,13,17Me31C	3205.4	3199.67	5.73	3200.66	4.74	26.3108
284	07,13,17Me31C	3191.3	3194.51	-3.21	3195.51	-4.21	26.2691
285	11,15,19Me31C	3181	3184.78	-3.78	3185.79	-4.79	26.1904
286	02,10,16Me32C	3324	3315.30	8.70	3316.06	7.94	27.2454
287	04,12,16Me32C	3316	3304.26	11.74	3305.05	10.95	27.1562
288	06,14,18Me32C	3299	3295.65	3.35	3296.45	2.55	27.0866
289	12,16,20Me32C	3281	3282.18	-1.18	3283.01	-2.01	26.9777
290	03,07,15Me33C	3436.5	3433.67	2.83	3434.20	2.30	28.2022
291	05,13,17Me33C	3405	3399.71	5.29	3400.31	4.69	27.9277
292	07,11,15Me33C	3389	3397.25	-8.25	3397.85	-8.85	27.9078
293	11,15,19Me33C	3379.6	3384.82	-5.22	3385.44	-5.84	27.8073
294	02,10,16Me34C	3524	3515.35	8.65	3515.72	8.28	28.8624
295	04,08,12Me34C	3515.5	3510.21	5.29	3510.59	4.92	28.8208
296	06,14,18Me34C	3497	3495.71	1.29	3496.11	0.89	28.7036
297	08,12,16Me34C	3486.4	3493.79	-7.39	3494.20	-7.80	28.6881
298	12,16,20Me34C	3478	3482.23	-4.23	3482.67	-4.67	28.5947
299	03,07,15Me35C	3636.3	3634.86	1.44	3635.00	1.30	29.8284
300	05,09,13Me35C	3605	3605.38	-0.38	3605.57	-0.57	29.5901
301	07,11,15Me35C	3588.3	3597.30	-9.00	3597.51	-9.21	29.5248
302	13,17,21Me35C	3577	3579.80	-2.80	3580.04	-3.04	29.3833
303	13,17,23Me35C	3583	3579.02	3.98	3579.26	3.74	29.3770
304	04,08,16Me36C	3715	3708.36	6.64	3708.36	6.64	30.4225
305	08,12,16Me36C	3685	3693.84	-8.84	3693.86	-8.86	30.3051
306	14,18,22Me36C	3676	3677.48	-1.48	3677.54	-1.54	30.1729
307	03,07,15Me37C	3835	3836.05	-1.05	3835.80	-0.80	31.4546
308	05,13,17Me37C	3803	3799.82	3.18	3799.63	3.37	31.1617
309	07,13,19Me37C	3784	3793.80	-9.80	3793.63	-9.63	31.1131
310	15,19,23Me37C	3775	3775.30	-0.30	3775.16	-0.16	30.9635
311	16,20,24Me38C	3873.5	3873.21	0.29	3872.88	0.62	31.7549
312	05,13,17Me39C	4001	3999.86	1.14	3999.28	1.72	32.7786
313	15,19,23Me39C	3972.4	3975.34	-2.94	3974.80	-2.40	32.5804
314	14,18,22Me40C	4071	4077.59	-6.59	4076.86	-5.86	33.4069
315	03,07,11,15Me29C	3062	3059.78	2.22	3061.05	0.95	25.1801
316	03,07,11,15Me31C	3261	3260.96	0.04	3261.83	-0.83	26.8062
317	04,08,12,16Me31C	3249	3235.91	13.09	3236.83	12.17	26.6037
318	03,07,11,15Me33C	3459	3462.15	-3.15	3462.63	-3.63	28.4324
319	04,08,12,16Me33C	3448	3435.95	12.05	3436.47	11.53	28.2206
320	03,07,11,15Me35C	3658	3663.34	-5.34	3663.42	-5.42	30.0586
321	07,11,15,19Me35C	3628	3621.37	6.63	3621.53	6.47	29.7193
322	09,13,17,21Me35C	3617	3613.62	3.38	3613.80	3.20	29.6567
323	11,15,19,24Me35C	3605	3606.41	-1.41	3606.60	-1.60	29.5984
324	06,10,12,16Me36C	3723	3727.89	-4.89	3727.84	-4.84	30.5803
325	08,12,16,20Me36C	3713	3717.37	-4.37	3717.35	-4.35	30.4953
326	10,14,18,22Me36C	3703.5	3710.17	-6.67	3710.16	-6.66	30.4371
327	03,07,11,15Me37C	3855	3864.53	-9.53	3864.22	-9.22	31.6848
328	07,11,15,19Me37C	3823	3821.42	1.58	3821.19	1.81	31.3363
329	09,13,17,21Me37C	3813	3813.67	-0.67	3813.46	-0.46	31.2737
330	11,15,19,24Me37C	3803	3806.46	-3.46	3806.26	-3.26	31.2154

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{\text{exp}}$	$RI_{\text{calc}}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{\text{calc}}$ (Eq. 3)	$\Delta RI$ (Eq. 3)	$I_{ET}$
331	10,14,18,22Me38C	3900	3910.22	-10.22	3909.82	-9.82	32.0541
<b>Linear alkenes</b>							
332	1–Pentene	482.6	472.95	9.65	479.28	3.32	4.2710
333	1–Hexene	583.8	572.97	10.83	579.11	4.69	5.0795
334	1–Heptene	683.1	673.00	10.10	678.94	4.16	5.8880
335	1–Octene	782.6	773.02	9.58	778.77	3.83	6.6965
336	1–Nonene	882.5	873.05	9.45	878.60	3.90	7.5050
337	1–Decene	982.5	973.08	9.42	978.43	4.07	8.3135
338	1–Undecene	1082.4	1073.10	9.30	1078.26	4.14	9.1220
339	1–Dodecene	1183	1173.13	9.87	1178.09	4.91	9.9305
340	1–Tridecene	1283.1	1273.16	9.94	1277.92	5.18	10.7390
341	1–Tetradecene	1383.2	1373.18	10.02	1377.75	5.45	11.5475
342	<i>Trans</i> -2–Pentene	499.5	489.61	9.89	495.91	3.59	4.4057
343	<i>Cis</i> -2–Pentene	505.4	496.89	8.51	503.17	2.23	4.4645
344	<i>Trans</i> -2–Hexene	596.5	589.64	6.86	595.74	0.76	5.2142
345	<i>Cis</i> -2–Hexene	604.9	596.91	7.99	603.00	1.90	5.2730
346	<i>Trans</i> -2–Heptene	698.7	689.66	9.04	695.57	3.13	6.0227
347	<i>Cis</i> -2–Heptene	704.7	696.94	7.76	702.83	1.87	6.0815
348	<i>Trans</i> -2–Octene	797.5	789.69	7.81	795.40	2.10	6.8312
349	<i>Cis</i> -2–Octene	803.2	796.96	6.24	802.66	0.54	6.8900
350	<i>Trans</i> -2–Nonene	896.4	889.72	6.68	895.23	1.17	7.6397
351	<i>Cis</i> -2–Nonene	901.9	896.99	4.91	902.49	-0.59	7.6985
352	<i>Trans</i> -2–Decene	996.7	989.74	6.96	995.06	1.64	8.4482
353	<i>Cis</i> -2–Decene	1001.7	997.02	4.68	1002.32	-0.62	8.5070
354	<i>Trans</i> -2–Undecene	1096.6	1089.77	6.83	1094.89	1.71	9.2567
355	<i>Cis</i> -2–Undecene	1101.5	1097.04	4.46	1102.15	-0.65	9.3155
356	<i>Trans</i> -2–Dodecene	1196.9	1189.79	7.11	1194.72	2.18	10.0652
357	<i>Cis</i> -2–Dodecene	1201.7	1197.07	4.63	1201.98	-0.28	10.1240
358	<i>Trans</i> -2–Tridecene	1297	1289.82	7.18	1294.55	2.45	10.8737
359	<i>Cis</i> -2–Tridecene	1301.6	1297.10	4.50	1301.81	-0.21	10.9325
360	<i>Trans</i> -2–tetradecene	1396.9	1389.85	7.05	1394.38	2.52	11.6822
361	<i>Trans</i> -3–Hexene	591.1	579.81	11.29	585.94	5.16	5.1348
362	<i>Cis</i> -3–Hexene	593.3	584.74	8.56	590.85	2.45	5.1746
363	<i>Trans</i> -3–Heptene	687.4	679.83	7.57	685.75	1.65	5.9432
364	<i>Cis</i> -3–Heptene	692	684.76	7.24	690.68	1.32	5.9831
365	<i>Trans</i> -3–Octene	788.2	779.85	8.35	785.59	2.61	6.7517
366	<i>Cis</i> -3–Octene	789.8	784.79	5.01	790.51	-0.71	6.7916
367	<i>Trans</i> -3–Nonene	886.4	879.88	6.52	885.42	0.98	7.5602
368	<i>Cis</i> -3–Nonene	887.5	884.82	2.68	890.34	-2.84	7.6001
369	<i>Trans</i> -3–Decene	985.8	979.91	5.89	985.25	0.55	8.3687
370	<i>Cis</i> -3–Decene	985.8	984.84	0.96	990.17	-4.37	8.4086
371	<i>Trans</i> -3–Undecene	1085.4	1084.87	0.53	1090.00	-4.60	9.2171
372	<i>Cis</i> -3–Undecene	1085.3	1079.93	5.37	1085.08	0.22	9.1772
373	<i>Trans</i> -3–Dodecene	1185.1	1184.90	0.20	1189.83	-4.73	10.0256
374	<i>Cis</i> -3–Dodecene	1185.1	1179.96	5.14	1184.91	0.19	9.9857
375	<i>Trans</i> -3–Tridecene	1284.9	1284.92	-0.02	1289.66	-4.76	10.8341
376	<i>Cis</i> -3–Tridecene	1284.4	1279.98	4.42	1284.74	-0.34	10.7942
377	<i>Trans</i> -3–Tetradecene	1384.6	1384.95	-0.35	1389.49	-4.89	11.6426
378	<i>Cis</i> -3–Tetradecene	1384.1	1380.01	4.09	1384.57	-0.47	11.6027
379	<i>Trans</i> -4–Octene	784.1	774.94	9.16	780.68	3.42	6.7120
380	<i>Cis</i> -4–Octene	788.2	777.42	10.78	783.15	5.05	6.7320
381	<i>Trans</i> -4–Nonene	884.2	874.97	9.23	880.51	3.69	7.5205
382	<i>Cis</i> -4–Nonene	885.4	877.44	7.96	882.98	2.42	7.5405
383	<i>Trans</i> -4–Decene	982.5	974.99	7.51	980.34	2.16	8.3290
384	<i>Cis</i> -4–Decene	982.8	977.47	5.33	982.81	-0.01	8.3490
385	<i>Trans</i> -4–Undecene	1081.1	1077.50	3.60	1082.64	-1.54	9.1575

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
386	<i>Cis</i> -4–Undecene	1080.5	1075.02	5.48	1080.17	0.33	9.1375
387	<i>Trans</i> -4–Dodecene	1180.6	1177.52	3.08	1182.47	-1.87	9.9660
388	<i>Cis</i> -4–Dodecene	1179.6	1175.05	4.55	1180.00	-0.40	9.9460
389	<i>Trans</i> -4–Tridecene	1279.9	1277.55	2.35	1282.30	-2.40	10.7745
390	<i>Cis</i> -4–Tridecene	1278.6	1275.07	3.53	1279.83	-1.23	10.7545
391	<i>Trans</i> -4–Tetradecene	1379.3	1377.57	1.73	1382.13	-2.83	11.5830
392	<i>Cis</i> -4–Tetradecene	1377.7	1375.10	2.60	1379.66	-1.96	11.5630
393	<i>Trans</i> -5–Decene	984.1	974.99	9.11	980.34	3.76	8.3290
394	<i>Cis</i> -5–Decene	981.6	970.00	11.60	975.35	6.25	8.2886
395	<i>Trans</i> -5–Undecene	1081.8	1075.02	6.78	1080.17	1.63	9.1375
396	<i>Cis</i> -5–Undecene	1078.2	1070.02	8.18	1075.19	3.01	9.0971
397	<i>Trans</i> -5–Dodecene	1180.6	1175.05	5.55	1180.00	0.60	9.9460
398	<i>Cis</i> -5–Dodecene	1175.6	1170.05	5.55	1175.02	0.58	9.9056
399	<i>Trans</i> -5–Tridecene	1279.5	1275.07	4.43	1279.83	-0.33	10.7545
400	<i>Cis</i> -5–Tridecene	1273.8	1270.08	3.72	1274.85	-1.05	10.7141
401	<i>Trans</i> -5–Tetradecene	1378.4	1375.10	3.30	1379.66	-1.26	11.5630
402	<i>Cis</i> -4–Tetradecene	1372	1370.10	1.90	1374.68	-2.68	11.5226
403	<i>Trans</i> -6–Dodecene	1179.6	1172.52	7.08	1177.48	2.12	9.9256
404	<i>Cis</i> -6–Dodecene	1175	1167.57	7.43	1172.55	2.45	9.8856
405	<i>Trans</i> -6–Tridecene	1277.4	1272.55	4.85	1277.32	0.08	10.7341
406	<i>Cis</i> -6–Tridecene	1271.2	1267.60	3.60	1272.38	-1.18	10.6941
407	<i>Trans</i> -6–Tetradecene	1375.7	1372.58	3.12	1377.15	-1.45	11.5426
408	<i>Cis</i> -6–Tetradecene	1368.6	1367.63	0.97	1372.21	-3.61	11.5026
409	<i>Trans</i> -7–Tetradecene	1374.5	1371.36	3.14	1375.94	-1.44	11.5328
410	<i>Cis</i> -7–Tetradecene	1366.7	1365.10	1.60	1369.69	-2.99	11.4822
<b>Branched alkenes</b>							
411	2–Methyl–1–propene	383	376.17	6.83	382.70	0.30	3.4888
412	1–Butene	384	373.29	10.71	379.82	4.18	3.4655
413	<i>trans</i> -2–Butene	405	389.57	15.43	396.07	8.93	3.5971
414	<i>cis</i> -2–Butene	417	396.87	20.13	403.35	13.65	3.6561
415	3–Methyl–1–butene	451	444.76	6.24	451.15	-0.15	4.0432
416	2–Methyl–1–butene	488	476.20	11.80	482.53	5.47	4.2973
417	3,3–Dimethyl–1–butene	509	498.05	10.95	504.33	4.67	4.4739
418	2–Methyl–2–butene	514	494.08	19.92	500.37	13.63	4.4418
419	4–Methyl–1–pentene	551	533.43	17.57	539.65	11.35	4.7599
420	3–Methyl–1–pentene	554	545.42	8.58	551.61	2.39	4.8568
421	<i>cis</i> -4–Methyl–2–pentene	557	548.33	8.67	554.51	2.49	4.8803
422	2,3–Dimethyl–1–butene	560	543.68	16.32	549.87	10.13	4.8427
423	<i>trans</i> -4–Methyl–2–pentene	562	555.03	6.97	561.20	0.80	4.9345
424	2–Methyl–1–pentene	581	576.23	4.77	582.36	-1.36	5.1058
425	2–Ethyl–1–butene	592	576.23	15.77	582.36	9.64	5.1058
426	2–Methyl–2–pentene	598	594.10	3.90	600.20	-2.20	5.2503
427	4,4–Dimethyl–1–pentene	608	596.92	11.08	603.01	4.99	5.2731
428	<i>trans</i> -3–Methyl–2–pentene	613	602.69	10.31	608.77	4.23	5.3197
429	<i>trans</i> -4,4–Dimethyl–2–pentene	615	615.35	-0.35	621.40	-6.40	5.4220
430	2,3–Dimethyl–2–butene	626	597.34	28.66	603.43	22.57	5.2765
431	3,3–Dimethyl–1–pentene	630	616.09	13.91	622.14	7.86	5.4280
432	2,3,3–Trimethyl–1–butene	632	614.33	17.67	620.39	11.61	5.4138
433	<i>cis</i> -4,4–Dimethyl–2–pentene	639	619.00	20.00	625.04	13.96	5.4515
434	2,4–Dimethyl–1–pentene	640	631.71	8.29	637.74	2.26	5.5543
435	3,4–Dimethyl–1–pentene	641	632.12	8.88	638.14	2.86	5.5576
436	3–Methyl–1–hexene	647	645.45	1.55	651.44	-4.44	5.6653
437	2,3–Dimethyl–1–pentene	654	643.70	10.30	649.70	4.30	5.6512
438	<i>cis</i> -4–Methyl–2–hexene	657	648.35	8.65	654.34	2.66	5.6888
439	<i>trans</i> -4–Methyl–2–hexene	667	655.11	11.89	661.08	5.92	5.7434
440	<i>cis</i> -3,4–Dimethyl–2–pentene	672	658.00	14.00	663.97	8.03	5.7668

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
441	2–Methyl–1–hexene	677	676.24	0.76	682.17	–5.17	5.9142
442	<i>trans</i> –3,4–Dimethyl–2–pentene	679	667.48	11.52	673.43	5.57	5.8434
443	<i>cis</i> –3–Methyl–3–hexene	685	683.51	1.49	689.43	–4.43	5.9730
444	2–Methyl–2–hexene	691	694.13	–3.13	700.03	–9.03	6.0588
445	<i>cis</i> –3–Methyl–2–hexene	695	687.68	7.32	693.60	1.40	6.0067
446	2,3–Dimethyl–2–pentene	705	697.37	7.63	703.26	1.74	6.0850
447	2,4,4–Trimethyl –1–pentene	708	695.19	12.81	701.09	6.91	6.0674
448	2,4,4–Trimethyl –2–pentene	718	719.22	–1.22	725.07	–7.07	6.2616
449	<i>cis</i> –2,2–Dimethyl –3–hexene	720	712.93	7.07	718.80	1.20	6.2108
450	2,3–Dimethyl–1–hexene	741	743.72	–2.72	749.52	–8.52	6.4596
451	2,5–Dimethyl–2–hexene	751	754.60	–3.60	760.38	–9.38	6.5476
452	<i>trans</i> –2–Methyl–3–heptene	757	750.22	6.78	756.01	0.99	6.5122
453	2,3–Dimethyl–2–hexene	790	797.40	–7.40	803.09	–13.09	6.8935
<b>Esters</b>							
454	Methyl acetate	457.6	474.52	–16.92	480.85	–23.25	4.2837
455	Ethyl acetate	546	549.92	–3.92	556.11	–10.11	4.8932
456	Propyl formate	560.8	558.21	2.59	564.38	–3.58	4.9602
457	Methyl propionate	565.9	561.03	4.87	567.19	–1.29	4.9803
458	2–Propyl acetate	601	593.19	7.81	599.28	1.72	5.2429
459	Methyl methylpropionate	628.9	615.05	13.85	621.10	7.80	5.4196
460	Tert–butyl acetate	637	628.04	8.96	634.07	2.93	5.5246
461	Ethyl propionate	645.7	636.43	9.27	642.44	3.26	5.5924
462	Propyl acetate	648.6	645.05	3.55	651.05	–2.45	5.6621
463	Methyl butyrate	661.3	653.70	7.60	659.68	1.62	5.7320
464	Butyl formate	665.9	655.80	10.10	661.78	4.12	5.7490
465	Ethyl methylpropionate	701.6	690.45	11.15	696.36	5.24	6.0291
466	Methyl 2–methylbutyrate	720.5	707.73	12.77	713.60	6.90	6.1687
467	Ethyl butyrate	739.2	737.84	1.36	743.65	–4.45	6.4121
468	Propyl propionate	746.1	731.58	14.52	737.40	8.70	6.3615
469	Butyl acetate	751.7	742.64	9.06	748.44	3.26	6.4509
470	Methyl pentanoate	764.4	752.99	11.41	758.78	5.62	6.5346
471	Pentyl formate	766.6	755.83	10.77	761.61	4.99	6.5575
472	Isopropyl butyrate	779.3	772.36	6.94	778.10	1.20	6.6911
473	Ethyl 2–methylbutyrate	792.3	783.12	9.18	788.84	3.46	6.7781
474	Ethyl 3–methylbutyrate	795.2	792.78	2.42	798.49	–3.29	6.8562
475	Propyl isobutyrate	796	785.59	10.41	791.31	4.69	6.7981
476	3–Methylbutyl acetate	816.5	811.80	4.70	817.47	–0.97	7.0099
477	Propyl butyrate	837.5	832.97	4.53	838.59	–1.09	7.1810
478	Isopropyl isopentanoate	837.9	836.05	1.85	841.67	–3.77	7.2059
479	Ethyl pentanoate	840.2	828.40	11.80	834.04	6.16	7.1441
480	Butyl propionate	846.8	829.16	17.64	834.79	12.01	7.1502
481	Pentyl acetate	852.1	842.67	9.43	848.27	3.83	7.2594
482	Methylpropyl methylpropionate	855	843.28	11.72	848.89	6.11	7.2644
483	Methyl hexanoate	864.8	853.02	11.78	858.61	6.19	7.3431
484	Hexyl formate	868.9	855.84	13.06	861.42	7.48	7.3659
485	Isopropyl pentanoate	878.7	871.65	7.05	877.20	1.50	7.4937
486	Propyl 2–methylbutyrate	887.9	878.26	9.64	883.80	4.10	7.5471
487	Butyl methylpropionate	893.8	883.17	10.63	888.70	5.10	7.5868
488	Isobutyl butyrate	898.6	882.80	15.80	888.33	10.27	7.5838
489	Propyl isopentanoate	902.5	887.92	14.58	893.44	9.06	7.6252
490	Ethyl 4–methylpentanoate	905.8	899.24	6.56	904.74	1.06	7.7167
491	Isopentyl propionate	912.9	898.30	14.60	903.80	9.10	7.7091
492	Butyl butyrate	936.3	930.55	5.75	935.99	0.31	7.9698
493	Propyl pentanoate	937.1	923.53	13.57	928.98	8.12	7.9130
494	Ethyl hexanoate	938.9	928.43	10.47	933.87	5.03	7.9526
495	Methylpropyl 2–methylbutyrate	945.6	935.95	9.65	941.37	4.23	8.0134

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
496	Pentyl propionate	946.1	929.18	16.92	934.62	11.48	7.9587
497	Hexyl acetate	950.3	942.69	7.61	948.10	2.20	8.0679
498	3–Methylbutyl methylpropionate	951.6	952.33	–0.73	957.72	–6.12	8.1458
499	Methyl heptanoate	964	953.05	10.95	958.44	5.56	8.1516
500	Heptyl formate	971.3	955.87	15.43	961.25	10.05	8.1744
501	Isopropyl hexanoate	976.1	971.68	4.42	977.03	–0.93	8.3022
502	Butyl 2–methylbutyrate	983.5	975.85	7.65	981.20	2.30	8.3359
503	Pentyl methylpropionate	989.4	983.20	6.20	988.53	0.87	8.3953
504	Isobutyl pentanoate	994.9	982.10	12.80	987.43	7.47	8.3864
505	Isopentyl butyrate	999.9	990.97	8.93	996.28	3.62	8.4581
506	Propyl hexanoate	1031.5	1023.55	7.95	1028.81	2.69	8.7215
507	Pentyl butyrate	1034.2	1030.58	3.62	1035.82	–1.62	8.7783
508	Butyl pentanoate	1034.6	1021.12	13.48	1026.38	8.22	8.7018
509	Ethyl heptanoate	1036.8	1028.44	8.36	1033.68	3.12	8.7610
510	3–Methylbutyl 2–methylbutyrate	1041.2	1044.99	–3.79	1050.21	–9.01	8.8948
511	Hexyl propionate	1044.4	1029.21	15.19	1034.45	9.95	8.7672
512	Heptyl acetate	1053.4	1042.72	10.68	1047.93	5.47	8.8764
513	Methyl octanoate	1064	1053.07	10.93	1058.27	5.73	8.9601
514	Octyl formate	1073.6	1055.89	17.71	1061.08	12.52	8.9829
515	Isopropyl heptanoate	1074.8	1071.71	3.09	1076.86	–2.06	9.1107
516	Pentyl 2–methylbutyrate	1080.1	1075.87	4.23	1081.03	–0.93	9.1444
517	Hexyl methylpropionate	1089	1083.22	5.78	1088.36	0.64	9.2038
518	Isobutyl hexanoate	1090.9	1082.12	8.78	1087.26	3.64	9.1949
519	Isopentyl pentanoate	1093.1	1090.26	2.84	1095.39	–2.29	9.2607
520	Butyl hexanoate	1127	1121.14	5.86	1126.21	0.79	9.5103
521	Propyl heptanoate	1127.2	1123.58	3.62	1128.64	–1.44	9.5300
522	Pentyl pentanoate	1131.7	1121.14	10.56	1126.21	5.49	9.5103
523	Hexyl butyrate	1132.9	1130.61	2.29	1135.65	–2.75	9.5868
524	Ethyl octanoate	1136.6	1128.47	8.13	1133.52	3.08	9.5695
525	Heptyl propionate	1145	1129.22	15.78	1134.27	10.73	9.5756
526	Octyl acetate	1154.6	1142.74	11.86	1147.76	6.84	9.6849
527	Methyl nonanoate	1163.8	1153.10	10.70	1158.10	5.70	9.7686
528	Isopropyl octanoate	1173.2	1171.73	1.47	1176.69	–3.49	9.9192
529	Hexyl 2–methylbutyrate	1177.7	1175.90	1.80	1180.86	–3.16	9.9529
530	Isopentyl hexanoate	1184.8	1190.29	–5.49	1195.22	–10.42	10.0692
531	Isobutyl heptanoate	1186.9	1182.14	4.76	1187.08	–0.18	10.0033
532	Methyl decanoate	1263.6	1253.13	10.47	1257.93	5.67	10.5771
533	Isobutyl octanoate	1283	1282.16	0.84	1286.91	–3.91	10.8118
534	Ethyl decanoate	1332	1328.52	3.48	1333.18	–1.18	11.1865
<b>Ketones and aldehydes</b>							
535	Propanone	469.7	461.19	8.51	467.55	2.15	4.1760
536	2–Butanone	574.7	561.22	13.48	567.38	7.32	4.9845
537	3–Methyl–2–butanone	639.9	624.50	15.40	630.54	9.36	5.4960
538	2–Pentanone	665.4	661.24	4.16	667.21	–1.81	5.7930
539	3–Pentanone	675.4	657.51	17.89	663.48	11.92	5.7628
540	2,2–Dimethyl–3–butanone	691.8	674.12	17.68	680.06	11.74	5.8971
541	3,3–Dimethyl–2–butanone	692.1	677.86	14.24	683.79	8.31	5.9273
542	4–Methyl–2–pentanone	720.1	714.05	6.05	719.91	0.19	6.2198
543	2–Methyl–3–pentanone	731.9	720.79	11.11	726.64	5.26	6.2743
544	4–Methyl–3–pentanone	731.9	720.79	11.11	726.64	5.26	6.2743
545	3–Methyl–2–pentanone	733.5	724.53	8.97	730.37	3.13	6.3045
546	3–Hexanone	764.1	757.52	6.58	763.30	0.80	6.5712
547	2–Hexanone	767	761.26	5.74	767.03	–0.03	6.6014
548	5–Methyl–3–hexanone	815.6	812.21	3.39	817.87	–2.27	7.0132
549	2–Methyl–3–hexanone	818.9	820.82	–1.92	826.47	–7.57	7.0828
550	5–Methyl–2–hexanone	835.4	827.98	7.42	833.62	1.78	7.1407

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
551	4-Heptanone	851.8	840.53	11.27	846.14	5.66	7.2421
552	3-Heptanone	864.9	857.55	7.35	863.13	1.77	7.3797
553	2-Heptanone	867.5	861.29	6.21	866.86	0.64	7.4099
554	2-Methyl-3-heptanone	917.5	920.83	-3.33	926.29	-8.79	7.8912
555	5-Methyl-3-heptanone	921.7	910.35	11.35	915.83	5.87	7.8065
556	2,2-Dimethyl-3-heptanone	963.4	974.19	-10.79	979.54	-16.14	8.3225
557	3-Octanone	964.8	959.44	5.36	964.82	-0.02	8.2033
558	2-Octanone	967.5	961.31	6.19	966.69	0.81	8.2184
559	5-Nonanone	1051.4	1040.58	10.82	1045.80	5.60	8.8591
560	2-Nonanone	1068.7	1061.34	7.36	1066.52	2.18	9.0269
561	3-Methyl-2-nonanone	1122	1124.62	-2.62	1129.68	-7.68	9.5384
562	3-Decanone	1164.8	1157.63	7.17	1162.62	2.18	9.8052
563	2-Decanone	1168.9	1161.36	7.54	1166.35	2.55	9.8354
564	6-Undecanone	1249.2	1240.63	8.57	1245.46	3.74	10.4761
565	2- Undecanone	1269.2	1261.39	7.81	1266.18	3.02	10.6439
566	2-Dodecanone	1369.5	1361.42	8.08	1366.01	3.49	11.4524
567	7-Tridecanone	1447.6	1440.67	6.93	1445.11	2.49	12.0930
568	2-Tridecanone	1469.7	1461.43	8.27	1465.83	3.87	12.2608
569	2-Tetradecanone	1570	1561.46	8.54	1565.66	4.34	13.0693
570	8-Pentadecanone	1646.7	1640.72	5.98	1644.77	1.93	13.7100
571	2-Pentadecanone	1670.2	1661.48	8.72	1665.49	4.71	13.8778
572	2-Hexadecanone	1770.5	1761.51	8.99	1765.32	5.18	14.6863
573	9-Heptadecanone	1845.9	1840.78	5.12	1844.43	1.47	15.3270
574	2-Heptadecanone	1870.8	1861.54	9.26	1865.15	5.65	15.4948
575	2-Octadecanone	1971	1961.56	9.44	1964.98	6.02	16.3033
576	10-Nonadecanone	2044.9	2040.83	4.07	2044.09	0.81	16.9440
577	2-Nonadecanone	2071.3	2061.58	9.72	2064.79	6.51	17.1117
578	Isobutanal	540.3	530.35	9.95	536.57	3.73	4.7350
579	Butanal	571.1	567.10	4.00	573.24	-2.14	5.0320
580	Isovaleraldehyde	635	619.90	15.10	625.94	9.06	5.4588
581	2-Methyl butanal	645.3	630.38	14.92	636.40	8.90	5.5435
582	Valeraldehyde	674.4	667.11	7.29	673.06	1.34	5.8404
583	3,3-Dimethyl butanal	689.1	683.74	5.36	689.66	-0.56	5.9748
584	2-Ethyl butanal	742.1	730.39	11.71	736.22	5.88	6.3519
585	Hexanal	776.5	767.14	9.36	772.89	3.61	6.6489
586	Heptanal	877.2	867.16	10.04	872.72	4.48	7.4574
587	2-Ethyl hexanal	933.2	930.44	2.76	935.88	-2.68	7.9689
588	Octanal	977.8	967.19	10.61	972.55	5.25	8.2659
<b>Alcohols</b>							
589	1-Butanol	646.48	645.64	0.84	651.64	-5.16	5.6669
590	1-Pentanol	750.4	745.68	4.72	751.48	-1.08	6.4755
591	1-Hexanol	852.96	845.70	7.26	851.30	1.66	7.2839
592	1-Heptanol	955.05	945.72	9.33	951.13	3.92	8.0924
593	1-Octanol	1057.34	1045.75	11.59	1050.96	6.38	8.9009
594	1-Nonanol	1158.66	1145.78	12.88	1150.79	7.87	9.7094
595	1-Decanol	1256.01	1245.80	10.21	1250.62	5.39	10.5179
596	2-Butanol	582.51	576.03	6.48	582.16	0.35	5.1042
597	2-Pentanol	682.66	676.05	6.61	681.99	0.67	5.9127
598	2-Hexanol	782.18	776.08	6.10	781.82	0.36	6.7212
599	2-Heptanol	885.57	876.11	9.46	881.65	3.92	7.5297
600	2-Nonanol	1084.16	1076.16	8.00	1081.31	2.85	9.1467
601	3-Pentanol	684.21	674.21	10.00	680.15	4.06	5.8978
602	3-Hexanol	780.36	774.24	6.12	779.98	0.38	6.7063
603	3-Heptanol	880.52	874.26	6.26	879.81	0.71	7.5148
604	3-Octanol	981.75	974.29	7.46	979.64	2.11	8.3233
605	4-Heptanol	875.42	867.00	8.42	872.56	2.86	7.4561

**Table 1.** (Continued).

No	Compounds <sup>a</sup>	$RI_{exp}$	$RI_{calc}$ (Eq. 2)	$\Delta RI$ (Eq. 2)	$RI_{calc}$ (Eq. 3)	$\Delta RI$ (Eq.3)	$I_{ET}$
606	4-Octanol	975.5	967.01	8.49	972.38	3.12	8.2645
607	2-Methyl-1-butanol	722.58	715.76	6.82	721.61	0.97	6.2336
608	2-Methyl-1-pentanol	813.35	815.78	-2.43	821.44	-8.09	7.0421
609	2-Methyl-2-pentanol	717.57	708.89	8.68	714.76	2.81	6.1781
610	2-Methyl-2-hexanol	817.33	808.92	8.41	814.59	2.74	6.9866
611	2-Methyl-2-heptanol	916.43	908.93	7.50	914.41	2.02	7.7950
612	2-Methyl-3-pentanol	757.96	744.32	13.64	750.12	7.84	6.4645
613	2-Methyl-3-hexanol	852.71	844.35	8.36	849.95	2.76	7.2730
614	3-Methyl-1-butanol	719.03	708.93	10.10	714.80	4.23	6.1784
615	3-Methyl-1-pentanol	828.82	808.93	19.89	814.60	14.22	6.9867
616	3-Methyl-2-butanol	666.02	646.14	19.88	652.13	13.89	5.6709
617	3-Methyl-3-hexanol	826.62	818.90	7.72	824.55	2.07	7.0673
618	4-Methyl-1-pentanol	821.19	832.37	-11.18	838.00	-16.81	7.1762
619	4-Methyl-2-pentanol	744.14	739.34	4.80	745.15	-1.01	6.4242
620	5-Methyl-3-hexanol	838.15	837.52	0.63	843.14	-4.99	7.2178
621	5-Methyl-3-heptanol	943.58	937.55	6.03	942.97	0.61	8.0263
622	2-Ethyl-1-butanol	825.94	815.78	10.16	821.44	4.50	7.0421
623	2-Ethyl-1-hexanol	1012.64	1015.83	-3.19	1021.10	-8.46	8.6591
624	4-Ethyl-3-hexanol	953.26	944.37	8.89	949.78	3.48	8.0815
625	2,2-Dimethyl-1-propanol	657.34	662.27	-4.93	668.23	-10.89	5.8013
626	2,2-Dimethyl-1-pentanol	867.57	862.31	5.26	867.88	-0.31	7.4182
627	2,2-Dimethyl-3-pentanol	805.63	790.85	14.78	796.56	9.07	6.8406
628	2,2-Dimethyl-3-hexanol	900.39	890.88	9.51	896.39	4.00	7.6491
629	2,4-Dimethyl-2-pentanol	775.91	772.16	3.75	777.90	-1.99	6.6895
630	2,4-Dimethyl-3-pentanol	821.18	814.42	6.76	820.08	1.10	7.0311
631	3,3-Dimethyl-1-butanol	778.77	771.69	7.08	777.44	1.33	6.6857
632	3,5-Dimethyl-3-hexanol	883.13	882.18	0.95	887.71	-4.58	7.5788

\* Branched alkanes considered as outliers.

<sup>a</sup> Alkanes notation = *mAnC*: *m* indicates the position of alkyl group(s) (Me = methyl, Et = ethyl, Isoprop = isopropyl) on the carbon backbone; *n* indicates the number of carbon atoms in the backbone.