調査報告

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メチルシリコンキャピラリーカラムによる環境 化学物質のための GC・保持指標 (PTRI)

奥村 為 男

大阪府公害監視センター

(〒537 大阪市東成区中道 1-3-62)

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Retention Indices of Environmental Chemicals on Methyl Silicone Capillary Column

Tameo Okumura

Environmental Pollution Control Center, Osaka Prefecture

(3-62, 1-Chome, Nakamichi, Higashinari-ku, Osaka 537)

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Summary

In this paper, the author has presented the Temperature Programed Retention Indices (PTRI) of 1,340 environmental chemicals on methyl silicone capillary column. PTRI is defined as follows :

$$\text{PTRI} = 100 \times Z + 100 \times (T_x - T_z) / (T_{z+1} - T_z)$$

Z : Carbon number of n-alkane eluted just before the target compound.

T_x , T_z and T_{z+1} : Retention times of the target compound (x), n-alkane of z and z + 1 carbon number, respectively.

The author expects these data are applied to identifications of environmental chemicals using GC/MS.

1. はじめに

化学物質による環境汚染問題は重要な課題であり、多くの調査研究が行われている。なかでも GC/MS・コンピュータシステムによる検索同定は、これらによる汚染をいち早く発見する手段として必要不可欠なものになっている。通常、試料中の未知物質を検索同定する場合、ガスクロマトグラフィー・質量分析器 (GC/MS) により得られたマススペクトルを、コンピュータにより、リファレンスのマススペクトルと照合することによって行われる。検索結果の評価としては、標準品と比較してマススペクトルが一致すること及び GC の保持時間が一致することが最高のレベルである。マススペクトルの一致については、極めて類似したマススペクトルが数多く存

在すること及びキャピラリーカラムによる高度の分離にもかわらず、実試料では単一物質のスペクトルが得にくい等の問題が存在する。このような場合に、GC の保持指標が検索同定に対して有力な情報となる。特に、鎖状化合物の同族体では、そのマススペクトルが酷似しており、マススペクトルのみからの同定は困難である。一例として、n-アルキルアルデヒドのマススペクトルを Fig. 1 に示した。フラグメントパターンは酷似していることから、このような物質を検索すると、一連のアルキルアルデヒドが検索されてくる。更に、分子イオンは見られず、水の脱離による M-18 がかるうじて認められるが、実試料ではこのフラグメントイオンからアルデヒドの炭素数を特定することは不可能に近い。このような場合、化合物を特定出来るのは GC の保持時間情報のみと

Fig. 1. Mass spectra of n-alkyl aldehyde

なる。また、同族化合物では、保持指標 (PTRI ; temperature programed retention index) とその化合物の炭素数の間に直線関係が存在することから、目的の標準品が入手出来なくとも、入手可能な同族体の情報から化合物の特定が可能となる。

保持指標に関しては多くの報告が見られるが、環境試料中の有機物の検索同定と言う観点からは、その利用について問題点も多い。問題点を列挙すると、(1)分子構造から保持指標を推定する報告が多く見られるが、同定への利用と言う点からは至便性に欠ける。(2)同族化合物間で、置換基の保持指標への影響を検討したものも多く見られるが、これらのものは環境汚染物質の検索同定と言う点からは、その化合物の種類に難点がある。(3)相対保持時間を表す基準化合物が一つの場合は、基準化合物から保持時間が大きく離れると、測定条件等により差が大きくなる。また、基準化合物が報告によりまちまちであるのも不便であり、一連のn-アルカンに統一することが望ましいと思われる。(4)充填式カラムが多用されていた時代の報告には、多種類の液相について比較検討したものが多く。しかし、最近では検索同定に関しては殆どキャピラリーカラムが使用されている。しかもその液相は無極性であるメチルシリコン系が圧倒的に多い。これは、このカラムの使用限界温度が高いため適用範囲が広いこと及び無極性であってもキャピラリーカラムでは殆どの物質に対して良好なピークを与えることによるものと思われる。従って、検索同定という点においてはメチルシリコン系のキャピラリーカラムが最適であり、このカラムでのPTRIデータを蓄積することが、化学物質による環境汚染の未然防止に寄与するであろう。

今回、著者は河川水中の有機物をキャピラリー・GC

/MSにより検索同定する機会があり、検索結果をより確実にするため1340種の物質についてPTRIを測定した。本PTRIデータはGC/MSによる環境汚染物質の検索同定に有用と思われるので報告する。

なお、PTRIは次式で定義される。

$$\text{PTRI} = 100 \times z + 100 \times (T_x - T_z) / (T_{z+1} - T_z)$$

ただし、z：溶質xの直前に溶出するn-アルカンの炭素数。T_x, T_z, T_{z+1}：それぞれ溶質x, n-アルカンC_z, C_{z+1}の保持容量または保持時間。

2. 測定方法

2.1 試薬

市販品として入手できるものは、主として和光純薬(株)、東京化成(株)及びPolyScience社から入手した。農薬の標準品は和光純薬(株)及びNANOGENから入手した。入手困難な標準物質については合成した。以下に合成した化合物と合成法の概略について記す。

塩素化多環芳香族炭化水素：各多環芳香族炭化水素の酢酸溶液に塩素を通じて合成した。生成物は、逆相薄層クロマトグラフィー(ポリアミドTLC/メタノール展開)で分離し、結晶として単離した。但し、塩素の置換位置については特定していない。

塩素化スチレン：よう素の存在下、スチレンに塩素を通じて得られた生成物を、1N-水酸化カリウムエタノール溶液で処理した。この生成物は、ベンゼン環及び側鎖に塩素が置換されているが、その位置については特定していない。

塩素化ベンゾフラン：塩素化スチレンと同様塩素の付加及び置換反応後、脱離反応によって合成した。塩素の導入位置については特定していない。

アニソール同族体：それぞれ相当するフェノール類をジメチル硫酸で常法によりメチル化した。

臭素化ジフェニルエーテル：よう素存在化、ジフェニルエーテルに臭素を作用させて合成した。このものは、各臭素置換体の主成分を逆相薄層クロマトグラフィー（塩素化多環芳香族炭化水素と同じ）で単離した。

n-アルキルアルデヒド：炭素数8,9,10,11及び14のものは市販品を入手出来たが、他のものは河川水をオゾン処理した試料から得た。これらは、そのマスペクトル及び炭素数とPTRIの直線性から容易に確定出来た。

多環系炭化水素の酸化生成物（ケトン及びキノン）：多環系炭化水素を酢酸中無水クロム酸で酸化して合成した。これらのものは単離せず、マスペクトルを確認して保持時間を求めた。

カルボン酸エステル：これらのものは、単一物を合成するのではなく混合物として合成した。即ち、種々のカルボン酸の混合物に塩酸存在下で過剰の単一アルコールでエステル化、あるいは、その逆に種々のアルコール混合物を単一のカルボン酸と縮合反応させて合成した。これらのものは単離せずGC/MSによりマスペクトルを確認してその保持時間を求めた。

N-メチル及びN,N-ジメチルアミン：1級アミンの混合物をよう化メチルで常法によりN-メチル化して合成した。それぞれのアミンは単離せず、GC/MSによりマスペクトルを確認して保持時間を求めた。

N-エチル及びN,N-ジエチルアミン：よう化エチルで、上記と同様にして合成した。

多価アルコールのエステル：それぞれの多価アルコールとカルボン酸の塩酸酸性下での縮合反応により合成した。

多価アルコールのメチル及びエチルエーテル：それぞれの多価アルコールを金属ナトリウムと反応させ、アルコールとした後、よう化メチルまたはよう化エチルとの反応により合成した。

農薬のオキシソニン体及びスルホキシンド、スルホン体：農薬

の標準品100 mgをメタノール50 mlに溶解し、室温で塩素飽和水中により酸化して合成した。

2.2 測定条件

測定条件をTable 1に示した。また、PTRI測定に先だってn-アルカン（C₁₀～C₂₈）の混合ヘキサン溶液（100 ppm）1 µlをGC/MSに注入し、基準となる保持時間を測定した。従って、今回PTRI測定対象としたのは、PTRIが1000～2800の物質である。

Table 1. Operational conditions of GC/MS

Gas chromatograph :	HP 5790 (Hewlett-Packard)
Column :	Ultra-1 ; Crosslinked methyl silicone (25 m × 0.32 mm I.D. 0.25 micron film)
Temperature :	Column ; 80℃ , programmed to 260℃ at 3℃ min ⁻¹ Injection port ; 250℃ Interface ; 250℃
Carrier gas :	He (2 ml min ⁻¹ 7.5 psi)
Injection mode :	Splitless (purge off ; 1 min)
Mass spectrometer :	JEOL JMS-DX 303 / JMA-DA 5000 Ionization energy ; 70eV Ionization current ; 300 µA Accelerate voltage ; 3 kv Ion multiplier voltage ; 1.0-1.3 kv Scan range ; m/z 30-500 Scan rate ; 1 scan sec ⁻¹

3. 測定結果及び考察

得られた結果をTable 2に示した。なおPTRIが1000未満のものは<1000で表示した。

ここでは、できるだけ広範な化合物を対象とした検索同定のため、異性体の中で置換基の位置を特定していない物質のPTRIデータも集積した。環境中の化学物質をGC/MSで検索する場合、どの程度まで化合物を特定するかと言う問題がある。例えば、鎖状炭化水素の場合、環境試料の検索同定においては、通常n-アルカンの同定は容易であるが、側鎖炭化水素の場合は特定が困難であり、例えばC₁₂（側鎖）或はC₁₂（branched）といった表示に留まっている場合が多い。また、アルキルベンゼン同族体のような場合でも完全な特定は困難であり、C₃-ベンゼンという表示に留まっている例が多い。アルキル化多環芳香族炭化水素も、環境中には広く存在するが、同様に特定は困難である。検索同定もこの程度の同定で満足出来る場合もあり、一方、ダイオキシンのように、完全な特定が要求される場合もある。このような場合においては、ある特定の範ちゅうで詳細に検討されたデータを参考にする必要がある。

Table 2. PTRI of chemicals on methyl silicone capillary column

	compound	formula	M.W.	PTRI
1	acenaphthene	C12H10	154	1437
2	acenaphthenone	C12H8O	168	1589
3	acenaphthylene	C12H8	152	1403
4	acephate	C4H10N03PS	183	1373
5	acetophenone	C8H8O	120	1033
6	acridine	C13H9N	179	1731
7	allyl arachidate	C23H44O2	352	2450
8	allyl behenoate	C25H48O2	380	2654
9	allyl caprate	C13H24O2	212	1456
10	allyl caproate	C9H16O2	156	1057
11	allyl caprylate	C11H20O2	184	1257
12	allyl n-heneicosanoate	C24H46O2	366	2549
13	allyl n-heptadecanoate	C20H38O2	310	2152
14	allyl n-heptanoate	C10H18O2	170	1156
15	allyl myristate	C17H32O2	268	1852
16	allyl n-nonadecanoate	C22H42O2	338	2351
17	allyl n-nonanoate	C12H22O2	198	1355
18	allyl palmitate	C19H36O2	296	2053
19	allyl n-pentadecanoate	C18H34O2	282	1953
20	allyl n-pentanoate	C8H14O2	142	< 1000
21	allyl stearate	C21H40O2	324	2251
22	allyl n-tricosanoate	C26H50O2	394	2744
23	allyl n-tridecanoate	C16H30O2	254	1755
24	allyl n-undecanoate	C14H26O2	226	1555
25	2-aminodiphenyl	C12H11N	169	1534
26	4-aminodiphenyl	C12H11N	169	1683
27	3-aminopyridine	C5H6N2	94	1051
28	amyl benzoate	C12H16O2	192	1440
29	anilazine	C9H5Cl3N4	274	1978
30	aniline	C6H7N	93	< 1000
31	p-anisaldehyde	C8H8O2	136	1208
32	o-anisidine	C7H9NO	123	1136
33	p-anisidine	C7H9NO	123	1174
34	anisole	C7H8O	108	< 1000
35	anthracene	C14H10	178	1725
36	anthraquinone	C14H8O2	208	1880
37	bentazone	C10H12N2O3S	240	1926
38	benz(a)anthraquinone	C18H10O2	258	2479
39	benzaldehyde	C7H6O	106	< 1000
40	benzo(a)anthracene	C18H12	228	2359
41	1,2-benzofluorene	C17H12	216	2127
42	2,3-benzofluorene	C17H12	216	2146
43	1,2-benzofluorenone	C17H10O	230	2252
44	benzofuran	C8H6O	118	< 1000
45	benzoic acid	C7H6O2	122	1149
46	benzophenone	C13H10O	182	1572
47	benzothiazole	C7H5NS	135	1184
48	benzothiophene	C8H6S	134	1159
49	benzyl acetate	C9H10O2	150	1133
50	benzyl n-butyl phthalate	C19H20O4	312	2271
51	benzyl butyrate	C11H14O2	178	1311
52	benzyl caprate	C17H26O2	262	1911
53	benzyl caproate	C13H18O2	206	1506
54	benzyl caprylate	C15H22O2	234	1707
55	benzyl n-heptadecanoate	C24H40O2	360	2634
56	benzyl n-heptanoate	C14H20O2	220	1606
57	benzyl myristate	C21H34O2	318	2321
58	benzyl n-nonanoate	C16H24O2	248	1808
59	benzyl palmitate	C23H38O2	346	2527
60	benzyl n-pentadecanoate	C22H36O2	332	2424
61	benzyl n-pentanoate	C12H16O2	192	1408
62	benzyl propionate	C10H12O2	164	1225
63	benzyl stearate	C25H42O2	374	2727
64	benzyl n-tridecanoate	C20H32O2	304	2218
65	benzyl n-undecanoate	C18H28O2	276	2013
66	benzylamine	C7H9N	107	< 1000
67	α -bromoacetophenone	C8H7BrO	198	1304
68	p-bromoacetophenone	C8H7BrO	198	1278
69	m-bromoaniline	C6H6BrN	171	1242
70	o-bromoaniline	C6H6BrN	171	1172

Table 2. (Continued)

compound	formula	M.W.	PTR
71 p-bromoaniline	C6H6BrN	171	1245
72 m-bromoanisole	C7H7BrO	186	1149
73 o-bromoanisole	C7H7BrO	186	1163
74 p-bromoanisole	C7H7BrO	186	1160
75 p-bromobenzophenone	C13H9BrO	260	1841
76 4-bromodiphenylether	C12H9BrO	248	1641
77 o-bromonitrobenzene	C6H4BrNO2	201	1276
78 m-bromophenol	C6H5BrO	172	1255
79 o-bromophenol	C6H5BrO	172	1039
80 p-bromophenol	C6H5BrO	172	1252
81 n-butyl arachidate	C24H48O2	368	2570
82 n-butyl behenoate	C26H52O2	396	2769
83 n-butyl benzoate	C11H14O2	178	1338
84 sec.-butyl benzoate	C11H14O2	178	1297
85 n-butyl p-tert.-butylbenzoate	C15H22O2	234	1689
86 n-butyl caprate	C14H28O2	228	1568
87 n-butyl 3,4-dimethylbenzoate	C13H18O2	206	1587
88 n-butyl n-heneicosanoate	C25H50O2	382	2676
89 n-butyl n-heptadecanoate	C21H42O2	326	2269
90 butyl methyl phthalate	C13H16O4	236	1663
91 n-butyl myristate	C18H36O2	284	1967
92 n-butyl n-nonadecanoate	C23H46O2	354	2469
93 n-butyl n-nonanoate	C13H26O2	214	1467
94 n-butyl palmitate	C20H40O2	312	2169
95 n-butyl n-pentadecanoate	C19H38O2	298	2068
96 n-butyl 2-phenoxybenzoate	C17H18O3	270	1941
97 n-butyl 2-phenoxybutyrate	C14H20O3	236	1565
98 n-butyl 2-phenoxypropionate	C13H18O3	222	1492
99 butyl phenyl ether	C10H14O	150	1164
100 n-butyl salicylate	C11H14O3	194	1436
101 n-butyl stearate	C22H44O2	340	2369
102 n-butyl m-toluate	C12H16O2	192	1444
103 n-butyl n-tridecanoate	C17H34O2	270	1868
104 n-butyl n-undecanoate	C15H30O2	242	1668
105 m-tert.-butylanisole	C11H16O	164	1206
106 o-sec.-butylanisole	C11H16O	164	1193
107 o-tert.-butylanisole	C11H16O	164	1170
108 p-sec.-butylanisole	C11H16O	164	1236
109 p-tert.-butylanisole	C11H16O	164	1218
110 butylated hydroxyanisole	C11H16O2	180	1456
111 butylated hydroxytoluene	C15H24O	220	1488
112 p-tert.-butylbenzoic acid	C11H14O2	178	1472
113 m-tert.-butylphenol	C10H14O	150	1267
114 o-sec.-butylphenol	C10H14O	150	1252
115 o-tert.-butylphenol	C10H14O	150	1247
116 p-sec.-butylphenol	C10H14O	150	1285
117 p-tert.-butylphenol	C10H14O	150	1265
118 n-capric acid	C10H20O2	172	1389
119 caproamide	C6H13NO	115	1135
120 carbazole	C12H9N	167	1766
121 n-cetylamine	C16H29N	235	1843
122 chloro 1,2-benzofluorene	C17H11Cl	250	2346
123 chloro 2,3-benzofluorene	C17H11Cl	250	2374
124 4-chloro-3-methylanisole	C8H9ClO	156	1180
125 4-chloro-3-methylphenol	C7H7ClO	142	1258
126 chloroacacenaphthene	C12H9Cl	188	1646
127 m-chloroaniline	C6H6ClN	127	1155
128 o-chloroaniline	C6H6ClN	127	1094
129 p-chloroaniline	C6H6ClN	127	1157
130 m-chloroanisole	C7H7ClO	142	1068
131 o-chloroanisole	C7H7ClO	142	1089
132 p-chloroanisole	C7H7ClO	142	1077
133 chloroanthracene	C14H9Cl	212	1930
134 chlorobenzo(a)anthracene	C18H11Cl	262	2584
135 chlorochrysene	C18H11Cl	262	2570
136 chlorodiphenylether	C12H9ClO	204	1526
137 chlorodiphenylether	C12H9ClO	204	1548
138 chlorofluoranthene	C16H9Cl	236	2187
139 chlorofluorene	C13H9Cl	200	1734
140 chloronaphthalene	C10H7Cl	162	1334

	compound	formula	M.W.	PTI
141	chloronaphthalene	C10H7Cl	162	1339
142	o-chloronitrobenzene	C6H4ClNO2	157	1195
143	p-chloronitrobenzene	C6H4ClNO2	157	1189
144	chlorophenanthrene	C14H9Cl	212	1915
145	m-chlorophenol	C6H5ClO	128	1170
146	o-chlorophenol	C6H5ClO	128	< 1000
147	p-chlorophenol	C6H5ClO	128	1168
148	chloropyrene	C16H9Cl	236	2241
149	chlorostyrene	C8H7Cl	138	1043
150	chlorotriphenylene	C18H11Cl	262	2556
151	chlorpyrifos oxon	C9H11Cl13N04P	334	1916
152	chrysene	C18H12	228	2361
153	cinnamaldehyde	C9H8O	132	1223
154	clodrin	C14H19O6P	314	2032
155	citronellal	C10H18O	154	1128
156	p-cresidine	C8H11NO	137	1234
157	m-cresol	C7H8O	108	1044
158	o-cresol	C7H8O	108	1024
159	p-cresol	C7H8O	108	1044
160	15-crown-5	C10H20O5	220	1554
161	cyclohexyl acetate	C8H14O2	142	1017
162	cyclohexyl butyrate	C10H18O2	170	1202
163	cyclohexyl caprate	C16H30O2	254	1805
164	cyclohexyl caproate	C12H22O2	198	1398
165	cyclohexyl caprylate	C14H26O2	226	1600
166	cyclohexyl n-heptadecanoate	C23H44O2	352	2523
167	cyclohexyl n-heptanoate	C13H24O2	212	1499
168	cyclohexyl myristate	C20H38O2	310	2214
169	cyclohexyl n-nonadecanoate	C25H48O2	380	2722
170	cyclohexyl n-nonanoate	C15H28O2	240	1702
171	cyclohexyl palmitate	C22H42O2	338	2420
172	cyclohexyl n-pentadecanoate	C21H40O2	324	2318
173	cyclohexyl n-pentanoate	C11H20O2	184	1299
174	cyclohexyl propionate	C9H16O2	156	1111
175	cyclohexyl stearate	C24H46O2	366	2628
176	cyclohexyl n-tridecanoate	C19H36O2	296	2113
177	cyclohexyl n-undecanoate	C17H32O2	268	1906
178	2,4-D methyl ester	C9H8Cl2O3	234	1581
179	2,4-DB methyl ester	C11H12Cl2O3	262	1794
180	2,4-DB	C10H10Cl2O3	248	1869
181	n-decanal	C10H20O	156	1186
182	n-decanamide	C10H21NO	171	1521
183	1-decanol	C10H22O	158	1254
184	2-decanone	C10H20O	156	1169
185	1-decene	C10H20	140	< 1000
186	n-decyl acetate	C12H24O2	200	1391
187	n-decyl butyrate	C14H28O2	228	1573
188	n-decyl caproate	C16H32O2	256	1765
189	n-decyl caprylate	C18H36O2	284	1959
190	n-decyl formate	C11H22O2	186	1310
191	n-decyl laurate	C22H44O2	340	2356
192	n-decyl myristate	C24H48O2	368	2555
193	n-decyl palmitate	C26H52O2	396	2758
194	n-decyl propionate	C13H26O2	214	1486
195	n-decylamine	C10H23N	157	1232
196	delnav	C12H26O6P2S4	456	2642
197	di-n-butyl adipate	C14H26O4	258	1732
198	di-n-butyl fumarate	C12H20O4	228	1556
199	di-n-butyl phthalate	C16H22O4	278	1909
200	di-n-butylamine	C8H19N	129	< 1000
201	di-n-decylamine	C20H43N	297	2142
202	di(1,3-dimethylbutyl) adipate	C18H34O4	314	1864
203	di(1,3-dimethylbutyl) azelate	C21H40O4	356	2163
204	di(1,3-dimethylbutyl) glutarate	C17H32O4	300	1756
205	di(1,3-dimethylbutyl) malonate	C15H28O4	272	1544
206	di(1,3-dimethylbutyl) oxalate	C14H26O4	258	1454
207	di(1,3-dimethylbutyl) pimelate	C19H36O4	328	1962
208	di(1,3-dimethylbutyl) suberate	C20H38O4	342	2062
209	di(1,3-dimethylbutyl) succinate	C16H30O4	286	1659
210	di(2-ethylbutyl) adipate	C18H34O4	314	2033

	compound	formula	M.W.	PTRI
211	di(2-ethylbutyl) azelate	C21H40O4	356	2335
212	di(2-ethylbutyl) glutarate	C17H32O4	300	1925
213	di(2-ethylbutyl) malonate	C15H28O4	272	1698
214	di(2-ethylbutyl) oxalate	C14H26O4	258	1619
215	di(2-ethylbutyl) pimelate	C19H36O4	328	2132
216	di(2-ethylbutyl) suberate	C20H38O4	342	2235
217	di(2-ethylbutyl) succinate	C16H30O4	286	1826
218	di(2-ethylhexyl) adipate	C22H42O4	370	2361
219	di(2-ethylhexyl) azelate	C25H48O4	412	2669
220	di(2-ethylhexyl) glutarate	C21H40O4	356	2255
221	di(2-ethylhexyl) malonate	C19H36O4	328	2025
222	di(2-ethylhexyl) oxalate	C18H34O4	314	1956
223	di(2-ethylhexyl) phthalate	C24H38O4	390	2498
224	di(2-ethylhexyl) pimelate	C23H44O4	384	2460
225	di(2-ethylhexyl) suberate	C24H46O4	398	2563
226	di(2-ethylhexyl) succinate	C20H38O4	342	2157
227	di(2-ethylhexyl)amine	C16H35N	241	1579
228	di(1-ethylpentyl) adipate	C20H38O4	342	2113
229	di(1-ethylpentyl) azelate	C23H44O4	384	2413
230	di(1-ethylpentyl) glutarate	C19H36O4	328	2005
231	di(1-ethylpentyl) malonate	C17H32O4	300	1791
232	di(1-ethylpentyl) oxalate	C16H30O4	286	1696
233	di(1-ethylpentyl) pimelate	C21H40O4	356	2210
234	di(1-ethylpentyl) suberate	C22H42O4	370	2311
235	di(1-ethylpentyl) succinate	C18H34O4	314	1904
236	di(1-ethylpropyl) adipate	C16H30O4	286	1788
237	di(1-ethylpropyl) azelate	C19H36O4	328	2089
238	di(1-ethylpropyl) glutarate	C15H28O4	272	1680
239	di(1-ethylpropyl) malonate	C13H24O4	244	1467
240	di(1-ethylpropyl) oxalate	C12H22O4	230	1366
241	di(1-ethylpropyl) pimelate	C17H32O4	300	1887
242	di(1-ethylpropyl) suberate	C18H34O4	314	1987
243	di(1-ethylpropyl) succinate	C14H26O4	258	1578
244	di-n-hexyl ether	C12H26O	186	1265
245	di-n-hexylamine	C12H27N	185	1345
246	di(3-methoxybutyl) adipate	C16H30O6	318	2038
247	di(3-methoxybutyl) azelate	C19H36O6	360	2342
248	di(3-methoxybutyl) glutarate	C15H28O6	304	1931
249	di(3-methoxybutyl) malonate	C13H24O6	276	1699
250	di(3-methoxybutyl) oxalate	C12H22O6	262	1619
251	di(3-methoxybutyl) pimelate	C17H32O6	332	2139
252	di(3-methoxybutyl) sebacate	C20H38O6	374	2447
253	di(3-methoxybutyl) suberate	C18H34O6	346	2239
254	di(3-methoxybutyl) succinate	C14H26O6	290	1829
255	di(2-methoxyethyl) adipate	C12H22O6	262	1746
256	di(2-methoxyethyl) azelate	C15H28O6	304	2048
257	di(2-methoxyethyl) glutarate	C11H20O6	248	1644
258	di(2-methoxyethyl) malonate	C9H16O6	220	1430
259	di(2-methoxyethyl) oxalate	C8H14O6	206	1327
260	di(2-methoxyethyl) pimelate	C13H24O6	276	1847
261	di(2-methoxyethyl) sebacate	C16H30O6	318	2151
262	di(2-methoxyethyl) suberate	C14H26O6	290	1947
263	di(2-methoxyethyl) succinate	C10H18O6	234	1550
264	di(1-methyl-2-methoxyethyl) adipate	C14H26O6	290	1790
265	di(1-methyl-2-methoxyethyl) azelate	C17H32O6	332	2088
266	di(1-methyl-2-methoxyethyl) glutarate	C13H24O6	276	1684
267	di(1-methyl-2-methoxyethyl) malonate	C11H20O6	248	1477
268	di(1-methyl-2-methoxyethyl) oxalate	C10H18O6	234	1375
269	di(1-methyl-2-methoxyethyl) pimelate	C15H28O6	304	1888
270	di(1-methyl-2-methoxyethyl) sebacate	C18H34O6	346	2188
271	di(1-methyl-2-methoxyethyl) suberate	C16H30O6	318	1987
272	di(1-methyl-2-methoxyethyl) succinate	C12H22O6	262	1594
273	di(1-methylhexyl) adipate	C20H38O4	342	2138
274	di(1-methylhexyl) azelate	C23H44O4	384	2436
275	di(1-methylhexyl) glutarate	C19H36O4	328	2033
276	di(1-methylhexyl) malonate	C17H32O4	300	1822
277	di(1-methylhexyl) oxalate	C16H30O4	286	1737
278	di(1-methylhexyl) pimelate	C21H40O4	356	2237
279	di(1-methylhexyl) suberate	C22H42O4	370	2336
280	di(1-methylhexyl) succinate	C18H34O4	314	1938

compound	formula	M.W.	PTR
281 di-n-octyl fumalate	C20H36O4	340	2207
282 di-n-octyl maleate	C20H36O4	340	2262
283 di-n-octyl phthalate	C24H38O4	390	2686
284 diallyl adipate	C12H18O4	226	1510
285 diallyl azelate	C15H24O4	268	1808
286 diallyl glutarate	C11H16O4	212	1405
287 diallyl maleate	C10H12O4	196	1283
288 diallyl malonate	C9H12O4	184	1178
289 diallyl oxalate	C8H10O4	170	1050
290 diallyl phthalate	C14H14O4	246	1692
291 diallyl pimelate	C13H20O4	240	1610
292 diallyl suberate	C14H22O4	254	1708
293 diallyl succinate	C10H14O4	198	1310
294 diamyl adipate	C16H30O4	286	1921
295 diamyl azelate	C19H36O4	328	2221
296 diamyl glutarate	C15H28O4	272	1816
297 diamyl malonate	C13H24O4	244	1594
298 diamyl oxalate	C12H22O4	230	1518
299 diamyl pimelate	C17H32O4	300	2019
300 diamyl suberate	C18H34O4	314	2121
301 diamyl succinate	C14H26O4	258	1718
302 diamylamine (isomer mix.)	C10H23N	157	1061
303 diamylamine (isomer mix.)	C10H23N	157	1106
304 diamylamine (isomer mix.)	C10H23N	157	1145
305 diazinon oxon	C12H21N2O4P	288	1732
306 dibenzofuran	C12H8O	168	1470
307 dibenzothiophene	C12H8S	184	1689
308 dibenzylamine	C14H15N	197	1670
309 4,4'-dibromodiphenylether	C12H8Br2O	326	1936
310 dibutyl adipate	C14H26O4	258	1730
311 dibutyl azelate	C17H32O4	300	2029
312 dibutyl glutarate	C13H24O4	244	1625
313 dibutyl isophthalate	C16H22O4	278	1996
314 dibutyl malonate	C11H20O4	216	1405
315 dibutyl oxalate	C10H18O4	202	1325
316 dibutyl phthalate	C16H22O4	278	1903
317 dibutyl pimelate	C15H28O4	272	1830
318 dibutyl suberate	C16H30O4	286	1930
319 dibutyl succinate	C12H22O4	230	1526
320 dichlone	C10H4Cl2O2	226	1712
321 dichloro 1,2-benzofluorene	C17H10Cl2	284	2553
322 dichloro 1,2-benzofluorene	C17H10Cl2	284	2579
323 dichloro 2,3-benzofluorene	C17H10Cl2	284	2543
324 dichloro benzo(a)anthracene	C18H10Cl2	296	2779
325 2,4-dichloro-1-methoxynaphthalene	C11H8Cl2O	226	1670
326 2,4-dichloro-1-naphthol	C10H6Cl2O	212	1648
327 2,4-dichloroaniline	C6H5Cl2N	161	1284
328 2,5-dichloroaniline	C6H5Cl2N	161	1284
329 2,6-dichloroaniline	C6H5Cl2N	161	1203
330 3,5-dichloroaniline	C6H5Cl2N	161	1347
331 2,3-dichloroaniline	C6H5Cl2N	161	1302
332 3,4-dichloroaniline	C6H5Cl2N	161	1372
333 2,3-dichloroanisole	C7H6Cl2O	176	1280
334 2,4-dichloroanisole	C7H6Cl2O	176	1249
335 2,5-dichloroanisole	C7H6Cl2O	176	1241
336 2,6-dichloroanisole	C7H6Cl2O	176	1163
337 3,4-dichloroanisole	C7H6Cl2O	176	1253
338 3,5-dichloroanisole	C7H6Cl2O	176	1217
339 dichloroanthracene	C14H8Cl2	246	2120
340 m-dichlorobenzene	C6H4Cl2	146	< 1000
341 o-dichlorobenzene	C6H4Cl2	146	1013
342 p-dichlorobenzene	C6H4Cl2	146	< 1000
343 dichlorobenzofuran	C8H4Cl2O	186	1292
344 dichlorochrysene	C18H10Cl2	296	2782
345 dichlorodiphenyl	C12H8Cl2	222	1568
346 dichlorodiphenyl	C12H8Cl2	222	1637
347 dichlorodiphenyl	C12H8Cl2	222	1647
348 dichlorodiphenylether	C12H8Cl2O	238	1686
349 dichlorodiphenylether	C12H8Cl2O	238	1697
350 dichlorodiphenylether	C12H8Cl2O	238	1712

compound	formula	M.W.	PTR
351 dichlorodiphenylether	C12H8Cl2O	238	1740
352 dichlorofluoranthene	C16H8Cl2	270	2360
353 dichlorofluorene	C13H8Cl2	234	1946
354 dichloronaphthalene	C10H6Cl2	196	1497
355 dichloronaphthalene	C10H6Cl2	196	1507
356 dichloronaphthalene	C10H6Cl2	196	1511
357 dichloronaphthalene	C10H6Cl2	196	1519
358 dichloronaphthalene	C10H6Cl2	196	1528
359 dichloronaphthalene	C10H6Cl2	196	1581
360 2,3-dichlorophenol	C6H4Cl2O	162	1144
361 2,4-dichlorophenol	C6H4Cl2O	162	1138
362 2,5-dichlorophenol	C6H4Cl2O	162	1140
363 2,6-dichlorophenol	C6H4Cl2O	162	1168
364 3,4-dichlorophenol	C6H4Cl2O	162	1385
365 3,5-dichlorophenol	C6H4Cl2O	162	1370
366 dichloropyrene	C16H8Cl2	270	2451
367 dichloropyrene	C16H8Cl2	270	2457
368 dichlorostyrene	C8H6Cl2	172	1162
369 dichlorostyrene	C8H6Cl2	172	1174
370 dichlorostyrene	C8H6Cl2	172	1208
371 dichlorostyrene	C8H6Cl2	172	1210
372 dichlorostyrene	C8H6Cl2	172	1243
373 dichlorostyrene	C8H6Cl2	172	1256
374 dichlorotriphenylene	C18H10Cl2	296	2700
375 dichlorotriphenylene	C18H10Cl2	296	2724
376 dicyclohexyl adipate	C18H30O4	310	2234
377 dicyclohexyl azelate	C21H36O4	352	2554
378 dicyclohexyl glutarate	C17H28O4	296	2124
379 dicyclohexyl malonate	C15H24O4	268	1888
380 dicyclohexyl oxalate	C14H22O4	254	1805
381 dicyclohexyl phthalate	C20H26O4	330	2434
382 dicyclohexyl pimelate	C19H32O4	324	2338
383 dicyclohexyl suberate	C20H34O4	338	2446
384 dicyclohexyl succinate	C16H26O4	282	2019
385 dicyclohexylamine	C12H23N	181	1392
386 didodecylamine	C24H51N	353	2543
387 diethyl adipate	C10H18O4	202	1352
388 diethyl azelate	C13H24O4	244	1652
389 N,N-diethyl decylamine	C14H31N	213	1442
390 N,N-diethyl dodecylamine	C16H35N	241	1642
391 diethyl fumalate	C8H12O4	172	1153
392 diethyl glutarate	C9H16O4	188	1247
393 N,N-diethyl hexadecylamine	C20H43N	297	2043
394 diethyl isophthalate	C12H14O4	222	1606
395 diethyl maleate	C8H12O4	172	1130
396 diethyl malonate	C7H12O4	160	1032
397 N,N-diethyl octadecylamine	C22H47N	325	2241
398 N,N-diethyl octylamine	C12H27N	185	1244
399 N,N-diethyl sec.-octylamine	C12H27N	185	1200
400 diethyl oxalate	C6H10O4	146	< 1000
401 diethyl phthalate	C12H14O4	222	1541
402 diethyl pimelate	C11H20O4	216	1453
403 diethyl suberate	C12H22O4	230	1552
404 diethyl succinate	C8H14O4	174	1145
405 N,N-diethyl tetradecylamine	C18H39N	269	1842
406 di(2-ethylhexyl) isophthalate	C24H38O4	390	2631
407 di(2-ethylhexyl) phthalate	C24H38O4	390	2488
408 dihexyl adipate	C18H34O4	314	2113
409 dihexyl azelate	C21H40O4	356	2416
410 dihexyl glutarate	C17H32O4	300	2008
411 dihexyl isophthalate	C20H38O4	334	2394
412 dihexyl malonate	C15H28O4	272	1783
413 dihexyl oxalate	C14H26O4	258	1711
414 dihexyl phthalate	C20H38O4	334	2281
415 dihexyl pimelate	C19H36O4	328	2212
416 dihexyl suberate	C20H38O4	342	2313
417 dihexyl succinate	C16H38O4	286	1910
418 9,10-dihydroanthracene	C14H12	180	1622
419 diisoamyl adipate (isomer)	C16H38O4	286	1848
420 diisoamyl adipate (isomer)	C16H38O4	286	1851

compound	formula	M.W.	PTR1
421 diisoamyl adipate (isomer)	C16H30O4	286	1855
422 diisoamyl azelate (isomer)	C19H36O4	328	2149
423 diisoamyl azelate (isomer)	C19H36O4	328	2153
424 diisoamyl azelate (isomer)	C19H36O4	328	2157
425 diisoamyl glutarate (isomer)	C15H28O4	272	1743
426 diisoamyl glutarate (isomer)	C15H28O4	272	1746
427 diisoamyl glutarate (isomer)	C15H28O4	272	1749
428 diisoamyl malonate (isomer)	C13H24O4	244	1519
429 diisoamyl malonate (isomer)	C13H24O4	244	1522
430 diisoamyl malonate (isomer)	C13H24O4	244	1525
431 diisoamyl oxalate	C12H22O4	230	1443
432 diisoamyl pimelate (isomer)	C17H32O4	300	1947
433 diisoamyl pimelate (isomer)	C17H32O4	300	1951
434 diisoamyl pimelate (isomer)	C17H32O4	300	1954
435 diisoamyl suberate (isomer)	C18H34O4	314	2048
436 diisoamyl suberate (isomer)	C18H34O4	314	2052
437 diisoamyl suberate (isomer)	C18H34O4	314	2056
438 diisoamyl succinate (isomer)	C14H26O4	258	1644
439 diisoamyl succinate (isomer)	C14H26O4	258	1647
440 diisoamyl succinate (isomer)	C14H26O4	258	1649
441 diisobutyl adipate	C14H26O4	258	1652
442 diisobutyl azelate	C17H32O4	300	1952
443 diisobutyl glutarate	C13H24O4	244	1546
444 diisobutyl malonate	C11H20O4	216	1327
445 diisobutyl oxalate	C10H18O4	202	1236
446 diisobutyl phthalate	C16H22O4	278	1819
447 diisobutyl pimelate	C15H28O4	272	1751
448 diisobutyl suberate	C16H30O4	286	1852
449 diisobutyl succinate	C12H22O4	230	1447
450 diisopropyl adipate	C12H22O4	230	1425
451 diisopropyl adipate	C12H22O4	230	1427
452 diisopropyl azelate	C15H28O4	272	1722
453 diisopropyl glutarate	C11H20O4	216	1322
454 diisopropyl malonate	C9H16O4	188	1116
455 diisopropyl oxalate	C8H14O4	174	1026
456 diisopropyl pimelate	C13H24O4	244	1523
457 diisopropyl suberate	C14H26O4	258	1622
458 diisopropyl succinate	C10H18O4	202	1225
459 dimedone	C8H12O2	140	1101
460 o-dimethoxybenzene	C8H10O2	138	1111
461 p-dimethoxybenzene	C8H10O2	138	1131
462 dimethyl adipate	C8H14O4	174	1206
463 dimethyl azelate	C11H20O4	216	1510
464 N,N-dimethyl decylamine	C12H27N	185	1298
465 N,N-dimethyl dodecylamine	C14H31N	213	1496
466 dimethyl fumarate	C6H8O4	144	< 1000
467 dimethyl fumalate	C6H8O4	144	< 1000
468 dimethyl glutarate	C7H12O4	160	1103
469 dimethyl glutarate	C7H12O4	160	1103
470 N,N-dimethyl heptylamine	C9H21N	143	1002
471 N,N-dimethyl hexadecylamine	C18H39N	269	1894
472 N,N-dimethyl hexylamine	C10H23N	157	1046
473 dimethyl isophthalate	C10H10O4	194	1457
474 dimethyl maleate	C6H8O4	144	< 1000
475 dimethyl malonate	C5H8O4	132	< 1000
476 N,N-dimethyl octadecylamine	C20H43N	297	2096
477 N,N-dimethyl octylamine	C10H23N	157	1099
478 N,N-dimethyl sec.-octylamine	C10H23N	157	1083
479 dimethyl phthalate	C10H10O4	194	1400
480 dimethyl phthalate	C10H10O4	194	1405
481 dimethyl pimelate	C9H16O4	188	1308
482 dimethyl sebacate	C12H22O4	230	1616
483 dimethyl suberate	C10H18O4	202	1410
484 dimethyl succinate	C6H10O4	146	1000
485 dimethyl terephthalate	C10H10O4	194	1468
486 N,N-dimethyl tetradecylamine	C16H35N	241	1694
487 p-dimethylaminobenzaldehyde	C9H11NO	149	1481
488 N,N-dimethylaniline	C8H11N	121	1061
489 2,3-dimethylanisole	C9H12O	136	1111
490 2,4-dimethylanisole	C9H12O	136	1088

compound	formula	M.W.	PTR
491 2,5-dimethylanisole	C9H12O	136	1091
492 2,6-dimethylanisole	C9H12O	136	1040
493 3,4-dimethylanisole	C9H12O	136	1121
494 3,5-dimethylanisole	C9H12O	136	1099
495 3,4-dimethylbenzoic acid	C9H10O2	150	1387
496 2,6-dimethylnaphthalene	C12H12	156	1370
497 1,8-dinitronaphthalene	C10H6N2O4	218	2035
498 dioctyl adipate	C22H42O4	370	2499
499 dioctyl glutarate	C21H40O4	356	2397
500 dioctyl malonate	C19H36O4	328	2168
501 dioctyl oxalate	C18H34O4	314	2101
502 dioctyl pimelate	C23H44O4	384	2599
503 dioctyl suberate	C24H46O4	398	2690
504 dioctyl succinate	C20H38O4	342	2299
505 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2156
506 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2180
507 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2192
508 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2200
509 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2211
510 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2223
511 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2245
512 dioxyethylene nonylphenylether (isomer)	C19H32O3	308	2258
513 diphenyl	C12H10	154	1342
514 diphenyl ether	C12H10O	170	1364
515 diphenyl phthalate	C20H14O4	318	2445
516 diphenylamine	C12H11N	169	1568
517 diphenylmethane	C13H12	168	1393
518 dipropyl adipate	C12H22O4	230	1540
519 dipropyl azelate	C15H28O4	272	1841
520 dipropyl glutarate	C11H20O4	216	1436
521 dipropyl malonate	C9H16O4	188	1220
522 dipropyl oxalate	C8H14O4	174	1084
523 dipropyl pimelate	C13H24O4	244	1641
524 dipropyl suberate	C14H26O4	258	1741
525 dipropyl succinate	C10H18O4	202	1336
526 dipropylene glycol (isomer)	C6H14O3	134	< 1000
527 dipropylene glycol (isomer)	C6H14O3	134	1009
528 dipropylene glycol (isomer)	C6H14O3	134	1013
529 dipropylene glycol (isomer)	C6H14O3	134	1036
530 dipropylene glycol diacetate (isomer)	C10H18O5	218	1288
531 dipropylene glycol diacetate (isomer)	C10H18O5	218	1296
532 dipropylene glycol dibutyrate (isomer)	C14H26O5	274	1621
533 dipropylene glycol dibutyrate (isomer)	C14H26O5	274	1628
534 dipropylene glycol dibutyrate (isomer)	C14H26O5	274	1632
535 dipropylene glycol dibutyrate (isomer)	C14H26O5	274	1643
536 dipropylene glycol dipropionate (isomer)	C12H22O5	246	1459
537 dipropylene glycol dipropionate (isomer)	C12H22O5	246	1464
538 dipropylene glycol dipropionate (isomer)	C12H22O5	246	1467
539 dipropylene glycol dipropionate (isomer)	C12H22O5	246	1476
540 dipropylene glycol monoacetate (isomer)	C8H16O4	176	1135
541 dipropylene glycol monoacetate (isomer)	C8H16O4	176	1137
542 dipropylene glycol monoacetate (isomer)	C8H16O4	176	1145
543 dipropylene glycol monoacetate (isomer)	C8H16O4	176	1149
544 dipropylene glycol monobutyrate (isomer)	C10H20O4	204	1309
545 dipropylene glycol monobutyrate (isomer)	C10H20O4	204	1313
546 dipropylene glycol monobutyrate (isomer)	C10H20O4	204	1315
547 dipropylene glycol monobutyrate (isomer)	C10H20O4	204	1318
548 dipropylene glycol monobutyrate (isomer)	C10H20O4	204	1324
549 dipropylene glycol monobutyrate (isomer)	C10H20O4	204	1339
550 dipropylene glycol monopropionate (isomer)	C9H18O4	190	1222
551 dipropylene glycol monopropionate (isomer)	C9H18O4	190	1226
552 dipropylene glycol monopropionate (isomer)	C9H18O4	190	1228
553 dipropylene glycol monopropionate (isomer)	C9H18O4	190	1231
554 dipropylene glycol monopropionate (isomer)	C9H18O4	190	1236
555 dipropylene glycol monopropionate (isomer)	C9H18O4	190	1250
556 divinyl adipate	C10H14O4	198	1295
557 n-docosanal	C22H44O	324	2408
558 n-docosanyl acetate	C24H48O2	368	2594
559 n-docosanyl butyrate	C26H52O2	396	2781
560 n-docosanyl formate	C23H46O2	354	2524

compound	formula	M.W.	PTR
561 n-docosanyl propionate	C25H50O2	382	2699
562 1-docosene	C22H44	308	2189
563 n-dodecanal	C12H24O	184	1387
564 1-dodecanol	C12H26O	186	1457
565 2-dodecanone	C12H24O	184	1373
566 1-dodecene	C12H24	168	1188
567 n-dodecyl acetate	C14H28O2	228	1592
568 n-dodecyl butyrate	C16H32O2	256	1773
569 n-dodecyl caproate	C18H36O2	284	1966
570 n-dodecyl caprylate	C20H40O2	312	2160
571 n-dodecyl formate	C13H26O2	214	1513
572 n-dodecyl laurate	C24H48O2	368	2553
573 n-dodecyl myristate	C26H52O2	396	2753
574 n-dodecyl propionate	C15H30O2	242	1686
575 n-dodecylamine	C12H25N	183	1435
576 n-eicosanal	C20H40O	296	2203
577 n-eicosanamide	C20H41NO	311	2540
578 1-eicosanol	C20H42O	298	2267
579 n-eicosanyl acetate	C22H44O2	340	2393
580 n-eicosanyl butyrate	C24H48O2	368	2579
581 n-eicosanyl caproate	C26H52O2	396	2771
582 n-eicosanyl formate	C21H42O2	326	2323
583 n-eicosanyl propionate	C23H46O2	354	2490
584 1-eicosene	C20H40	280	1988
585 11-eicosenyl alcohol	C20H40O	296	2238
586 erucyl alcohol	C22H44O	324	2443
587 ethyl arachidate	C22H44O2	340	2373
588 ethyl behenoate	C24H48O2	368	2573
589 ethyl benzoate	C9H10O2	150	1139
590 ethyl p-tert.-butylbenzoate	C13H18O2	206	1486
591 ethyl caprate	C12H24O2	200	1375
592 N-ethyl decylamine	C12H27N	185	1355
593 ethyl 3,4-dimethylbenzoate	C11H14O2	178	1385
594 N-ethyl dodecylamine	C14H31N	213	1555
595 ethyl n-heneicosanoate	C23H46O2	354	2474
596 ethyl n-heptadecanoate	C19H38O2	298	2075
597 N-ethyl hexadecylamine	C18H39N	269	1953
598 ethyl methyl phthalate	C11H12O4	208	1499
599 ethyl myristate	C16H32O2	256	1774
600 ethyl n-nonadecanoate	C21H42O2	326	2274
601 ethyl n-nonanoate	C11H22O2	186	1275
602 N-ethyl octadecylamine	C20H43N	297	2153
603 N-ethyl octylamine	C10H23N	157	1154
604 ethyl palmitate	C18H36O2	284	1974
605 ethyl n-pentadecanoate	C17H34O2	270	1875
606 ethyl 2-phenoxybenzoate	C15H14O3	242	1758
607 ethyl 2-phenoxybutyrate	C12H16O3	208	1392
608 ethyl 2-phenoxypropionate	C11H14O3	194	1318
609 ethyl salicylate	C9H10O3	166	1238
610 ethyl stearate	C20H40O2	312	2174
611 N-ethyl tetradecylamine	C16H35N	241	1752
612 ethyl m-toluate	C10H12O2	164	1246
613 ethyl n-tricosanoate	C25H50O2	382	2679
614 ethyl n-tridecanoate	C15H30O2	242	1675
615 ethyl n-undecanoate	C13H26O2	214	1475
616 N-ethylaniline	C8H11N	121	1100
617 o-ethylaniline	C8H11N	121	1119
618 p-ethylaniline	C8H11N	121	1132
619 m-ethylanisole	C9H12O	136	1088
620 o-ethylanisole	C9H12O	136	1060
621 p-ethylanisole	C9H12O	136	1091
622 2-ethylanthraquinone	C16H12O2	236	2122
623 2-ethylhexyl acetate	C10H20O2	172	1161
624 2-ethylhexyl benzoate	C15H22O2	234	1674
625 2-ethylhexyl p-tert.-butylbenzoate	C19H30O2	290	2019
626 2-ethylhexyl butyrate	C12H24O2	200	1314
627 2-ethylhexyl caprate	C18H36O2	284	1885
628 2-ethylhexyl caproate	C14H28O2	228	1497
629 2-ethylhexyl caprylate	C16H32O2	256	1688
630 2-ethylhexyl 3,4-dimethylbenzoate	C17H26O2	262	1920

	compound	formula	M.W.	PTR1
631	2-ethylhexyl n-heptadecanoate	C25H50O2	382	2579
632	2-ethylhexyl n-heptanoate	C15H30O2	242	1592
633	2-ethylhexyl methyl phthalate	C17H24O4	292	1951
634	2-ethylhexyl myristate	C22H44O2	340	2281
635	2-ethylhexyl n-nonadecanoate	C27H54O2	410	2775
636	2-ethylhexyl n-nonanoate	C17H34O2	270	1787
637	2-ethylhexyl palmitate	C24H48O2	368	2479
638	2-ethylhexyl n-pentadecanoate	C23H46O2	354	2378
639	2-ethylhexyl n-pentanoate	C13H26O2	214	1404
640	2-ethylhexyl 2-phenoxybenzoate	C21H26O3	326	2256
641	2-ethylhexyl 2-phenoxybutyrate	C18H28O3	292	1871
642	2-ethylhexyl 2-phenoxypropionate	C17H26O3	278	1803
643	2-ethylhexyl propionate	C11H22O2	186	1236
644	2-ethylhexyl salicylate	C15H22O3	250	1769
645	2-ethylhexyl stearate	C26H52O2	396	2684
646	2-ethylhexyl m-toluate	C16H24O2	248	1774
647	2-ethylhexyl n-tridecanoate	C21H42O2	326	2181
648	2-ethylhexyl n-undecanoate	C19H38O2	298	1983
649	m-ethylphenol	C8H10O	122	1139
650	o-ethylphenol	C8H10O	122	1111
651	p-ethylphenol	C8H10O	122	1137
652	fenitrothion oxon	C9H12N06P	261	1800
653	fenthion sulfoxide	C10H15O4PS2	295	2038
654	fenthioate oxon	C12H17O5PS	304	1925
655	fluoranthene	C16H10	202	1981
656	fluoranthene-quinone	C16H8O2	232	2394
657	fluorene	C13H10	166	1531
658	fluorenone	C13H8O	180	1663
659	folpet	C9H4Cl3N02S	295	1980
660	1,2,3,4,7,8-HCDD	C12H2Cl6O2	388	2674
661	1,2,3,4,7,8-HCDF	C12H2Cl6O	372	2620
662	n-heneicosanal	C21H42O	310	2307
663	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2261
664	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2333
665	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2343
666	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2376
667	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2384
668	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2393
669	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2441
670	heptachlorodiphenyl (isomer)	C12H3Cl7	392	2494
671	heptachloronaphthalene	C10HCl7	366	2505
672	n-heptadecanal	C17H34O	254	1898
673	n-heptadecanamide	C17H35NO	269	2233
674	n-heptadecanoic acid	C17H34O2	270	2059
675	2-heptadecanone	C17H34O	254	1881
676	n-heptylamine	C7H17N	115	< 1000
677	hexachlorobenzene	C6Cl6	282	1661
678	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2120
679	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2160
680	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2184
681	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2230
682	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2238
683	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2261
684	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2288
685	hexachlorodiphenyl (isomer)	C12H4Cl6	358	2393
686	hexachloroethane	C2Cl6	234	1056
687	hexachloronaphthalene	C10H2Cl6	332	2287
688	hexachlorophene-dimethyl ether	C15H10Cl6O2	432	2666
689	n-hexadecanal	C16H32O	240	1795
690	1-hexadecanol	C16H34O	240	1863
691	1-hexadecene	C16H32	224	1588
692	n-hexadecyl acetate	C18H36O2	284	1990
693	n-hexadecyl butyrate	C20H40O2	312	2174
694	n-hexadecyl caproate	C22H44O2	340	2366
695	n-hexadecyl caprylate	C24H48O2	368	2562
696	n-hexadecyl formate	C17H34O2	270	1914
697	n-hexadecyl propionate	C19H38O2	298	2088
698	n-hexyl acetate	C8H16O2	144	< 1000
699	n-hexyl arachidate	C26H52O2	396	2760
700	n-hexyl benzoate	C13H18O2	206	1540

compound	formula	M.W.	PTR1
701 n-hexyl p-tert.-butylbenzoate	C17H26O2	262	1892
702 n-hexyl butyrate	C10H20O2	172	1173
703 n-hexyl caprate	C16H32O2	256	1763
704 n-hexyl caproate	C12H24O2	200	1368
705 n-hexyl caprylate	C14H28O2	228	1565
706 n-hexyl 3,4-dimethylbenzoate	C15H22O2	234	1645
707 n-hexyl formate	C7H14O2	130	< 1000
708 n-hexyl n-heptadecanoate	C23H46O2	354	2464
709 n-hexyl laurate	C18H36O2	284	1963
710 hexyl methyl phthalate	C15H20O4	264	1848
711 n-hexyl myristate	C20H40O2	312	2162
712 n-hexyl n-nonadecanoate	C25H50O2	382	2669
713 n-hexyl n-nonanoate	C15H30O2	242	1663
714 n-hexyl palmitate	C22H44O2	340	2364
715 n-hexyl n-pentadecanoate	C21H42O2	326	2262
716 n-hexyl 2-phenoxybenzoate	C19H22O3	298	2137
717 n-hexyl 2-phenoxybutyrate	C16H24O3	264	1756
718 n-hexyl 2-phenoxypropionate	C15H22O3	250	1684
719 n-hexyl propionate	C9H18O2	158	1086
720 n-hexyl salicylate	C13H18O3	222	1639
721 n-hexyl stearate	C24H48O2	368	2564
722 n-hexyl m-toluate	C14H28O2	220	1645
723 n-hexyl n-tridecanoate	C19H38O2	298	2062
724 n-hexyl n-undecanoate	C17H34O2	270	1862
725 2-hydroxydiphenyl	C12H10O	170	1466
726 4-hydroxydiphenyl	C12H10O	170	1660
727 2-hydroxyethyl butyrate	C6H12O3	132	1000
728 2-hydroxyethyl caprate	C12H24O3	216	1595
729 2-hydroxyethyl caproate	C8H16O3	160	1194
730 2-hydroxyethyl caprylate	C10H20O3	188	1396
731 2-hydroxyethyl n-heptadecanoate	C19H38O3	314	2326
732 2-hydroxyethyl n-heptanoate	C9H18O3	174	1294
733 2-hydroxyethyl myristate	C16H32O3	272	2011
734 2-hydroxyethyl n-nonadecanoate	C21H42O3	342	2555
735 2-hydroxyethyl n-nonanoate	C11H22O3	202	1498
736 2-hydroxyethyl palmitate	C18H36O3	300	2214
737 2-hydroxyethyl n-pentadecanoate	C17H34O3	286	2115
738 2-hydroxyethyl n-pentanoate	C7H14O3	146	1096
739 2-hydroxyethyl stearate	C20H40O3	328	2436
740 2-hydroxyethyl n-undecanoate	C13H26O3	230	1712
741 2-hydroxyethyl n-tridecanoate	C15H30O3	258	1914
742 indazole	C7H6N2	118	1260
743 indole	C8H7N	117	1248
744 indoline	C8H9N	119	1166
745 isoamyl benzoate	C12H16O2	192	1402
746 isoamyl ether	C10H22O	158	< 1000
747 isobutyl arachidate	C24H48O2	368	2530
748 isobutyl behenoate	C26H52O2	396	2724
749 isobutyl caprate	C14H28O2	228	1528
750 isobutyl n-heneicosanoate	C25H50O2	382	2634
751 isobutyl n-heptadecanoate	C21H42O2	326	2229
752 isobutyl myristate	C18H36O2	284	1927
753 isobutyl n-pentadecanoate	C19H38O2	298	2029
754 isobutyl n-nonadecanoate	C23H46O2	354	2428
755 isobutyl n-nonanoate	C13H26O2	214	1428
756 isobutyl palmitate	C20H40O2	312	2129
757 isobutyl stearate	C22H44O2	340	2328
758 isobutyl n-tridecanoate	C17H34O2	270	1826
759 isobutyl n-undecanoate	C15H30O2	242	1627
760 isochroman	C9H10O	134	1151
761 isofenphos	C15H24N04PS	345	2018
762 isofenphos oxon	C15H24N05P	329	1948
763 isopropyl benzoate	C10H12O2	164	1177
764 o-isopropylanisole	C10H14O	150	1118
765 β -isopropyl naphthalene	C13H14	170	1422
766 o-isopropylphenol	C9H12O	136	1173
767 isoprothiolane sulfoxide	C12H18O5S2	295	2193
768 isoquinoline	C9H7N	129	1217
769 isoxathion oxon	C13H16N05P	297	2089
770 kelthane (isomer)	C14H9Cl5O	368	2364

	compound	formula	M.W.	PTRI
771	kelthane (isomer)	C14H9Cl5O	368	2386
772	kepone	C10Cl11O	486	2222
773	lauramide	C12H25NO	199	1715
774	linuron	C9H10Cl12N2O2	248	1884
775	malathion oxon	C10H19O7PS	314	1838
776	MDBA	C8H6Cl12O3	220	1617
777	methidathion	C6H11N2O4PS3	302	2015
778	3-methoxybutyl arachidate	C25H50O3	398	2691
779	3-methoxybutyl butyrate	C9H18O3	174	1136
780	3-methoxybutyl caprate	C15H30O3	258	1725
781	3-methoxybutyl caproate	C11H22O3	202	1330
782	3-methoxybutyl caprylate	C13H26O3	230	1526
783	3-methoxybutyl n-heptadecanoate	C22H44O3	356	2422
784	3-methoxybutyl n-heptanoate	C12H24O3	216	1428
785	3-methoxybutyl myristate	C19H38O3	314	2123
786	3-methoxybutyl n-nonadecanoate	C24H48O3	384	2603
787	3-methoxybutyl n-nonanoate	C14H28O3	244	1625
788	3-methoxybutyl palmitate	C21H42O3	342	2323
789	3-methoxybutyl n-pentadecanoate	C20H40O3	328	2222
790	3-methoxybutyl n-pentanoate	C10H20O3	188	1232
791	3-methoxybutyl propionate	C8H16O3	160	1048
792	3-methoxybutyl stearate	C23H46O3	370	2513
793	3-methoxybutyl n-tridecanoate	C18H36O3	300	2023
794	3-methoxybutyl n-undecanoate	C16H32O3	272	1823
795	2-methoxydiphenyl	C13H12O	184	1511
796	4-methoxydiphenyl	C13H12O	184	1606
797	2-methoxyethyl arachidate	C23H46O3	338	2581
798	2-methoxyethyl benzoate	C10H12O3	180	1349
799	2-methoxyethyl p-tert.-butylbenzoate	C14H20O3	236	1700
800	2-methoxyethyl butyrate	C7H14O3	146	< 1000
801	2-methoxyethyl caprate	C13H26O3	230	1577
802	2-methoxyethyl caproate	C9H18O3	174	1183
803	2-methoxyethyl caprylate	C11H22O3	202	1375
804	2-methoxyethyl 3,4-dimethylbenzoate	C12H16O3	208	1599
805	2-methoxyethyl n-heptadecanoate	C20H40O3	328	2275
806	2-methoxyethyl n-heptanoate	C10H20O3	188	1281
807	2-methoxyethyl myristate	C17H34O3	286	1975
808	2-methoxyethyl n-nonadecanoate	C22H44O3	356	2477
809	2-methoxyethyl n-nonanoate	C12H24O3	216	1477
810	2-methoxyethyl palmitate	C19H38O3	314	2176
811	2-methoxyethyl n-pentadecanoate	C18H36O3	300	2076
812	2-methoxyethyl n-pentanoate	C8H16O3	160	1086
813	2-methoxyethyl 2-phenoxybenzoate	C16H16O4	272	1964
814	2-methoxyethyl 2-phenoxybutyrate	C13H18O4	238	1585
815	2-methoxyethyl 2-phenoxypropionate	C12H16O4	224	1512
816	2-methoxyethyl propionate	C6H12O3	132	< 1000
817	2-methoxyethyl salicylate	C10H12O4	196	1448
818	2-methoxyethyl stearate	C21H42O3	342	2374
819	2-methoxyethyl m-toluate	C11H14O3	194	1454
820	2-methoxyethyl n-undecanoate	C14H28O3	244	1676
821	1-methoxynaphthalene	C11H10O	158	1403
822	2-methoxynaphthalene	C11H10O	158	1407
823	2-methoxyethyl n-tridecanoate	C16H32O3	272	1875
824	methyl arachidate	C21H42O2	326	2309
825	methyl behenoate	C23H46O2	354	2511
826	methyl benzoate	C8H8O2	136	1064
827	methyl benzoate	C8H8O2	136	1066
828	methyl p-tert.-butylbenzoate	C12H16O2	192	1410
829	methyl n-caprate	C11H22O2	186	1306
830	methyl n-decanoate	C14H28O2	228	1607
831	N-methyl decylamine	C11H25N	171	1285
832	methyl 3,4-dimethylbenzoate	C10H12O2	164	1311
833	N-methyl dodecylamine	C13H29N	199	1486
834	methyl cis-11-eicosenoate	C21H40O2	324	2278
835	methyl n-heneicosanoate	C22H44O2	340	2409
836	methyl n-heptadecanoate	C18H36O2	284	2007
837	N-methyl hexadecylamine	C17H37N	255	1888
838	1-methyl-2-methoxyethyl arachidate	C24H48O3	384	2592
839	1-methyl-2-methoxyethyl behenoate	C26H52O3	412	2792
840	1-methyl-2-methoxyethyl benzoate	C11H14O3	194	1373

	compound	formula	M.W.	PIRI
841	1-methyl-2-methoxyethyl p-tert.-butylbenzoate	C15H22O3	250	1719
842	1-methyl-2-methoxyethyl butyrate	C8H16O3	160	1017
843	1-methyl-2-methoxyethyl caprate	C14H28O3	244	1601
844	1-methyl-2-methoxyethyl caproate	C10H20O3	188	1210
845	1-methyl-2-methoxyethyl caprylate	C12H24O3	216	1405
846	1-methyl-2-methoxyethyl 3,4-dimethylbenzoate	C13H18O3	222	1620
847	1-methyl-2-methoxyethyl n-heneicosanoate	C25H50O3	398	2700
848	1-methyl-2-methoxyethyl n-heptadecanoate	C21H42O3	342	2293
849	1-methyl-2-methoxyethyl n-heptanoate	C11H22O3	202	1307
850	1-methyl-2-methoxyethyl myristate	C18H36O3	300	1995
851	1-methyl-2-methoxyethyl n-nonadecanoate	C23H46O3	370	2491
852	1-methyl-2-methoxyethyl n-nonanoate	C13H26O3	230	1503
853	1-methyl-2-methoxyethyl palmitate	C20H40O3	328	2194
854	1-methyl-2-methoxyethyl n-pentadecanoate	C19H38O3	314	2094
855	1-methyl-2-methoxyethyl n-pentanoate	C9H18O3	174	1114
856	1-methyl-2-methoxyethyl 2-phenoxybenzoate	C17H18O4	286	1976
857	1-methyl-2-methoxyethyl propionate	C7H14O3	146	< 1000
858	1-methyl-2-methoxyethyl stearate	C22H44O3	356	2392
859	1-methyl-2-methoxyethyl m-toluate	C12H16O3	208	1477
860	1-methyl-2-methoxyethyl n-undecanoate	C16H32O3	260	1699
861	1-methyl-2-methoxyethyl n-tridecanoate	C17H34O3	286	1897
862	methyl myristate	C15H30O2	242	1707
863	methyl myristoleate	C15H28O2	240	1689
864	methyl n-nonadecanoate	C20H40O2	312	2209
865	methyl n-nonanoate	C10H20O2	172	1206
866	N-methyl octadecylamine	C19H41N	283	2088
867	N-methyl octylamine	C9H21N	143	1085
868	methyl oleate	C19H36O2	296	2078
869	methyl palmitate	C17H34O2	270	1909
870	methyl palmitoleate	C17H32O2	268	1882
871	methyl n-pentadecanoate	C16H32O2	256	1808
872	methyl 2-phenoxybenzoate	C14H12O3	228	1969
873	methyl 2-phenoxybutyrate	C11H14O3	194	1334
874	methyl 2-phenoxypropionate	C10H12O3	180	1258
875	methyl salicylate	C8H8O3	152	1161
876	methyl stearate	C19H38O2	298	2109
877	N-methyl tetradecylamine	C15H33N	227	1686
878	methyl m-toluate	C9H10O2	150	1171
879	methyl n-tricosanoate	C24H48O2	368	2614
880	methyl 2,4,6-trimethylbenzoate	C11H14O2	178	1311
881	methyl n-undecanoate	C12H24O2	200	1405
882	N-methylaniline	C7H9N	107	1031
883	m-methylanisole	C8H10O	122	1001
884	o-methylanisole	C8H10O	122	< 1000
885	p-methylanisole	C8H10O	122	1001
886	4-methyldiphenyl	C13H12	168	1455
887	1-methylnaphthalene	C11H10	142	1277
888	2-methylnaphthalene	C11H10	142	1263
889	4-methylphenanthrene	C15H12	192	1856
890	MGK264	C17H25NO2	275	1965
891	MGK264	C17H25NO2	275	1978
892	myristic acid	C14H28O2	228	1764
893	naphthalene	C10H8	128	1154
894	1-naphthol	C10H8O	144	1464
895	2-naphthol	C10H8O	144	1471
896	α -naphthoquinoline	C13H9N	179	1720
897	β -naphthoquinoline	C13H9N	179	1750
898	α -naphthoquinone	C10H6O2	158	1349
899	1-naphthylamine	C10H9N	143	1471
900	2-naphthylamine	C10H9N	143	1486
901	nicotine	C10H14N2	162	1307
902	m-nitroanisole	C7H7NO3	153	1273
903	o-nitroanisole	C7H7NO3	153	1296
904	9-nitroanthracene	C14H9NO2	223	2046
905	2-nitrodiphenyl	C12H9NO2	199	1627
906	3-nitrofluoranthene	C16H9NO2	247	2433
907	2-nitrofluorene	C13H9NO2	211	2013
908	1-nitronaphthalene	C10H7NO2	173	1535
909	2-nitronaphthalene	C10H7NO2	173	1574
910	1-nitropyrene	C16H9NO2	247	2481

compound	formula	M.W.	PTI
911 n-nonadecanal	C19H38O	282	2102
912 2-nonadecanone	C19H38O	282	2085
913 1-nonadecene	C19H38	266	1890
914 n-nonanal	C9H18O	142	1082
915 n-nonanoic acid	C9H18O2	158	1272
916 2-nonanone	C9H18O	142	1067
917 nonylphenol (isomer)	C15H24O	220	1582
918 nonylphenol (isomer)	C15H24O	220	1593
919 nonylphenol (isomer)	C15H24O	220	1620
920 nonylphenol (isomer)	C15H24O	220	1632
921 nonylphenol (isomer)	C15H24O	220	1643
922 nonylphenol (isomer)	C15H24O	220	1665
923 nonylphenol (isomer)	C15H24O	220	1673
924 nonylphenol (isomer)	C15H24O	220	1682
925 nonylphenol (isomer)	C15H24O	220	1684
926 nonylphenol (isomer)	C15H24O	220	1690
927 nonylphenol (isomer)	C15H24O	220	1698
928 nonylphenol (isomer)	C15H24O	220	1702
929 nonylphenol (isomer)	C15H24O	220	1706
930 nonylphenol (isomer)	C15H24O	220	1710
931 nonylphenol (isomer)	C15H24O	220	1717
932 nonylphenol (isomer)	C15H24O	220	1724
933 octachlorodiphenyl (isomer)	C12H2Cl8	426	2526
934 octachlorodiphenyl (isomer)	C12H2Cl8	426	2539
935 octachlorodiphenyl (isomer)	C12H2Cl8	426	2651
936 octachloronaphthalene	C10Cl8	400	2694
937 n-octadecanal	C18H36O	268	1999
938 1-octadecanol	C18H38O	270	2066
939 n-octadecyl acetate	C20H40O2	312	2192
940 n-octadecyl butyrate	C22H44O2	340	2377
941 n-octadecyl caproate	C24H48O2	368	2569
942 n-octadecyl caprylate	C26H52O2	396	2765
943 n-octadecyl formate	C19H38O2	298	2118
944 n-octadecyl propionate	C21H42O2	326	2291
945 n-octanal	C8H16O	128	< 1000
946 n-octanamide	C8H17NO	143	1326
947 1-octanol	C8H18O	130	1051
948 2-octanone	C8H16O	128	< 1000
949 n-octyl acetate	C10H20O2	172	1192
950 octyl benzoate	C15H22O2	234	1745
951 n-octyl butyrate	C12H24O2	200	1372
952 n-octyl caproate	C14H28O2	228	1567
953 n-octyl caprylate	C16H32O2	256	1763
954 n-octyl formate	C9H18O2	158	1109
955 n-octyl laurate	C20H40O2	312	2158
956 octyl methyl phthalate	C17H24O4	292	2022
957 n-octyl myristate	C22H44O2	340	2359
958 n-octyl palmitate	C24H48O2	368	2560
959 n-octyl propionate	C11H22O2	186	1286
960 n-octyl stearate	C26H52O2	396	2763
961 n-octylamine	C8H19N	129	1028
962 sec-octylamine	C8H19N	129	< 1000
963 p-tert.-octylphenol	C14H22O	206	1572
964 oleamide	C18H35NO	281	2307
965 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1621
966 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1877
967 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1903
968 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1911
969 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1931
970 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1944
971 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1963
972 oxyethylene nonylphenylether (isomer)	C17H28O2	264	1973
973 palmitamide	C16H33NO	255	2127
974 palmitic acid	C16H32O2	256	1964
975 PAP (phenthoate)	C12H17O4PS2	320	2008
976 1,2,3,4,7-PCDD	C12H3Cl5O2	354	2467
977 1,2,3,7,8-PCDF	C12H3Cl5O	338	2422
978 PCP	C6HCl5O	300	1695
979 pentabromodiphenylether	C12H5Br5O	560	2692
980 pentachloroanisole	C7H4Cl5O	279	1672

	compound	formula	M.W.	PTRI
981	pentachlorobenzene	C6HCl5	248	1478
982	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2010
983	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2047
984	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2062
985	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2070
986	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2098
987	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2107
988	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2128
989	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2230
990	pentachlorodiphenyl (isomer)	C12H5Cl5	324	2238
991	pentachloroethane	C2HCl5	200	< 1000
992	pentachloronaphthalene (isomer)	C10H3Cl5	298	2030
993	pentachloronaphthalene (isomer)	C10H3Cl5	298	2055
994	pentachloronaphthalene (isomer)	C10H3Cl5	298	2094
995	pentachloronaphthalene (isomer)	C10H3Cl5	298	2103
996	pentachloronaphthalene (isomer)	C10H3Cl5	298	2111
997	pentachloronaphthalene (isomer)	C10H3Cl5	298	2123
998	pentachlorophenol	C6H2Cl5O	265	1698
999	n-pentadecanal	C15H30O	226	1692
1000	n-pentadecanamide	C15H31NO	241	2025
1001	n-pentadecanoic acid	C15H30O2	242	1861
1002	2-pentadecanone	C15H30O	226	1678
1003	phenanthrene	C14H10	178	1715
1004	phenanthrene-quinone (isomer)	C14H8O2	208	1873
1005	phenanthrene-quinone (isomer)	C14H8O2	208	1880
1006	phenanthrene-quinone (isomer)	C14H8O2	208	1935
1007	phenazine	C12H8N2	180	1670
1008	phenetole	C8H10O	122	< 1000
1009	phenol	C6H6O	94	< 1000
1010	2-phenoxybutyric acid	C10H12O3	180	1450
1011	2-phenoxyethyl acetate	C10H12O3	180	1344
1012	2-phenoxyethyl butyrate	C12H16O3	208	1522
1013	2-phenoxyethyl caprate	C18H28O3	292	2118
1014	2-phenoxyethyl caproate	C14H28O3	236	1717
1015	2-phenoxyethyl caprylate	C16H24O3	264	1916
1016	2-phenoxyethyl n-heptanoate	C15H22O3	250	1816
1017	2-phenoxyethyl myristate	C22H36O3	348	2534
1018	2-phenoxyethyl n-nonanoate	C17H26O3	278	2015
1019	2-phenoxyethyl palmitate	C24H40O3	376	2744
1020	2-phenoxyethyl n-pentadecanoate	C23H38O3	362	2650
1021	2-phenoxyethyl n-pentanoate	C13H18O3	222	1619
1022	2-phenoxyethyl propionate	C11H14O3	194	1436
1023	2-phenoxyethyl n-undecanoate	C19H38O3	306	2221
1024	2-phenoxypropionic acid	C9H10O3	166	1372
1025	2-phenoxyethyl n-tridecanoate	C21H34O3	334	2427
1026	phenyl benzoate	C13H10O2	198	1604
1027	phenyl glycidyl ether	C9H10O2	150	1251
1028	N-phenyl-1-naphthylamine	C16H13N	219	2060
1029	N-phenyl-2-naphthylamine	C16H13N	219	2169
1030	phenylacetaldehyde	C8H8O	120	1009
1031	1-phenylnaphthalene	C16H12	204	1835
1032	phthalic acid	C8H6O4	166	1245
1033	piperophos oxon	C14H28N04PS	337	2311
1034	n-propyl arachidate	C23H46O2	354	2472
1035	n-propyl behenoate	C25H50O2	382	2679
1036	propyl benzoate	C10H12O2	164	1238
1037	n-propyl caprate	C13H26O2	214	1472
1038	n-propyl n-heptadecanoate	C20H40O2	312	2172
1039	n-propyl n-heneicosanoate	C24H48O2	368	2573
1040	propyl methyl phthalate	C12H14O4	222	1578
1041	n-propyl myristate	C17H34O2	270	1870
1042	n-propyl n-nonadecanoate	C22H44O2	340	2373
1043	n-propyl n-nonanoate	C12H24O2	200	1372
1044	n-propyl palmitate	C19H38O2	298	2072
1045	n-propyl n-pentadecanoate	C18H36O2	284	1972
1046	n-propyl stearate	C21H42O2	326	2273
1047	n-propyl n-tricosanoate	C26H52O2	396	2771
1048	n-propyl n-tridecanoate	C16H32O2	256	1771
1049	n-propyl n-undecanoate	C14H28O2	228	1571
1050	o-propylanisole	C10H14O	150	1143

	compound	formula	M.W.	PTR
1051	propylene glycol dibutyrate	C10H18O4	202	1340
1052	propylene glycol dipropionate	C9H16O4	188	1170
1053	propylene glycol monobutyrate (isomer)	C7H14O3	146	1028
1054	propylene glycol monobutyrate (isomer)	C7H14O3	146	1035
1055	propylene glycol monopropionate	C6H12O3	132	< 1000
1056	o-propylphenol	C9H10O	136	1195
1057	prothiofos oxon	C11H15Cl2O3PS	328	2008
1058	pyrene	C16H10	202	2025
1059	pyridaphenthion oxon	C14H17N2O5P	324	2311
1060	quinazoline	C8H6N2	130	1201
1061	quinoline	C9H7N	129	1199
1062	8-quinolinol	C9H7NO	145	1312
1063	quinomethionate	C10H6N2O5S2	234	2016
1064	quinoxaline	C8H6N2	130	1169
1065	ronnel	C8H8Cl3O3PS	320	1862
1066	salicylaldehyde	C7H6O2	122	1012
1067	silvex	C9H7Cl3O3	268	1869
1068	silvex methyl ester	C10H9Cl3O3	282	1709
1069	simetryn sulfone	C8H15N5O2S	245	2216
1070	skatole	C9H9N	131	1339
1071	stearamide	C18H37NO	283	2332
1072	stearic acid	C18H36O2	284	2155
1073	stearylamine	C18H31N	261	2047
1074	2,4,5-T methyl ester	C9H7Cl3O3	268	1728
1075	2,4,5-T	C8H5Cl3O3	254	1870
1076	1,2,3,4-TCDD	C12H4Cl4O2	320	2279
1077	2,3,7,8-TCDD	C12H4Cl4O2	320	2286
1078	2,3,7,8-TCDF	C12H4Cl4O	304	2250
1079	tedion	C12H6Cl4O2S	354	2422
1080	terephthalaldehyde	C8H6O2	134	1166
1081	m-terphenyl	C18H14	230	2083
1082	o-terphenyl	C18H14	230	1835
1083	p-terphenyl	C18H14	230	2116
1084	tetrabromodiphenylether	C12H6Br4O	482	2428
1085	2,3,4,6-tetrachloroanisole	C7H4Cl4O	244	1484
1086	1,2,3,4-tetrachlorobenzene	C642Cl4	214	1336
1087	1,2,3,5-tetrachlorobenzene	C642Cl4	214	1294
1088	1,2,4,5-tetrachlorobenzene	C642Cl4	214	1294
1089	tetrachlorobenzofuran (isomer)	C8H2Cl4O	254	1549
1090	tetrachlorobenzofuran (isomer)	C8H2Cl4O	254	1580
1091	tetrachlorobenzofuran (isomer)	C8H2Cl4O	254	1596
1092	tetrachlorobenzofuran (isomer)	C8H2Cl4O	254	1625
1093	tetrachlorobenzofuran (isomer)	C8H2Cl4O	254	1646
1094	tetrachlorobenzofuran (isomer)	C8H2Cl4O	254	1653
1095	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1845
1096	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1856
1097	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1886
1098	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1894
1099	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1902
1100	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1922
1101	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1927
1102	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1944
1103	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1956
1104	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	1993
1105	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	2002
1106	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	2006
1107	tetrachlorodiphenyl (isomer)	C12H6Cl4	290	2035
1108	tetrachloronaphthalene (isomer)	C10H4Cl4	264	1812
1109	tetrachloronaphthalene (isomer)	C10H4Cl4	264	1843
1110	tetrachloronaphthalene (isomer)	C10H4Cl4	264	1866
1111	tetrachloronaphthalene (isomer)	C10H4Cl4	264	1886
1112	tetrachloronaphthalene (isomer)	C10H4Cl4	264	1915
1113	tetrachloronaphthalene (isomer)	C10H4Cl4	264	1927
1114	tetrachloronaphthalene (isomer)	C10H4Cl4	264	1955
1115	2,3,4,6-tetrachlorophenol	C6H3Cl4O	231	1506
1116	n-tetracosanal	C24H48O	352	2614
1117	n-tetracosanyl formate	C25H50O2	382	2728
1118	n-tetradecanamide	C14H29NO	227	1921
1119	1-tetradecanol	C14H30O	214	1659
1120	n-tetradecenol	C14H28O	212	1591

	compound	formula	M.W.	PTR I
1121	1-tetradecene	C14H28	196	1389
1122	n-tetradecyl acetate	C16H32O2	256	1793
1123	n-tetradecyl butyrate	C18H36O2	284	1974
1124	n-tetradecyl caproate	C20H40O2	312	2166
1125	n-tetradecyl caprylate	C22H44O2	340	2360
1126	n-tetradecyl formate	C15H30O2	242	1710
1127	n-tetradecyl laurate	C26H52O2	396	2750
1128	n-tetradecyl propionate	C17H34O2	270	1888
1129	n-tetradecylamine	C14H27N	209	1638
1130	thianaphthene	C8H6S	134	1159
1131	thianthrene	C12H8S2	216	1883
1132	tolclofos-methyl	C9H11Cl2O3PS	301	1832
1133	tolclofos-methyl oxon	C9H11Cl2O4P	285	1794
1134	m-tolualdehyde	C8H8O	120	1034
1135	o-tolualdehyde	C8H8O	120	1034
1136	p-tolualdehyde	C8H8O	120	1046
1137	m-toluic acid	C8H8O2	136	1249
1138	m-toluidine	C7H9N	107	1043
1139	o-toluidine	C7H9N	107	1037
1140	p-toluidine	C7H9N	107	1037
1141	tri-n-amyamine	C15H33N	227	1456
1142	tri-n-butylamine	C12H27N	185	1189
1143	tri-n-hexylamine	C18H39N	269	1730
1144	tri-n-octylamine	C24H51N	353	2290
1145	tri-n-propylamine	C9H21N	143	< 1000
1146	triazimenol	C14H18ClN3O2	295	2023
1147	tribenzylamine	C21H21N	287	2235
1148	2,4,6-tribromoaniline	C6H4Br3N	327	1635
1149	2,4,6-tribromoanisole	C7H5Br3O	342	1564
1150	tribromodiphenylether	C12H7Br3O	404	2177
1151	2,4,6-tribromophenol	C6H3Br3O	328	1576
1152	tri-n-butyl phosphate	C12H27O4P	266	1615
1153	2,4,6-trichloroaniline	C6H4Cl3N	195	1362
1154	2,4,5-trichloroanisole	C7H5Cl3O	210	1407
1155	2,4,6-trichloroanisole	C7H5Cl3O	210	1298
1156	1,2,3-trichlorobenzene	C6H3Cl3	180	1182
1157	1,2,4-trichlorobenzene	C6H3Cl3	180	1149
1158	1,3,5-trichlorobenzene	C6H3Cl3	180	1112
1159	trichlorobenzofuran (isomer)	C8H3Cl3O	220	1407
1160	trichlorobenzofuran (isomer)	C8H3Cl3O	220	1444
1161	trichlorodiphenyl (isomer)	C12H7Cl3	256	1681
1162	trichlorodiphenyl (isomer)	C12H7Cl3	256	1728
1163	trichlorodiphenyl (isomer)	C12H7Cl3	256	1732
1164	trichlorodiphenyl (isomer)	C12H7Cl3	256	1747
1165	trichlorodiphenyl (isomer)	C12H7Cl3	256	1760
1166	trichlorodiphenyl (isomer)	C12H7Cl3	256	1763
1167	trichlorodiphenyl (isomer)	C12H7Cl3	256	1800
1168	trichlorodiphenyl (isomer)	C12H7Cl3	256	1815
1169	trichlorodiphenyl (isomer)	C12H7Cl3	256	1834
1170	trichlorodiphenyl (isomer)	C12H7Cl3	256	1845
1171	trichlorodiphenylether	C12H7Cl3O	272	1877
1172	trichloronaphthalene (isomer)	C10H5Cl3	230	1666
1173	trichloronaphthalene (isomer)	C10H5Cl3	230	1677
1174	trichloronaphthalene (isomer)	C10H5Cl3	230	1739
1175	2,4,5-trichlorophenol	C6H3Cl3O	196	1322
1176	2,4,6-trichlorophenol	C6H3Cl3O	196	1315
1177	trichloropyrene	C16H7Cl3	304	2644
1178	trichlorostyrene (isomer)	C8H5Cl3	206	1292
1179	trichlorostyrene (isomer)	C8H5Cl3	206	1311
1180	trichlorostyrene (isomer)	C8H5Cl3	206	1337
1181	trichlorostyrene (isomer)	C8H5Cl3	206	1346
1182	trichlorostyrene (isomer)	C8H5Cl3	206	1355
1183	trichlorostyrene (isomer)	C8H5Cl3	206	1375
1184	trichlorostyrene (isomer)	C8H5Cl3	206	1384
1185	trichlorostyrene (isomer)	C8H5Cl3	206	1387
1186	trichlorostyrene (isomer)	C8H5Cl3	206	1408
1187	trichlorostyrene (isomer)	C8H5Cl3	206	1411
1188	trichlorostyrene (isomer)	C8H5Cl3	206	1419
1189	trichlorostyrene (isomer)	C8H5Cl3	206	1462
1190	trichlorostyrene (isomer)	C8H5Cl3	206	1467

compound	formula	M.W.	PTI
1191 trichlorostyrene (isomer)	C8H5Cl3	206	1481
1192 trichlorostyrene (isomer)	C8H5Cl3	206	1499
1193 trichlorostyrene (isomer)	C8H5Cl3	206	1513
1194 trichlorostyrene (isomer)	C8H5Cl3	206	1543
1195 trichlorostyrene (isomer)	C8H5Cl3	206	1550
1196 trichlorostyrene (isomer)	C8H5Cl3	206	1594
1197 n-tricosanal	C23H46O	338	2511
1198 tricresyl phosphate (isomer)	C21H21O4P	368	2563
1199 tricresyl phosphate (isomer)	C21H21O4P	368	2591
1200 tricresyl phosphate (isomer)	C21H21O4P	368	2621
1201 n-tridecanoic acid	C13H26O2	214	1669
1202 n-tridecanol	C13H26O	198	1489
1203 2-tridecanone	C13H26O	198	1475
1204 triethyl phosphate	C6H15O4P	182	1087
1205 trimethyl phosphate	C3H9O4P	140	< 1000
1206 2,3,5-trimethylanisole	C10H14O	150	1208
1207 2,3,6-trimethylanisole	C10H14O	150	1163
1208 2,4,6-trimethylanisole	C10H14O	150	1139
1209 2,4,6-trimethylbenzoic acid	C10H12O2	164	1402
1210 2,3,5-trimethylphenol	C9H12O	136	1242
1211 2,3,6-trimethylphenol	C9H12O	136	1201
1212 2,4,6-trimethylphenol	C9H12O	136	1173
1213 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2427
1214 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2456
1215 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2474
1216 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2479
1217 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2490
1218 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2503
1219 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2512
1220 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2521
1221 trioxyethylene nonylphenylether (isomer)	C21H36O4	352	2537
1222 triphenyl phosphate	C18H15O4P	326	2311
1223 triphenylene	C18H12	228	2361
1224 triphenylene-quinone	C18H10O2	258	2488
1225 tripropylene glycol (isomer)	C9H20O4	192	1273
1226 tripropylene glycol (isomer)	C9H20O4	192	1278
1227 tripropylene glycol (isomer)	C9H20O4	192	1284
1228 tripropylene glycol (isomer)	C9H20O4	192	1288
1229 tripropylene glycol (isomer)	C9H20O4	192	1291
1230 tripropylene glycol (isomer)	C9H20O4	192	1297
1231 tripropylene glycol (isomer)	C9H20O4	192	1307
1232 tripropylene glycol diacetate (isomer)	C13H24O6	276	1560
1233 tripropylene glycol diacetate (isomer)	C13H24O6	276	1562
1234 tripropylene glycol diacetate (isomer)	C13H24O6	276	1567
1235 tripropylene glycol diacetate (isomer)	C13H24O6	276	1572
1236 tripropylene glycol diacetate (isomer)	C13H24O6	276	1574
1237 tripropylene glycol diacetate (isomer)	C13H24O6	276	1578
1238 tripropylene glycol dibutyl ether (isomer)	C17H36O4	304	1706
1239 tripropylene glycol dibutyl ether (isomer)	C17H36O4	304	1717
1240 tripropylene glycol dibutyl ether (isomer)	C17H36O4	304	1719
1241 tripropylene glycol dibutyl ether (isomer)	C17H36O4	304	1725
1242 tripropylene glycol dibutyl ether (isomer)	C17H36O4	304	1735
1243 tripropylene glycol dibutyl ether (isomer)	C17H36O4	304	1741
1244 tripropylene glycol dibutyrate (isomer)	C17H32O6	332	1883
1245 tripropylene glycol dibutyrate (isomer)	C17H32O6	332	1887
1246 tripropylene glycol dibutyrate (isomer)	C17H32O6	332	1899
1247 tripropylene glycol dibutyrate (isomer)	C17H32O6	332	1908
1248 tripropylene glycol dibutyrate (isomer)	C17H32O6	332	1913
1249 tripropylene glycol dibutyrate (isomer)	C17H32O6	332	1917
1250 tripropylene glycol dibutyrate (isomer)	C17H32O6	332	1921
1251 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1372
1252 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1380
1253 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1383
1254 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1389
1255 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1392
1256 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1395
1257 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1400
1258 tripropylene glycol diethyl ether (isomer)	C13H28O4	248	1405
1259 tripropylene glycol dihexyl ether (isomer)	C21H44O4	360	2065
1260 tripropylene glycol dihexyl ether (isomer)	C21H44O4	360	2076

	compound		formula	M.W.	PTR
1261	tripropylene glycol	dihexyl ether (isomer)	C21H44O4	360	2081
1262	tripropylene glycol	dihexyl ether (isomer)	C21H44O4	360	2084
1263	tripropylene glycol	dihexyl ether (isomer)	C21H44O4	360	2096
1264	tripropylene glycol	dihexyl ether (isomer)	C21H44O4	360	2102
1265	tripropylene glycol	dihexyl ether (isomer)	C21H44O4	360	2107
1266	tripropylene glycol	dioctyl ether (isomer)	C25H52O4	416	2430
1267	tripropylene glycol	dioctyl ether (isomer)	C25H52O4	416	2442
1268	tripropylene glycol	dioctyl ether (isomer)	C25H52O4	416	2450
1269	tripropylene glycol	dioctyl ether (isomer)	C25H52O4	416	2464
1270	tripropylene glycol	dioctyl ether (isomer)	C25H52O4	416	2474
1271	tripropylene glycol	dioctyl ether (isomer)	C25H52O4	416	2479
1272	tripropylene glycol	dipropionate (isomer)	C15H28O6	304	1727
1273	tripropylene glycol	dipropionate (isomer)	C15H28O6	304	1739
1274	tripropylene glycol	dipropionate (isomer)	C15H28O6	304	1751
1275	tripropylene glycol	dipropionate (isomer)	C15H28O6	304	1756
1276	tripropylene glycol	dipropionate (isomer)	C15H28O6	304	1759
1277	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1486
1278	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1492
1279	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1499
1280	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1505
1281	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1511
1282	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1523
1283	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1527
1284	tripropylene glycol	monobutyl ether (isomer)	C13H28O4	248	1532
1285	tripropylene glycol	monobutyrate (isomer)	C13H26O5	262	1582
1286	tripropylene glycol	monobutyrate (isomer)	C13H26O5	262	1594
1287	tripropylene glycol	monobutyrate (isomer)	C13H26O5	262	1599
1288	tripropylene glycol	monobutyrate (isomer)	C13H26O5	262	1604
1289	tripropylene glycol	monobutyrate (isomer)	C13H26O5	262	1607
1290	tripropylene glycol	monobutyrate (isomer)	C13H26O5	262	1621
1291	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1313
1292	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1314
1293	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1319
1294	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1325
1295	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1329
1296	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1332
1297	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1335
1298	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1341
1299	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1348
1300	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1350
1301	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1353
1302	tripropylene glycol	monoethyl ether (isomer)	C11H24O4	220	1360
1303	tripropylene glycol	monohexyl ether (isomer)	C15H32O4	276	1672
1304	tripropylene glycol	monohexyl ether (isomer)	C15H32O4	276	1687
1305	tripropylene glycol	monohexyl ether (isomer)	C15H32O4	276	1692
1306	tripropylene glycol	monohexyl ether (isomer)	C15H32O4	276	1695
1307	tripropylene glycol	monohexyl ether (isomer)	C15H32O4	276	1701
1308	tripropylene glycol	monooctyl ether (isomer)	C17H36O4	304	1864
1309	tripropylene glycol	monooctyl ether (isomer)	C17H36O4	304	1872
1310	tripropylene glycol	monooctyl ether (isomer)	C17H36O4	304	1879
1311	tripropylene glycol	monooctyl ether (isomer)	C17H36O4	304	1883
1312	tripropylene glycol	monooctyl ether (isomer)	C17H36O4	304	1888
1313	tripropylene glycol	monooctyl ether (isomer)	C17H36O4	304	1893
1314	tripropylene glycol	monooctyl ether (isomer)	C17H36O4	304	1908
1315	tripropylene glycol	monopropionate (isomer)	C12H24O5	248	1502
1316	tripropylene glycol	monopropionate (isomer)	C12H24O5	248	1512
1317	tripropylene glycol	monopropionate (isomer)	C12H24O5	248	1517
1318	tripropylene glycol	monopropionate (isomer)	C12H24O5	248	1524
1319	tripropylene glycol	monopropionate (isomer)	C12H24O5	248	1539
1320	tris(butoxyethyl) phosphate		C18H39O7P	398	2363
1321	tris(2-chloroethyl) phosphate		C6H12Cl3O4P	284	1689
1322	tris(1,3-dichloro-2-propyl)phosphate		C9H15Cl6O4P	428	2248
1323	tris(2-ethylhexyl) phosphate		C24H51O4P	434	2448
1324	n-undecanal		C11H22O	170	1285
1325	n-undecanoic acid		C11H22O2	186	1474
1326	2-undecanone		C11H22O	170	1271
1327	xanthene		C13H10O	182	1599
1328	xanthone		C13H8O2	196	1787
1329	2,3-xyleneol		C8H10O	122	1147
1330	2,4-xyleneol		C8H10O	122	1120

compound	formula	M.W.	PTRI
1331 2,6-xyleneol	C8H10O	122	1076
1332 3,4-xyleneol	C8H10O	122	1163
1333 3,5-xyleneol	C8H10O	122	1139
1334 2,5-xyleneol	C8H10O	122	1122
1335 2,3-xylylidine	C8H11N	121	1161
1336 2,4-xylylidine	C8H11N	121	1131
1337 2,5-xylylidine	C8H11N	121	1136
1338 2,6-xylylidine	C8H11N	121	1131
1339 3,4-xylylidine	C8H11N	121	1161
1340 3,5-xylylidine	C8H11N	121	1140

Table 3. Correlation PTRI and Carbon number in homologs

homologs	A	B	a)	b)
			R	N
n-Alkyl alcohol	240	101.39	1.000	7
n-Alkyl aldehyde	162	102.08	1.000	16
Methyl n-alkylcarboxylate	200	100.44	1.000	14
1-(n-Alkene)	-13	100.07	1.000	6
2-Alkanone	152	101.76	1.000	8
n-Alkylamine	213	101.87	1.000	6
Di-(n-alkylamine)	147	99.81	1.000	4
Tri-(n-alkylamine)	81	91.90	1.000	4
n-Alkylcarboxylic acid	405	97.28	1.000	9
Ethyl n-alkylcarboxylate	269	91.05	0.998	14
Allyl n-alkylcarboxylate	161	99.59	1.000	16
n-Propyl n-alkylcarboxylate	167	100.31	1.000	13
iso-Butyl n-alkylcarboxylate	122	100.33	1.000	12
n-Butyl n-alkylcarboxylate	161	100.42	1.000	12
n-Hexyl n-alkylcarboxylate	156	100.39	1.000	10
Cyclohexyl n-alkylcarboxylate	183	101.54	1.000	16
2-Ethylhexyl n-alkylcarboxylate	165	95.92	0.999	15
Benzyl n-alkylcarboxylate	206	100.69	1.000	15
Methoxyethyl n-alkylcarboxylate	285	99.54	1.000	13
Methoxypropyl n-alkylcarboxylate	222	98.71	1.000	17
Methoxybutyl n-alkylcarboxylate	247	98.72	1.000	14
Phenoxyethyl n-alkylcarboxylate	323	100.11	1.000	13
2-Hydroxyethyl n-alkylcarboxylate	362	103.51	1.000	14
Propyleneglycol ester of n-alkyl	328	100.63	1.000	14
n-Alkyl carbonamide	519	100.58	1.000	10

$$\text{PTRI} = A + B \times C_n$$

a) coefficient of correlation

b) compounds number determined

アリファチックな同族化合物群間には、分子内の炭素数と PTRI の間に直線関係がある。このことから、たとえ標準品が入手出来なくとも、他の同族体の PTRI から容易に推定出来る。本報では主な同族化合物群について、炭素数と PTRI の相関式を求め、Table 3 に示した。

GC の保持指標に関する報告は多数あるが、環境汚染物質の検索同定と言う観点から見ると、対象物質や液相及び基準化合物等の不統一性から至便性に問題点も多い。農薬や工業薬品等の環境汚染物質に関する保持指標の報告は利用価値が大きいが、その保持指標の表示法の不統一性から至便性に欠ける。そこで、それらのデータ

と本報との共通データの相関性から、PTRI に変換すべく現在検討中である。

農薬の PTRI に関しては、すでに約 140 種について報告（水質汚濁研究 14(2), 109-122, 1991）したが、今回若干の補充をするとともに、農薬の酸化生成物についても追加集積した。

なお、GC 保持指標に関する報告の中で、1984～1987 年の“Journal of Chromatography”誌に掲載されているものを参考資料として Table 4 に示した（著者名は筆頭者のみ示した）。

Table 4. List of Information for GC Retention Data in "Journal of Chromatography"

Compound	Column	Standard	Other	Vol.	Page	Year
chemicals from incinerator	DB-5		Tong	285	423-441	1984
alkanol, acetate, chloroacetate	SE-30 et al		Korhonen	285	443-455	1984
halogenated methyl propanoate & butanoate	OU-101		Korhonen	285	115-126	1984
alkanol, acetate, bromoacetate	SE-30 et al		Korhonen	287	399-406	1984
chlorinated veratrole (1,2-dimethoxybenzene)	SE-30 et al		Korhonen	287	293-303	1984
unsaturated alcohol, (acetyl, halogenoacetyl) deriv.	SE-30 et al		Korhonen	288	329-346	1984
halogenated acid ester	SE-30 et al		Korhonen	288	51-69	1984
phthalate (alkyl, benzyl)	OU-17		Dziwinski	288	221-226	1984
halogenated ester of carboxylic acid	OU-101 et al		Horna	290	45-55	1984
aromatic carboxylic acid	SE-52 et al		Wurst	291	145-153	1984
chlorinated phenoxyphenol	SE-54	time	Humppi	291	135-144	1984
chlorinated 4-hydroxybenzaldehyde	SE-30		Korhonen	292	345-353	1984
halogenoacetate of alcohol & halogenoethyl ester	SP-400		Komarek	292	105-115	1984
n-alkadiene (C8-C10)	squalane		Sojak	292	241-261	1984
perhydroaromatic hydrocarbon	SE-30 et al		Kiselev	292	97-103	1984
phthalate	SE-30 et al		Ishida	294	339-343	1984
chlorinated anisole	SE-30 et al		Korhonen	294	99-116	1984
anthraquinon deriv. (naturally occurring)	CP-sil 5 CB		Eijk	295	497-502	1984
chlorinated salicylaldehyde	SE-30 et al		Korhonen	298	101-114	1984
chloromethyl ester of n-carboxylic acid	SE-30 et al		Haken	298	150-158	1984
monochlorinated n-carboxylic ester	SE-30 et al		Haken	298	89-100	1984
wax ester	SP-2340		Itabashi	299	351-363	1984
mannitol acetal	OU-OU-101 et al		Tomori	299	87-96	1984
steroids	OU-1	time	Kwan	301	189-197	1984
hydroxy monocarboxylic acid (TMS)	OU-101 cap.		Allen	301	273-276	1984
meibomian gland lipid (deriv)	OU-1	time	Harvey	301	173-187	1984
hydroxy dicarboxylic acid (TMS)	OU-101 cap.		Allen	301	273-276	1984
alkene		PTRI	Raso	302	107-117	1984
alkyl iodide	C.W 20M pac. et al		Castello	303	61-66	1984
chlorophenol	SE-30 et al		Korhonen	303	197-205	1984
tetramethylguanidine	SE-30 pac.	PTRI	Oszczapowicz	315	95-100	1984
dimethylformamide	SE-30 pac.	PTRI	Oszczapowicz	315	95-100	1984
dimethylacetamide	SE-30 pac.	PTRI	Oszczapowicz	315	95-100	1984
alkyl alkoxysilane	Apiezon M et al	PTRI	Peetre	318	41-55	1985
carboxylic acid (aliphatic) ester	Squalane et al	PTRI	Bermejo	318	187-194	1985
PCB	M.S cap.	PTRI	Kozloski	318	211-219	1985
chlorobenzene	SE-30	PTRI	Sabljić	319	1-8	1985
monochlorobutanoate	SE-30 cap. et al		Korhonen	320	325-334	1985
butanoate	SE-30 cap. et al		Korhonen	320	325-334	1985
chloroanisole	SE-30 cap. et al		Korhonen	321	115-125	1985
chloroanisole	SE-30 cap. et al		Korhonen	321	467-474	1985
chloroveratrole	SE-30 cap. et al		Korhonen	321	467-474	1985
chlorophenol	SE-30 cap. et al		Korhonen	321	115-125	1985
chlorophenyl acetate	SE-30 cap. et al		Korhonen	321	115-125	1985
nitro polynuclear aromatic hydrocarbon	SE-30 cap. et al	C14	Korhonen	322	71-81	1985
benzoate	SE-30 cap. et al	PTRI	Korhonen	322	83-96	1985
carboxylic acid ester (ethyl, chloroethyl)	SE-30 cap. et al	C14	Korhonen	322	97-106	1985
monochlorobenzoate	SE-30 cap. et al	PTRI	Korhonen	322	83-96	1985
benzoate	SE-30 cap. et al	C14	Korhonen	323	331-342	1985
monochlorobenzoate	SE-30 cap. et al	C14	Korhonen	323	331-342	1985
pyrazine deriv.	OU-101 cap. et al	PTRI	Mihara	324	428-430	1985
propanoate	SE-30 cap. et al	C14	Korhonen	324	343-353	1985
carboxylic acid (branched) ester	OU-7 pac. et al		Chretien	324	355-362	1985
chloroethanol- ω	SE-30 cap. et al	C14	Korhonen	324	181-191	1985
alkyl bromide	Apiezon L pac et al	PTRI	Castello	324	363-371	1985
monochloropropanoate	SE-30 cap. et al	C14	Korhonen	324	343-353	1985
chlorinated hydroxybenzaldehyde	SE-30 cap. et al	C14	Korhonen	324	192-198	1985
benzoate (unsaturated ester)	SE-30 cap. et al	C14	Korhonen	324	113-127	1985
monochlorobenzoate (unsaturated ester)	SE-30 cap. et al	C14	Korhonen	324	113-127	1985
butanoate	SE-30 cap. et al	PTRI	Haken	325	61-73	1985
monochlorobenzoate (ethyl chloroethyl)	SE-30 cap. et al	C14	Korhonen	325	433-443	1985
benzoate (ethyl chloroethyl)	SE-30 cap. et al	C14	Korhonen	325	433-443	1985
acrylate	OU-101 cap. et al	PTRI	Horna	325	367-378	1985
ketone	SE-30 cap.	2-ketone	Raymer	325	13-22	1985
methacrylate	OU-101 cap. et al	PTRI	Horna	325	367-378	1985
monochlorobutanoate	SE-30 cap. et al	PTRI	Haken	325	61-73	1985

Table 4. (Continued)

Compound	Column	Standard	Other	Vol.	Page	Year
pentafluoro benzoate	SE-30 cap. et al	C14	Korhonen	328	325-332	1985
halogenated	M.S. cap.	bromoalka	Yasuhara	328	35-48	1985
benzoate	SE-30 cap. et al	C14	Korhonen	328	325-332	1985
benzoate	SE-30 cap. et al	C14	Korhonen	329	359-369	1985
pentafluoro benzoate	SE-30 cap. et al	C14	Korhonen	329	359-369	1985
carboxylic acid (aliphatic) chloroethyl ester	SE-30 cap. et al	PTRI	Korhonen	329	43-56	1985
polyoxyethylene glycol ether S-analogue		PTRI	Szymanowski	330	61-70	1985
dimethylbenzamide	SE-30 pac.	PTRI	Oszczapowicz	330	79-85	1985
polyoxyethylene glycol ether		PTRI	Szymanowski	330	61-70	1985
PCB	OU-101 pac. et al		William	330	203-216	1985
benzylideneamine	SE-30 pac.	PTRI	Oszczapowicz	330	79-85	1985
alkane deriv.	OU-1 cap. et al	PTRI	Kusmierz	331	219-228	1985
vesicant	DB-1 cap. et al	PTRI	D'agostino	331	47-54	1985
irritants	DB-1 cap. et al	PTRI	D'agostino	331	47-54	1985
phosphorous	DB-1 cap. et al	PTRI	D'agostino	331	47-54	1985
PCDD PCDF	SE-54 cap. et al		Humppi	331	410-418	1985
arylaliphatic acid	Apolane 87 pac.	PTRI	Kuchar	333	21-28	1985
fatty acid (methyl ester)	SP 2560		Alexander	342	1-12	1985
amino acid (TAB deriv.)	OU-101		Schneider	345	19-31	1985
alkylbenzene (long chain)	SE-54 cap		Takada	346	281-290	1985
N,N-dialkylformamide	SE-30	PTRI	Osek	351	177-182	1986
volatile (H.C S compound)	SE-52	PTRI	Langenhove	351	65-75	1986
hydrocarbon	squalane	PTRI	Krupcik	351	111-121	1986
alkylchloride	C.W 20M et al		Castello	354	65-74	1986
alkylbenzothiophene	DB-5 cap. et al		Andersson	354	83-98	1986
n-alkene, n-alkane	PBO		Sojak	356	105-114	1986
benzoic acid (4-nitro, 3,5-dinitro)ester	SE-30 cap. ea al		Korhonen	356	285-299	1986
carboxylic (aromatic)acid ester	SE-30 et al		Kuchar	356	95-103	1986
monochlorinated n-alkyl acetate	SE-30 cap. et al		Haken	356	79-94	1986
halopropionate	OU-101 et al		Komarek	357	273-281	1986
amine, dimethylformamide, dimethylacetamide	OU-225	PTRI	Oszczapowicz	357	93-99	1986
4-nitro, 3,5-dinitrobenzoic acid ester	SE-30 et al	C14	Korhonen	357	107-118	1986
chlorinated n-alkyl acetate	SE-30 et al		Haken	357	253-271	1986
polycyclic aromatic (alkyl deriv.)	SE-54	C20	Nishioka	357	79-91	1986
amino acid (t-butyl dimethylsilyl)	SE-30 OU-17		Mawhinney	358	231-242	1986
benzoic 4-nitro 3,5-dinitrobenzoic acid ester	SE-30 et al		Korhonen	360	63-78	1986
dicarboxylic acid dimethyl ester	ultra-1	PTRI	Herrmann	360	79-88	1986
non-ionic surfactant	OU-17 pac.		Szymanowski	360	43-52	1986
QM-siloxane	OU-1 cap.		Reiher	360	33-42	1986
acrylic acid and methacrylic acid ester	OU-101 et al		Horna	360	89-104	1986
mono di tricarboxylic acid (t-butyl dimethylsilyl)	SE-30 OU-17 cap.		Mawhinney	361	117-130	1986
amine	OU-101 et al		Osmialowski	361	63-69	1986
diol (1,2- 1,3-) cyclic ferroceneboronate	OU-1	PTRI	Brooks	362	113-116	1986
amidine	SE-30	PTRI	Oszczapowicz	362	383-389	1986
aromatic carboxylic acid ester	SE-30 ey al	C14	Korhonen	363	277-292	1986
alkylbenzene			Golovnya	364	193-202	1986
amine			Golovnya	364	193-202	1986
sulphur containing compound	Apiezon M OU-17		Grigoryeva	364	63-77	1986
halocarbon (C1-C2)	OU-1 Sp-1000 mix		Castello	366	59-68	1986
carboxylic acid halogenoethyl ester	SE-54		Horna	366	91-105	1986
alkyl halogenoacetate	SE-54		Horna	366	91-105	1986
alkyl benzyl maleate	OU-101 pac.		Dziwinski	367	201-206	1986
pesticide	SE-30 et al	PTRI	Osselton	368	265-271	1986
dicarboxylic acid (TMS)	ultra-1	PTRI	Herrmann	370	49-61	1986
pesticide, drug (N P contain)	ultra-1	PTRI	Tamayo	374	73-85	1986
non-ionic surfactant	SE-30 et al	PTRI	Voelkel	387	95-104	1987
pyridine (substituted)	DB-5 cap. et al	pyridine	Premecz	388	23-35	1987
halogenated cyclohexane, benzene, anisole	H.C. et al	PTRI	Evans	389	240-244	1987
alkylbezothiophene, alkyl dibenzothiophene	OU-73 cap.		Arpino	390	329-348	1987
alkylquinoline	OU-101 cap. et al		Buryan	391	89-96	1987
monoalkylcyclopentadien	squalane CW 20M	PTRI	Sojak	391	79-87	1987
PCDD	DB-5 cap.	PTRI	Donnelly	392	51-63	1987
hydrocarbon	OU-1	R Time	Onodera	392	295-308	1987
pesticide, industrial.	OU-101 pac.		Saxton	393	175-194	1987
alkylphenanthren	Silar 10c cap. et al		Garrigues	395	217-228	1987
aromatic carboxylic acid ester	SE-30 et al	PTRI	Kuchar	398	43-51	1987
PAH deriv.	DB-5		Naikwadi	398	227-237	1987
pyrazine	OU-101 et al		Mihara	402	309-317	1987
n-alkene	OU-101	PTRI	Rang	406	75-80	1987
hydrocarbon (gasoline)	OU-101		Krupcik	407	65-77	1987
volatile	OU-17	PTRI	Uehori	411	251-257	1987

4. おわりに

今回1340種の化合物のPTRIについて報告した。環境汚染物質に重点を置いたつもりであるが、必ずしも満足できるものではない。化学物質による環境汚染の未然防止と言う観点からGC/MS検索を考えると、マススペクトルデータの蓄積は当然であるが、PTRIデータの蓄積も重要である。さらに、キャピラリーカラムの普及から、PTRIデータもキャピラリーカラムしかもメチルシリコ

ン系に主眼を置き、n-アルカンを基準としたPTRI表示に統一したデータを蓄積することが至便的と考えられる。本PTRIデータが、化学物質安全対策に資することを期待したい。

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