Antoine Coefficients

log(P) = A-B/(T+C) where P is in mmHg and T is in Celsius

ID formula compound name A B C Tmin Tmax ?? ?

1 CCL4 carbon-tetrachloride 6.89410 1219.580 227.170 -20 101 Y2 0

2 CCL3F trichlorofluoromethane 6.88430 1043.010 236.860 -33 27 Y2 0

3 CCL2F2 dichlorodifluoromethane 6.68619 782.072 235.377 -119 -30 Y6 0

4 CCLF3 chlorotrifluoromethane 6.35109 522.061 231.677 -150 -81 Y6 0

5 CF4 carbon-tetrafluoride 6.97230 540.500 260.100 -180 -125 Y1 0

6 CO carbon-monoxide 6.24020 230.270 260.010 -210 -165 Y2 0

7 CO2 carbon-dioxide 9.81060 1347.790 273.000 -119 -69 Y2 0

8 COS carbonyl-sulfide 6.90723 804.480 250.000 -111 -49 Y5 0

9 CS2 carbon-disulfide 6.94190 1168.620 241.540 -45 69 Y2 0

10 CHCL3 chloroform 6.93710 1171.200 227.000 -13 97 Y2 0

11 CHCL2F dichlorofluoromethane 6.97575 996.267 234.172 -91 9 Y6 0

12 CHCLF2 chlorodifluoromethane 6.75770 740.390 231.860 -48 -33 Y2 0

13 CHF3 trifluoromethane 7.08860 705.330 249.780 -128 -82 Y4 0

14 CHI3 triiodomethane 6.59598 1567.8 204. 137 254 N 19

15 CHNS isothiocyanic-acid 0.00000 0.000 0.000 0 0 0

16 CH2CL2 dichloromethane 7.08030 1138.910 231.460 -44 59 Y2 0

17 CH2CLF chlorofluoromethane 6.20452 740.39 231.86 -55 12 N 12

18 CH2F2 difluoromethane 7.13890 821.700 244.700 -82 -32 Y4 0

19 CH2I2 diiodomethane 6.94246 1567.800 204.000 83 232 Y10 0

20 CH2O formaldehyde 7.15610 957.240 243.010 -88 -2 Y2 0

21 CH2O2 formic-acid 7.37790 1563.280 247.070 -2 136 Y1 0

22 CH3BR bromomethane 6.95970 986.590 238.330 -58 53 Y2 0

23 CH3CL chloromethane 6.99440 902.450 243.610 -93 -7 Y2 0

24 CH3F fluoromethane 7.09760 740.220 253.890 -132 -64 Y2 0

25 CH3I iodomethane 6.98800 1146.340 236.660 -13 52 Y2 0

26 CH3NO2 nitromethane 7.04400 1291.000 209.010 5 136 Y2 0

27 CH3NO2 methyl-nitrite 0.00000 0.000 0.000 0 0 0

28 CH3NO3 methyl-nitrate 0.00000 0.000 0.000 0 0 0

29 CH4 methane 6.69561 405.420 267.777 -181 -152 Y3 0

30 CH4O methanol 8.07240 1574.990 238.870 -16 91 Y2 0

31 CH4S methanethiol 7.03163 1015.547 238.706 -70 25 Y3 0

32 CH5N methylamine 7.49690 1079.150 240.240 -61 38 Y2 0

33 C2CL4 tetrachloroethene 7.02000 1415.490 221.010 34 187 Y2 0

34 C2CL6 hexachloroethane 7.08633 1626.945 197.048 33 186 Y6 0

35 C2CL3F3 112trichlorotrifluoroethane 6.88030 1099.900 227.500 -25 83 Y4 0

36 C2CL2F4 12dichlorotetrafluoroethane 6.87084 942.336 232.632 -95 4 Y6 0

37 C2CLF5 chloropentafluoroethane 6.83330 802.970 242.280 -98 -43 Y2 0

38 C2F4 tetrafluoroethene 6.89660 683.840 245.940 -133 -63 Y2 0

39 C2F6 hexafluoroethane 6.79330 657.060 246.220 -103 -73 Y2 0

40 C2N2 cyanogen 6.43629 576.579 182.308 -77 -4 Y7 0

41 C2HCL3 trichloroethene 7.02810 1315.100 230.010 -13 127 Y2 0

42 C2HCL5 pentachloroethane 6.74000 1378.000 197.000 25 162 Y4 0

43 C2HF3 trifluoroethene 5.68715 491.359 227.23 -93 -31 N 49

44 C2H2 acetylene(ethyne) 9.14020 1232.600 280.900 -129 -83 Y3 0

45 C2H2CL2 1,1-dichloroethene 6.97220 1099.400 237.200 -28 32 Y4 0

46 C2H2CL2 cis-1,2-dichloroethene 7.02230 1205.400 230.600 0 84 Y4 0

47 C2H2CL2 trans-1,2-dichloroethene 6.96510 1141.900 231.900 -38 85 Y4 0

48 C2H2CL4 1,1,2,2-tetrachloroethane 6.63170 1228.100 179.900 25 130 Y4 0

49 C2H2F2 1,1-difluoroethene 6.34918 491.359 227.239 -140 -86 Y7 0

50 C2H2F2 cis-1,2-difluoroethene 5.31401 491.359 227.23 -78 2.6 N 49

51 C2H2F2 trans-1,2-difluoroethene 5.31401 491.359 227.23 -78 2.6 N 49

52 C2H2O ketene 6.95730 803.100 238.010 -103 -18 Y2 0

53 C2H3BR bromoethylene 7.24379 1219.308 264.021 -88 16 Y6 0

54 C2H3CL chloroethene 6.49710 783.400 230.010 -88 17 Y2 0

55 C2H3CL3 1,1,2-trichloroethane 6.96530 1351.000 217.000 29 155 Y2 0

56 C2H3CLO acetyl-chloride 6.84070 1062.860 217.630 -36 82 Y2 0

57 C2H3F fluoroethene 6.33949 593.551 243.111 -149 -72 Y6 0

58 C2H3F3 1,1,1-trifluoroethane 6.90380 788.210 243.240 -3 27 Y2 0

59 C2H3N acetonitrile 7.07350 1279.200 224.010 -13 117 Y2 0

60 C2H4 ethylene 6.74756 585.000 255.000 -153 -91 Y3 0

61 C2H4BR2 1,2-dibromoethane 6.72148 1280.820 201.750 52 131 Y4 0

62 C2H4CL2 1,1-dichloroethane 6.98530 1171.420 228.130 -31 79 Y2 0

63 C2H4CL2 1,2-dichloroethane 7.02530 1271.250 222.940 -33 100 Y2 0

64 C2H4F2 1,1-difluoroethane 7.03000 910.000 244.000 -35 0 Y2 0

65 C2H4I2 1,2-diiodoethane 6.98834 1647.100 201.000 98 253 Y10 0

66 C2H4O ethylene-oxide 7.27010 1115.100 244.150 -73 37 Y2 0

67 C2H4O acetaldehyde 7.05650 1070.600 236.010 -63 47 Y2 0

68 C2H4O2 acetic-acid 7.29960 1479.020 216.820 17 157 Y2 0

69 C2H4O2 methyl-formate 7.17040 1125.200 230.560 -48 51 Y2 0

70 C2H4OS thioacetic-acid 7.74889 1479.02 216.82 40 106 N 68

71 C2H4S thiacyclopropane 7.03725 1194.370 232.420 -35 77 Y3 0

72 C2H5BR bromoethane 6.92000 1090.810 231.720 -47 60 Y2 0

73 C2H5CL chloroethane 6.94000 1012.780 236.680 -73 37 Y2 0

74 C2H5F fluoroethane 6.97850 854.210 246.160 -103 -21 Y2 0

75 C2H5I iodoethane 6.95900 1232.000 229.000 30 60 Y4 0

76 C2H5N ethylenimine 7.13230 1133.700 210.010 -25 86 Y2 0

77 C2H5NO2 nitroethane 7.58777 1671.266 241.187 -21 114 Y6 0

78 C2H5NO3 ethyl-nitrate 7.16370 1338.800 224.900 0 60 Y4 0

79 C2H6 ethane 6.83452 663.700 256.470 -143 -75 Y3 0

80 C2H6O methyl-ether 7.31640 1025.560 256.060 -94 -8 Y2 0

81 C2H6O ethyl-alcohol 8.21330 1652.050 231.480 -3 96 Y2 0

82 C2H6O2 ethylene-glycol 8.79450 2615.400 244.910 91 221 Y1 0

83 C2H6S methyl-sulfide 6.94879 1090.755 230.799 -47 58 Y3 0

84 C2H6S ethanethiol 6.95206 1084.531 231.385 -49 56 Y3 0

85 C2H6S2 methyl-disulfide 6.97792 1346.342 218.863 6 135 Y3 0

86 C2H7N ethylamine 7.38620 1137.300 235.860 -58 43 Y2 0

87 C2H7N dimethylamine 7.06390 1024.400 238.010 -55 37 Y2 0

88 C3H3N acrylonitrile 6.91630 1208.300 222.010 -18 112 Y1 0

89 C3H4 allene(propadiene) 5.71370 458.060 196.070 -99 -16 Y3 0

90 C3H4 propyne(methylacetylene) 6.78485 803.730 229.080 -90 -6 Y3 0

91 C3H4O2 acrylic-acid 7.19260 1441.500 193.010 42 177 Y1 0

92 C3H5BR 3-bromo-1-propene 7.05187 1259.83 232.04 17 93 N 109

93 C3H5CL 3-chloro-1-propene 6.93880 1099.600 226.010 -43 77 Y2 0

94 C3H5CL3 1,2,3-trichloropropane 7.00280 1484.100 204.010 42 197 Y1 0

95 C3H5I 3-iodo-1-propene 6.96930 1316.500 220.000 20 142 Y10 0

96 C3H5N propionitrile 6.93010 1277.200 218.010 -3 132 Y2 0

97 C3H6 propene 6.81960 785.000 247.000 -112 -32 Y3 0

98 C3H6 cyclopropane 6.88790 856.010 246.510 -93 -28 Y2 0

99 C3H6BR2 1,2-dibromopropane 6.89105 1419.600 212.000 50 250 Y4 0

100 C3H6CL2 1,2-dichloropropane 6.96540 1296.400 221.000 15 135 Y2 0

101 C3H6CL2 1,3-dichloropropane 6.97186 1376.200 216.000 34 162 Y10 0

102 C3H6CL2 2,2-dichloropropane 6.94820 1201.100 226.000 -6 105 Y10 0

103 C3H6I2 1,2-diiodopropane 6.0765 1507.41 244.7 125 275 N 115

104 C3H6O propylene-oxide 6.65460 915.310 208.290 -48 67 Y2 0

105 C3H6O allyl-alcohol 7.34240 1271.700 188.010 13 127 Y1 0

106 C3H6O propionaldehyde 7.04930 1154.800 229.010 -38 77 Y2 0

107 C3H6O acetone 7.23160 1277.030 237.230 -32 77 Y2 0

108 C3H6S thiacyclobutane 7.01667 1321.331 224.513 -5 120 Y3 0

109 C3H7BR 1-bromopropane 7.03766 1259.836 232.042 -53 71 Y6 0

110 C3H7BR 2-bromopropane 7.00463 1223.475 236.508 -62 60 Y6 0

111 C3H7CL 1-chloropropane 6.93110 1121.120 230.210 -43 77 Y2 0

112 C3H7CL 2-chloropropane 6.96540 1081.600 230.010 -48 67 Y1 0

113 C3H7F 1-fluoropropane 6.95330 965.180 239.500 -70 30 Y10 0

114 C3H7F 2-fluoropropane 7.07451 965.18 239.5 -49 8 N 113

115 C3H7I 1-iodopropane 7.22121 1507.410 244.701 -36 103 Y6 0

116 C3H7I 2-iodopropane 7.01670 1340.448 234.365 -43 90 Y6 0

117 C3H7NO2 1-nitropropane 7.11460 1467.450 215.230 59 131 Y4 0

118 C3H7NO2 2-nitropropane 7.48654 1664.036 240.995 -19 120 Y6 0

119 C3H7NO3 propyl-nitrate 7.73719 1721.723 245.490 0 70 Y6 0

120 C3H7NO3 isopropyl-nitrate 6.42006 1018.568 183.528 0 70 Y6 0

121 C3H8 propane 6.80398 803.810 246.990 -108 -25 Y3 0

122 C3H8O ethyl-methyl-ether 5.88190 504.490 160.760 -68 37 Y2 0

123 C3H8O propyl-alcohol 7.61920 1375.140 193.010 12 127 Y2 0

124 C3H8O isopropyl-alcohol 8.11820 1580.920 219.620 0 101 Y2 0

125 C3H8S ethyl-methyl-sulfide 6.93849 1182.562 224.784 -26 90 Y3 0

126 C3H8S 1-propanethiol 6.92846 1183.307 224.624 -25 91 Y3 0

127 C3H8S 2-propanethiol 6.87734 1113.895 226.157 -37 75 Y3 0

128 C3H9N propylamine 6.94680 1108.200 224.010 -38 77 Y2 0

129 C3H9N trimethylamine 6.97040 968.700 234.010 -58 32 Y2 0

130 C4F8 octafluorocyclobutane 6.81530 862.490 225.150 -32 1 Y1 0

131 C4H2 butadiyne(biacetylene) 5.51917 460.684 164.594 -78 0 Y6 0

132 C4H4 1buten3yne(vinylacetylene) 6.95300 957.000 230.010 -73 32 Y1 0

133 C4H4O furan 6.97530 1060.850 227.750 -35 90 Y1 0

134 C4H4S thiophene 6.95926 1246.020 221.350 -12 108 Y3 0

135 C4H6 1,2-butadiene 6.99383 1041.117 242.274 -26 30 Y3 0

136 C4H6 1,3-butadiene 6.84999 930.546 238.854 -58 14 Y3 0

137 C4H6 1-butyne(ethylacetylene) 6.98198 988.750 233.010 -68 27 Y3 0

138 C4H6 2-butyne(dimethylacetylene) 7.07338 1101.710 235.810 -30 47 Y3 0

139 C4H6 cyclobutene 6.95769 1009.320 244.986 -77 2 Y6 0

140 C4H6O3 acetic-anhydride 7.12160 1427.770 198.050 35 164 Y2 0

141 C4H7N butyronitrile 7.03960 1390.700 217.000 34 160 Y2 0

142 C4H7N isobutyronitrile 7.21591 1390.7 217 49 127 N 141

143 C4H8 1-butene 6.84290 926.100 240.000 -81 13 Y3 0

144 C4H8 2-butene,cis 6.86926 960.100 237.000 -73 23 Y3 0

145 C4H8 2-butene,trans 6.86952 960.800 240.000 -76 20 Y3 0

146 C4H8 2-methylpropene 6.84134 923.200 240.000 -82 12 Y3 0

147 C4H8 cyclobutane 6.91630 1024.540 241.380 -73 17 Y2 0

148 C4H8BR2 1,2-dibromobutane 7.25696 1759.076 235.009 8 166 Y6 0

149 C4H8BR2 2,3-dibromobutane 7.20023 1691.481 230.223 5 161 Y6 0

150 C4H8I2 1,2-diiodobutane 6.2433 1507.41 244.7 110 246 N 115

151 C4H8O butyraldehyde 7.02120 1233.000 223.010 -18 107 Y2 0

152 C4H8O 2-butanone 7.20870 1368.210 236.510 -16 103 Y2 0

153 C4H8O2 p-dioxane 7.00630 1288.500 211.010 2 137 Y2 0

154 C4H8O2 ethyl-acetate 7.01460 1211.900 216.010 -13 112 Y2 0

155 C4H8S thiacyclopentane 6.99540 1401.939 219.607 14 147 Y3 0

156 C4H9BR 1-bromobutane 6.92254 1298.608 219.700 19 141 Y10 0

157 C4H9BR 2-bromobutane 6.82724 1229.080 220.000 10 146 Y9 0

158 C4H9BR 2-bromo-2-methylpropane 6.66850 1129.700 225.000 -7 110 Y10 0

159 C4H9CL 1-chlorobutane 6.93790 1227.430 224.110 -18 112 Y2 0

160 C4H9CL 2-chlorobutane 6.94470 1195.800 226.010 -23 102 Y1 0

161 C4H9CL 1-chloro-2-methylpropane 6.95304 1205.079 227.046 -54 69 Y6 0

162 C4H9CL 2-chloro-2-methylpropane 6.86710 1114.900 229.010 -38 87 Y1 0

163 C4H9I 2-iodo-2-methylpropane 7.2539 1507.41 244.7 42 124 N 115

164 C4H9N pyrrolidine 6.92460 1179.990 205.260 27 127 Y2 0

165 C4H9NO2 1-nitrobutane 6.86715 1467.45 215.23 86 182 N 117

166 C4H9NO2 2-nitrobutane 7.25197 1664.03 240.99 75 167 N 118

167 C4H10 butane 6.80896 935.860 238.730 -78 19 Y3 0

168 C4H10 2-methylpropane(isobutane) 6.91048 946.350 246.680 -87 7 Y3 0

169 C4H10O ethyl-ether 6.92032 1064.070 228.800 -61 20 Y4 0

170 C4H10O methyl-propyl-ether 6.11860 708.690 179.900 0 39 Y4 0

171 C4H10O methyl-isopropyl-ether 6.24495 708.69 179.9 -12 51 N 170

172 C4H10O butyl-alcohol 7.47680 1362.390 178.730 15 131 Y2 0

173 C4H10O sec-butyl-alcohol 7.47430 1314.190 186.510 25 120 Y2 0

174 C4H10O tert-butyl-alcohol 7.31990 1154.480 177.660 20 103 Y2 0

175 C4H10S ethylsulfide 6.92836 1257.833 218.662 -6 117 Y3 0

176 C4H10S isopropyl-methyl-sulfide 6.90196 1232.170 221.670 -13 109 Y3 0

177 C4H10S methyl-propyl-sulfide 6.95545 1284.320 219.660 -4 120 Y3 0

178 C4H10S 1-butanethiol 6.92754 1281.018 218.100 -2 123 Y3 0

179 C4H10S 2-butanethiol 6.88698 1229.904 222.021 -13 109 Y3 0

180 C4H10S 2-methyl-1-propanethiol 6.88746 1237.282 220.313 -10 113 Y3 0

181 C4H10S 2-methyl-2-propanethiol 6.78781 1115.565 221.314 1 87 Y3 0

182 C4H10S2 ethyl-disulfide 6.97507 1485.970 208.958 40 182 Y3 0

183 C4H11N butylamine 7.21300 1308.400 224.200 -14 100 Y2 0

184 C4H11N sec-butylamine 7.15069 1238.300 227.000 -9 98 Y10 0

185 C4H11N tert-butylamine 6.78309 993.262 210.493 19 75 Y6 0

186 C4H11N diethylamine 6.97240 1127.000 220.010 -31 77 Y2 0

187 C5H5N pyridine 6.98820 1344.200 212.010 12 152 Y2 0

188 C5H6S 2-methylthiophene 6.93897 1326.480 214.310 9 138 Y3 0

189 C5H6S 3-methylthiophene 6.98611 1363.840 216.780 11 141 Y3 0

190 C5H8 1,2-pentadiene 6.91820 1104.991 228.851 -20 66 Y3 0

191 C5H8 1,3-pentadiene,cis 6.91089 1101.923 229.367 -17 65 Y3 0

192 C5H8 1,3-pentadiene,trans 6.91317 1103.840 231.724 -16 63 Y3 0

193 C5H8 1,4-pentadiene 6.83543 1017.995 231.461 -33 46 Y3 0

194 C5H8 2,3-pentadiene 6.96216 1126.837 227.841 -13 69 Y3 0

195 C5H8 3-methyl-1,2-butadiene 6.94350 1103.901 230.890 -20 62 Y3 0

196 C5H8 2-methyl-1,3-butadiene 6.88564 1071.578 233.513 -18 55 Y3 0

197 C5H8 1-pentyne 6.96730 1092.520 227.190 -43 62 Y1 0

198 C5H8 2-pentyne 7.04614 1189.870 229.600 -33 78 Y4 0

199 C5H8 3-methyl-1-butyne 6.88480 1014.810 227.110 -55 47 Y4 0

200 C5H8 cyclopentene 6.92070 1121.810 233.460 -29 105 Y1 0

201 C5H8 spiropentane 6.91700 1090.080 231.100 3 71 Y4 0

202 C5H10 1-pentene 6.84650 1044.895 233.516 -55 51 Y3 0

203 C5H10 2-pentene,cis 6.87274 1067.951 230.585 -49 58 Y3 0

204 C5H10 2-pentene,trans 6.90575 1083.987 232.965 -49 58 Y3 0

205 C5H10 2-methyl-1-butene 6.87314 1053.780 232.788 -53 52 Y3 0

206 C5H10 3-methyl-1-butene 6.82618 1013.474 236.816 -63 41 Y3 0

207 C5H10 2-methyl-2-butene 6.91562 1095.088 232.842 -48 60 Y3 0

208 C5H10 cyclopentane 6.88676 1124.162 231.361 -40 72 Y3 0

209 C5H10BR2 2,3-dibromo-2-methylbutane 7.36735 1695.900 207.000 81 218 Y10 0

210 C5H10O valeraldehyde 7.01920 1316.000 215.010 4 139 Y1 0

211 C5H10O 2-pentanone 6.95000 1274.600 210.910 2 137 Y1 0

212 C5H10S thiacyclohexane 6.90518 1422.470 211.720 29 170 Y3 0

213 C5H10S cyclopentanethiol 6.91497 1388.630 212.050 81 173 Y4 0

214 C5H11BR 1-bromopentane 6.95580 1401.634 214.380 41 173 Y10 0

215 C5H11CL 1-chloropentane 6.96617 1332.890 218.500 24 148 Y10 0

216 C5H11CL 1-chloro-3-methylbutane 6.79527 1258.5 223 39 124 N 217

217 C5H11CL 2-chloro-2-methylbutane 6.95902 1258.500 223.000 7 123 Y10 0

218 C5H12 pentane 6.87632 1075.780 233.205 -50 58 Y3 0

219 C5H12 2-methylbutane(isopentane) 6.83315 1040.730 235.445 -57 49 Y3 0

220 C5H12 2,2-dimethypropane 6.60427 883.420 227.782 -13 29 Y3 0

221 C5H12O methyl-tert-butyl-ether 5.896 708.69 179.9 2 80 N 170

222 C5H12O pentyl-alcohol 7.17760 1314.560 168.160 37 138 Y2 0

223 C5H12O tert-pentyl-alcohol 7.87530 1604.700 208.160 55 133 Y1 0

224 C5H12S butyl-methyl-sulfide 6.94583 1363.808 212.074 17 150 Y3 0

225 C5H12S ethyl-propyl-sulfide 6.93380 1341.570 212.510 14 145 Y3 0

226 C5H12S 2-methyl-2-butanethiol 6.82837 1254.885 218.759 -3 125 Y3 0

227 C5H12S 1-pentanethiol 6.93311 1369.479 211.314 20 153 Y3 0

228 C6CL6 hexachlorobenzene 9.78602 4597.570 355.961 114 309 Y6 0

229 C6F6 hexafluorobenzene 7.03300 1227.980 215.500 -3 117 Y2 0

230 C6H4CL2 o-dichlorobenzene 7.07030 1649.550 213.320 58 210 Y2 0

231 C6H4CL2 m-dichlorobenzene 7.30370 1782.400 230.010 53 202 Y2 0

232 C6H4CL2 p-dichlorobenzene 6.99800 1575.110 208.520 54 204 Y2 0

233 C6H4F2 m-difluorobenzene 7.06582 1310.27 222.58 36 114 N 234

234 C6H4F2 o-difluorobenzene 7.02031 1310.271 222.587 31 130 Y6 0

235 C6H4F2 p-difluorobenzene 7.08812 1310.27 222.58 34 112 N 234

236 C6H5BR bromobenzene 6.86060 1438.820 205.450 47 177 Y2 0

237 C6H5CL chlorobenzene 6.97810 1431.050 217.560 47 147 Y2 0

238 C6H5F fluorobenzene 7.18700 1381.830 235.570 -23 97 Y2 0

239 C6H5I iodobenzene 7.01190 1640.130 208.780 17 197 Y2 0

240 C6H6 benzene 6.90565 1211.033 220.790 -16 104 Y3 0

241 C6H6O phenol 7.13450 1516.070 174.570 72 208 Y2 0

242 C6H6S benzenethiol 6.99019 1529.454 203.048 52 198 Y3 0

243 C6H7N 2-picoline 7.03240 1415.730 211.580 79 169 Y1 0

244 C6H7N 3-picoline 7.05020 1481.770 211.210 74 185 Y1 0

245 C6H7N aniline 7.24180 1675.300 200.010 67 227 Y2 0

246 C6H10 1-hexyne 6.91212 1194.600 225.000 -8 118 Y9 0

247 C6H10 cyclohexene 6.87240 1221.900 223.180 27 87 Y1 0

248 C6H10 1-methylcyclopentene 6.86884 1199.600 225.000 -5 130 Y8 0

249 C6H10 3-methylcyclopentene 6.87259 1165.600 227.000 -10 119 Y8 0

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 250 | C6H10 | 4-methylcyclopentene | 6.87015 | 1197.600 | 225.000 | -2 | 130 | Y8 | 0 |
| 251 | C6H10O | cyclohexanone | 6.97851 | 1495.580 | 209.559 | 90 | 166 | Y6 | 0 |
| 252 | C6H12 | 1-hexene | 6.86572 | 1152.971 | 225.849 | -29 | 87 | Y3 | 0 |
| 253 | C6H12 | 2-hexene,cis | 7.03805 | 1258.571 | 233.851 | -25 | 92 | Y3 | 0 |
| 254 | C6H12 | 2-hexene,trans | 6.89342 | 1173.343 | 224.530 | -25 | 91 | Y3 | 0 |
| 255 | C6H12 | 3-hexene,cis | 6.87854 | 1164.134 | 224.749 | -27 | 90 | Y3 | 0 |
| 256 | C6H12 | 3-hexene,trans | 6.91780 | 1180.707 | 225.384 | -26 | 90 | Y3 | 0 |
| 257 | C6H12 | 2-methyl-1-pentene | 6.85030 | 1138.516 | 224.704 | -30 | 85 | Y3 | 0 |
| 258 | C6H12 | 3-methyl-1-pentene | 6.75523 | 1086.316 | 226.204 | -37 | 77 | Y3 | 0 |
| 259 | C6H12 | 4-methyl-1-pentene | 6.83529 | 1121.302 | 229.687 | -38 | 77 | Y3 | 0 |
| 260 | C6H12 | 2-methyl-2-pentene | 6.92367 | 1183.837 | 225.514 | -26 | 90 | Y3 | 0 |
| 261 | C6H12 | 3-methyl-2-pentene,cis | 6.91073 | 1186.402 | 226.696 | -26 | 91 | Y3 | 0 |
| 262 | C6H12 | 3-methyl-2-pentene,trans | 6.92634 | 1194.527 | 224.833 | -23 | 94 | Y3 | 0 |
| 263 | C6H12 | 4-methyl-2-pentene,cis | 6.84129 | 1120.707 | 226.586 | -35 | 79 | Y3 | 0 |
| 264 | C6H12 | 4-methyl-2-pentene,trans | 6.88030 | 1142.874 | 227.143 | -33 | 81 | Y3 | 0 |
| 265 | C6H12 | 2-ethyl-1-butene | 6.99712 | 1218.352 | 231.300 | -28 | 88 | Y3 | 0 |
| 266 | C6H12 | 2,3-dimethyl-1-butene | 6.86236 | 1134.675 | 229.367 | -36 | 78 | Y3 | 0 |
| 267 | C6H12 | 3,3-dimethyl-1-butene | 6.67751 | 1010.516 | 224.909 | -47 | 64 | Y3 | 0 |
| 268 | C6H12 | 2,3-dimethyl-2-butene | 6.95058 | 1215.428 | 225.443 | -21 | 97 | Y3 | 0 |
| 269 | C6H12 | cyclohexane | 6.84130 | 1201.531 | 222.647 | 6 | 105 | Y3 | 0 |
| 270 | C6H12 | methylcyclopentane | 6.86283 | 1186.059 | 226.042 | -24 | 96 | Y3 | 0 |
| 271 | C6H12O | cyclohexanol | 6.25530 | 912.870 | 109.130 | 94 | 161 | Y4 | 0 |
| 272 | C6H12O | hexanal | 6.71442 | 1316. | 215.01 | 64 | 156 | N | 210 |
| 273 | C6H12S | thiacycloheptane | 6.90523 | 1422.47 | 211.72 | 78 | 169 | N | 212 |
| 274 | C6H14 | hexane | 6.87024 | 1168.720 | 224.210 | -25 | 92 | Y3 | 0 |
| 275 | C6H14 | 2-methylpentane | 6.83910 | 1135.410 | 226.572 | -32 | 83 | Y3 | 0 |
| 276 | C6H14 | 3-methylpentane | 6.81887 | 1152.368 | 227.129 | -29 | 89 | Y3 | 0 |
| 277 | C6H14 | 2,2-dimethylbutane | 6.75483 | 1081.176 | 229.343 | -41 | 73 | Y3 | 0 |
| 278 | C6H14 | 2,3-dimethylbutane | 6.80983 | 1127.187 | 228.900 | -35 | 81 | Y3 | 0 |
| 279 | C6H14O | propyl-ether | 6.94760 | 1256.500 | 219.000 | 26 | 89 | Y4 | 0 |
| 280 | C6H14O | isopropyl-ether | 7.09710 | 1257.600 | 230.010 | -24 | 91 | Y2 | 0 |
| 281 | C6H14O | hexyl-alcohol | 7.86040 | 1761.260 | 196.670 | 35 | 157 | Y1 | 0 |
| 282 | C6H14S | butyl-ethyl-sulfide | 6.94102 | 1421.320 | 205.810 | 33 | 172 | Y3 | 0 |
| 283 | C6H14S | isopropyl-sulfide | 6.87118 | 1327.120 | 212.550 | 13 | 147 | Y3 | 0 |
| 284 | C6H14S | methyl-pentyl-sulfide | 7.11609 | 1413.44 | 205.73 | 70 | 153 | N | 285 |
| 285 | C6H14S | propyl-sulfide | 6.93577 | 1413.440 | 205.730 | 32 | 170 | Y3 | 0 |
| 286 | C6H14S | 1-hexanethiol | 6.94664 | 1454.004 | 204.954 | 40 | 181 | Y3 | 0 |
| 287 | C6H14S2 | propyl-disulfide | 6.97529 | 1603.793 | 195.848 | 73 | 226 | Y3 | 0 |
| 288 | C6H15N | triethylamine | 6.89890 | 1251.800 | 222.010 | -13 | 127 | Y2 | 0 |
| 289 | C7H5F3 | a,a,a-trifluorotoluene | 6.97045 | 1306.350 | 217.380 | 55 | 139 | Y4 | 0 |
| 290 | C7H5N | benzonitrile | 7.72911 | 2110.572 | 244.819 | 28 | 191 | Y6 | 0 |
| 291 | C7H6O2 | benzoic-acid | 7.45400 | 1820.000 | 147.960 | 132 | 287 | Y1 | 0 |
| 292 | C7H7F | p-fluorotoluene | 6.99426 | 1374.055 | 217.400 | 68 | 155 | Y4 | 0 |
| 293 | C7H8 | toluene | 6.95464 | 1344.800 | 219.482 | 6 | 136 | Y3 | 0 |
| 294 | C7H8 | 1,3,5-cycloheptatriene | 6.97433 | 1376.840 | 220.750 | 0 | 65 | Y4 | 0 |
| 295 | C7H8O | m-cresol | 7.50800 | 1856.360 | 199.070 | 97 | 207 | Y2 | 0 |
| 296 | C7H8O | o-cresol | 6.91170 | 1435.500 | 165.160 | 97 | 207 | Y2 | 0 |
| 297 | C7H8O | p-cresol | 7.03510 | 1511.080 | 161.860 | 97 | 207 | Y2 | 0 |
| 298 | C7H12 | 1-heptyne | 6.68593 | 1216.600 | 220.000 | 14 | 142 | Y9 | 0 |
| 299 | C7H14 | 1-heptene | 6.90069 | 1257.505 | 219.179 | -6 | 118 | Y3 | 0 |
| 300 | C7H14 | cycloheptane | 6.85390 | 1331.570 | 216.360 | 57 | 162 | Y1 | 0 |

301 C7H14 ethylcyclopentane 6.88709 1298.599 220.675 -3 129 Y3 0

302 C7H14 1,1-dimethylcyclopentane 6.81724 1219.474 221.946 -12 113 Y3 0

303 C7H14 c-1,2-dimethylcyclopentane 6.85008 1269.140 220.209 -3 125 Y3 0

304 C7H14 t-1,2-dimethylcyclopentane 6.84422 1242.748 221.686 -9 117 Y3 0

305 C7H14 c-1,3-dimethylcyclopentane 6.83715 1237.456 222.005 -10 116 Y3 0

306 C7H14 t-1,3-dimethylcyclopentane 6.83817 1240.023 221.621 -9 117 Y3 0

307 C7H14 methylcyclohexane 6.82300 1270.763 221.416 -3 127 Y3 0

308 C7H14O heptanal 5.47587 686.453 111.817 12 155 Y6 0

309 C7H16 heptane 6.89385 1264.370 216.636 -2 123 Y3 0

310 C7H16 2-methylhexane 6.87318 1236.026 219.545 -9 115 Y3 0

311 C7H16 3-methylhexane 6.86764 1240.196 219.223 -8 117 Y3 0

312 C7H16 3-ethylpentane 6.87564 1251.827 219.887 -7 118 Y3 0

313 C7H16 2,2-dimethylpentane 6.81480 1190.033 223.303 -19 104 Y3 0

314 C7H16 2,3-dimethylpentane 6.85382 1238.017 221.823 -10 115 Y3 0

315 C7H16 2,4-dimethylpentane 6.82621 1192.041 221.634 -17 105 Y3 0

316 C7H16 3,3-dimethylpentane 6.82667 1228.663 225.316 -14 111 Y3 0

317 C7H16 2,2,3-trimethylbutane 6.79230 1200.563 226.050 -19 106 Y3 0

318 C7H16O isopropyl-tert-butyl-ether 6.62913 1257.6 230.01 41 134 N 280

319 C7H16O heptyl-alcohol 6.64760 1140.640 126.560 60 176 Y1 0

320 C7H16S butyl-propyl-sulfide 6.65279 1421.32 205.81 99 203 N 282

321 C7H16S ethyl-pentyl-sulfide 6.65279 1421.32 205.81 99 203 N 282

322 C7H16S hexyl-methyl-sulfide 6.65279 1421.32 205.81 99 203 N 282

323 C7H16S 1-heptanethiol 6.95249 1525.311 197.696 59 206 Y3 0

324 C8H6 ethynylbenzene 6.957 1445.58 209.44 82 172 N 325

325 C8H8 styrene 6.95710 1445.580 209.440 32 187 Y2 0

326 C8H8 1,3,5,7-cyclooctatetraene 7.00669 1472.110 215.840 0 75 Y4 0

327 C8H10 ethylbenzene 6.95719 1424.255 213.206 26 163 Y3 0

328 C8H10 m-xylene 7.00908 1462.266 215.105 28 166 Y3 0

329 C8H10 o-xylene 6.99891 1474.679 213.686 32 172 Y3 0

330 C8H10 p-xylene 6.99052 1453.430 215.307 27 166 Y3 0

331 C8H14 1-octyne 7.02447 1413.800 215.000 25 170 Y9 0

332 C8H16 1-octene 6.93263 1353.486 212.764 15 148 Y3 0

333 C8H16 cyclooctane 6.86190 1437.780 209.980 94 197 Y1 0

334 C8H16 propylcyclopentane 6.90392 1384.386 213.159 21 158 Y3 0

335 C8H16 ethylcyclohexane 6.86728 1382.466 214.995 21 160 Y3 0

336 C8H16 1,1-dimethylcyclohexane 6.79821 1321.705 217.845 10 147 Y3 0

337 C8H16 c-1,2-dimethylcyclohexane 6.83746 1367.311 215.835 18 158 Y3 0

338 C8H16 t-1,2-dimethylcyclohexane 6.83308 1353.881 219.132 13 151 Y3 0

339 C8H16 c-1,3-dimethylcyclohexane 6.83883 1338.473 218.072 11 147 Y3 0

340 C8H16 t-1,3-dimethylcyclohexane 6.83455 1343.687 215.394 15 152 Y3 0

341 C8H16 c-1,4-dimethylcyclohexane 6.83287 1345.613 216.154 15 152 Y3 0

342 C8H16 t-1,4-dimethylcyclohexane 6.81773 1330.437 218.581 10 147 Y3 0

343 C8H16O octanal 12.51168 3977.531 244.532 73 169 Y6 0

344 C8H18 octane 6.90940 1349.820 209.385 19 152 Y3 0

345 C8H18 2-methylheptane 6.91735 1337.468 213.693 12 144 Y3 0

346 C8H18 3-methylheptane 6.89944 1331.530 212.414 13 145 Y3 0

347 C8H18 4-methylheptane 6.90065 1327.661 212.568 12 144 Y3 0

348 C8H18 3-ethylhexane 6.89098 1327.884 212.595 13 145 Y3 0

349 C8H18 2,2-dimethylhexane 6.83715 1273.594 215.072 3 133 Y3 0

350 C8H18 2,3-dimethylhexane 6.87004 1315.503 214.157 10 142 Y3 0

351 C8H18 2,4-dimethylhexane 6.85305 1287.876 214.790 5 135 Y3 0

352 C8H18 2,5-dimethylhexane 6.85984 1287.274 214.412 5 135 Y3 0

353 C8H18 3,3-dimethylhexane 6.85121 1307.882 217.439 6 138 Y3 0

354 C8H18 3,4-dimethylhexane 6.87986 1330.035 214.863 11 144 Y3 0

355 C8H18 3-ethyl-2-methylpentane 6.86358 1318.120 215.306 9 142 Y3 0

356 C8H18 3-ethyl-3-methylpentane 6.86731 1347.209 219.684 10 145 Y3 0

357 C8H18 2,2,3-trimethylpentane 6.82546 1294.875 218.420 4 136 Y3 0

358 C8H18 2,2,4-trimethylpentane 6.81189 1257.840 220.735 -4 125 Y3 0

359 C8H18 2,3,3-trimethylpentane 6.84353 1328.046 220.375 7 142 Y3 0

360 C8H18 2,3,4-trimethylpentane 6.85396 1315.084 217.526 7 140 Y3 0

361 C8H18 2,2,3,3-tetramethylbutane 6.87665 1329.930 226.360 103 133 Y3 0

362 C8H18O butyl-ether 6.98250 1431.500 207.010 32 182 Y2 0

363 C8H18O sec-butyl-ether 6.79153 1348.53 223.79 57 149 N 364

364 C8H18O tert-butyl-ether 6.93294 1348.533 223.790 4 109 Y5 0

365 C8H18O octyl-alcohol 6.83700 1310.620 136.060 70 195 Y2 0

366 C8H18S butyl-sulfide 6.54589 1421.32 205.81 106 215 N 282

367 C8H18S ethyl-hexyl-sulfide 6.42693 1421.32 205.81 115 231 N 282

368 C8H18S heptyl-methyl-sulfide 6.42693 1421.32 205.81 115 231 N 282

369 C8H18S pentyl-propyl-sulfide 6.42693 1421.32 205.81 115 231 N 282

370 C8H18S 1-octanethiol 6.96909 1593.000 190.610 76 229 Y3 0

371 C8H18S2 butyl-disulfide 6.96380 1684.100 181.300 101 263 Y3 0

372 C9H10 alpha-methylstyrene 7.09240 1582.700 206.010 75 220 Y1 0

373 C9H10 propenylbenzene,cis 7.44961 1909.083 238.874 18 179 Y6 0

374 C9H10 propenylbenzene,trans 7.54993 1909.08 238.87 105 197 N 373

375 C9H10 m-methylstyrene 6.87928 1471.440 200.000 72 250 Y4 0

376 C9H10 o-methylstyrene 6.88461 1485.410 200.000 75 255 Y4 0

377 C9H10 p-methylstyrene 7.01120 1535.100 200.700 68 170 Y4 0

378 C9H12 propylbenzene 6.95142 1491.297 207.140 43 188 Y3 0

379 C9H12 cumene 6.93666 1460.793 207.777 38 181 Y3 0

380 C9H12 m-ethyltoluene 7.01582 1529.184 208.509 46 190 Y3 0

381 C9H12 o-ethyltoluene 7.00314 1535.374 207.300 48 194 Y3 0

382 C9H12 p-ethyltoluene 6.99802 1527.113 208.921 46 191 Y3 0

383 C9H12 1,2,3-trimethylbenzene 7.04082 1593.958 207.078 57 205 Y3 0

384 C9H12 1,2,4-trimethylbenzene 7.04383 1573.267 208.564 52 198 Y3 0

385 C9H12 mesitylene 7.07436 1569.622 209.578 49 193 Y3 0

386 C9H16 1-nonyne 6.77410 1404.700 210.000 50 223 Y9 0

387 C9H18 1-nonene 6.95387 1435.359 205.535 36 174 Y3 0

388 C9H18 butylcyclopentane 6.89935 1457.080 205.990 41 185 Y3 0

389 C9H18 propylcyclohexane 6.88646 1460.800 207.939 40 186 Y3 0

390 C9H18 c-c-135trimethylcyclohexane 7.09743 1460.8 207.93 78 164 N 389

391 C9H18 c-t-135trimethylcyclohexane 7.07274 1460.8 207.93 80 166 N 389

392 C9H18O nonanal 7.81505 2036.854 227.486 33 185 Y6 0

393 C9H20 nonane 6.93440 1429.460 201.820 39 179 Y3 0

394 C9H20 2-methyloctane 6.91191 1398.420 203.650 33 171 Y3 0

395 C9H20 3-methyloctane 6.90920 1405.800 204.760 33 172 Y3 0

396 C9H20 4-methyloctane 6.90318 1399.120 205.410 32 170 Y3 0

397 C9H20 3-ethylheptane 6.90489 1406.500 206.500 32 171 Y3 0

398 C9H20 4-ethylheptane 6.89898 1399.800 207.200 30 169 Y3 0

399 C9H20 2,2-dimethylheptane 6.88174 1363.910 208.210 24 160 Y3 0

400 C9H20 2,3-dimethylheptane 6.87635 1389.500 207.300 29 168 Y3 0

401 C9H20 2,4-dimethylheptane 6.90252 1368.720 207.440 24 160 Y3 0

402 C9H20 2,5-dimethylheptane 6.89317 1375.400 206.800 27 163 Y3 0

403 C9H20 2,6-dimethylheptane 6.89385 1368.000 205.680 26 162 Y3 0

404 C9H20 3,3-dimethylheptane 6.87553 1385.360 209.790 26 165 Y3 0

405 C9H20 3,4-dimethylheptane 6.88359 1396.900 208.400 29 168 Y3 0

406 C9H20 3,5-dimethylheptane 6.90164 1382.800 207.900 26 163 Y3 0

407 C9H20 4,4-dimethylheptane 6.86968 1378.700 210.400 24 163 Y3 0

408 C9H20 3-ethyl-2-methylhexane 6.88690 1390.200 209.000 27 166 Y3 0

409 C9H20 4-ethyl-2-methylhexane 6.90030 1376.100 208.600 25 161 Y3 0

410 C9H20 3-ethyl-3-methylhexane 6.87787 1406.800 211.400 28 169 Y3 0

411 C9H20 3-ethyl-4-methylhexane 6.89430 1404.300 209.500 29 168 Y3 0

412 C9H20 2,2,3-trimethylhexane 6.86574 1375.720 211.630 23 161 Y3 0

413 C9H20 2,2,4-trimethylhexane 6.84922 1340.900 211.350 18 154 Y3 0

414 C9H20 2,2,5-trimethylhexane 6.83531 1324.049 210.737 16 151 Y3 0

415 C9H20 2,3,3-trimethylhexane 6.85417 1389.790 212.100 25 166 Y3 0

416 C9H20 2,3,4-trimethylhexane 6.85274 1387.220 210.220 27 167 Y3 0

417 C9H20 2,3,5-trimethylhexane 6.87078 1359.090 209.290 22 159 Y3 0

418 C9H20 2,4,4-trimethylhexane 6.85163 1368.723 214.047 20 158 Y3 0

419 C9H20 3,3,4-trimethylhexane 6.85761 1403.880 212.560 27 169 Y3 0

420 C9H20 3,3-diethylpentane 6.89262 1451.245 215.575 31 175 Y3 0

421 C9H20 3-ethyl-2,2-dimethylpentane 6.87166 1383.130 212.750 23 162 Y3 0

422 C9H20 3-ethyl-2,3-dimethylpentane 6.84463 1418.000 213.000 30 174 Y3 0

423 C9H20 3-ethyl-2,4-dimethylpentane 6.85293 1380.540 210.870 25 165 Y3 0

424 C9H20 2,2,3,3-tetramethylpentane 6.82876 1397.483 213.703 26 169 Y3 0

425 C9H20 2,2,3,4-tetramethylpentane 6.83173 1374.042 214.762 21 161 Y3 0

426 C9H20 2,2,4,4-tetramethylpentane 6.79710 1325.183 216.093 13 150 Y3 0

427 C9H20 2,3,3,4-tetramethylpentane 6.85961 1417.473 214.705 27 170 Y3 0

428 C9H20O nonyl-alcohol 6.67570 1276.630 123.060 90 214 Y1 0

429 C9H20S butyl-pentyl-sulfide 6.23448 1421.32 205.81 129 258 N 282

430 C9H20S ethyl-heptyl-sulfide 6.23448 1421.32 205.81 129 258 N 282

431 C9H20S hexyl-propyl-sulfide 6.23448 1421.32 205.81 129 258 N 282

432 C9H20S methyl-octyl-sulfide 6.23448 1421.32 205.81 129 258 N 282

433 C9H20S 1-nonanethiol 6.98390 1655.600 183.700 93 251 Y3 0

434 C10H8 naphthalene 7.01065 1733.710 201.859 87 250 Y3 0

435 C10H8 azulene 6.7868 1733.71 201.85 160 278 N 434

436 C10H14 butylbenzene 6.98317 1577.965 201.378 62 213 Y3 0

437 C10H14 m-diethylbenzene 7.00360 1575.310 200.960 61 211 Y3 0

438 C10H14 o-diethylbenzene 6.98780 1576.940 200.510 63 213 Y3 0

439 C10H14 p-diethylbenzene 6.99820 1588.310 201.970 63 214 Y3 0

440 C10H14 1,2,3,4-tetramethylbenzene 7.05940 1690.540 199.480 80 236 Y3 0

441 C10H14 1,2,3,5-tetramethylbenzene 7.07790 1675.430 201.140 75 228 Y3 0

442 C10H14 1,2,4,5-tetramethylbenzene 7.08000 1672.430 201.430 74 227 Y3 0

443 C10H18 1-decyne 7.10870 1606.600 206.000 78 246 Y9 0

444 C10H18 decahydronaphthalene,cis 6.87529 1594.460 203.392 68 228 Y3 0

445 C10H18 decahydronaphthalene,trans 6.85681 1564.683 206.259 61 219 Y3 0

446 C10H20 1-decene 6.96034 1501.872 197.578 54 199 Y3 0

447 C10H20 1-cyclopentylpentane 6.94140 1540.600 198.800 60 210 Y3 0

448 C10H20 butylcyclohexane 6.91030 1538.518 200.833 59 211 Y3 0

449 C10H20O decanal 8.20794 2378.316 237.905 52 209 Y6 0

450 C10H22 decane 6.96375 1508.750 195.374 58 203 Y3 0

451 C10H22 2-methylnonane 6.93372 1472.730 196.380 52 196 Y3 0

452 C10H22 3-methylnonane 6.92975 1479.100 197.500 52 197 Y3 0

453 C10H22 4-methylnonane 6.92234 1471.000 198.300 50 194 Y3 0

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 454 | C10H22 | 5-methylnonane | 6.91878 | 1468.400 | 198.500 | 50 | 194 | Y3 | 0 |
| 455 | C10H22 | 3-ethyloctane | 6.91845 | 1477.400 | 199.400 | 50 | 195 | Y3 | 0 |
| 456 | C10H22 | 4-ethyloctane | 6.90922 | 1466.680 | 200.440 | 48 | 192 | Y3 | 0 |
| 457 | C10H22 | 2,2-dimethyloctane | 6.90617 | 1439.600 | 200.700 | 43 | 185 | Y3 | 0 |
| 458 | C10H22 | 2,3-dimethyloctane | 6.89449 | 1462.220 | 200.000 | 48 | 193 | Y3 | 0 |
| 459 | C10H22 | 2,4-dimethyloctane | 6.92146 | 1439.800 | 200.400 | 43 | 184 | Y3 | 0 |
| 460 | C10H22 | 2,5-dimethyloctane | 6.90263 | 1442.500 | 200.200 | 44 | 187 | Y3 | 0 |
| 461 | C10H22 | 2,6-dimethyloctane | 6.93331 | 1450.530 | 199.400 | 45 | 187 | Y3 | 0 |
| 462 | C10H22 | 2,7-dimethyloctane | 6.91326 | 1444.190 | 198.270 | 46 | 188 | Y3 | 0 |
| 463 | C10H22 | 3,3-dimethyloctane | 6.88895 | 1457.600 | 202.500 | 45 | 190 | Y3 | 0 |
| 464 | C10H22 | 3,4-dimethyloctane | 6.89926 | 1465.900 | 201.400 | 47 | 192 | Y3 | 0 |
| 465 | C10H22 | 3,5-dimethyloctane | 6.89758 | 1448.800 | 201.300 | 44 | 188 | Y3 | 0 |
| 466 | C10H22 | 3,6-dimethyloctane | 6.91284 | 1456.900 | 200.500 | 46 | 189 | Y3 | 0 |
| 467 | C10H22 | 4,4-dimethyloctane | 6.88891 | 1446.900 | 203.500 | 42 | 186 | Y3 | 0 |
| 468 | C10H22 | 4,5-dimethyloctane | 6.89288 | 1460.520 | 201.900 | 46 | 191 | Y3 | 0 |
| 469 | C10H22 | 4-propylheptane | 6.94710 | 1458.700 | 201.200 | 44 | 186 | Y3 | 0 |
| 470 | C10H22 | 4-isopropylheptane | 6.88757 | 1449.800 | 202.900 | 43 | 188 | Y3 | 0 |
| 471 | C10H22 | 3-ethyl-2-methylheptane | 6.89294 | 1457.900 | 202.200 | 45 | 190 | Y3 | 0 |
| 472 | C10H22 | 4-ethyl-2-methylheptane | 6.89200 | 1438.200 | 202.300 | 42 | 185 | Y3 | 0 |
| 473 | C10H22 | 5-ethyl-2-methylheptane | 6.89424 | 1448.800 | 201.300 | 44 | 188 | Y3 | 0 |
| 474 | C10H22 | 3-ethyl-3-methylheptane | 6.88063 | 1472.900 | 204.500 | 46 | 193 | Y3 | 0 |
| 475 | C10H22 | 4-ethyl-3-methylheptane | 6.88689 | 1464.200 | 203.300 | 45 | 191 | Y3 | 0 |
| 476 | C10H22 | 3-ethyl-5-methylheptane | 6.91593 | 1455.200 | 202.400 | 44 | 187 | Y3 | 0 |
| 477 | C10H22 | 3-ethyl-4-methylheptane | 6.88827 | 1466.800 | 203.000 | 46 | 192 | Y3 | 0 |
| 478 | C10H22 | 4-ethyl-4-methylheptane | 6.88302 | 1464.900 | 205.200 | 44 | 190 | Y3 | 0 |
| 479 | C10H22 | 2,2,3-trimethylheptane | 6.87507 | 1446.100 | 204.400 | 42 | 187 | Y3 | 0 |
| 480 | C10H22 | 2,2,4-trimethylheptane | 6.87525 | 1409.400 | 204.500 | 35 | 177 | Y3 | 0 |
| 481 | C10H22 | 2,2,5-trimethylheptane | 6.87855 | 1417.400 | 203.800 | 37 | 179 | Y3 | 0 |
| 482 | C10H22 | 2,2,6-trimethylheptane | 6.89454 | 1411.090 | 202.630 | 37 | 177 | Y3 | 0 |
| 483 | C10H22 | 2,3,3-trimethylheptane | 6.87202 | 1457.800 | 205.000 | 43 | 189 | Y3 | 0 |
| 484 | C10H22 | 2,3,4-trimethylheptane | 6.87417 | 1451.700 | 203.600 | 44 | 189 | Y3 | 0 |
| 485 | C10H22 | 2,3,5-trimethylheptane | 6.83990 | 1440.000 | 203.000 | 44 | 190 | Y3 | 0 |
| 486 | C10H22 | 2,3,6-trimethylheptane | 6.88668 | 1433.700 | 201.900 | 42 | 184 | Y3 | 0 |
| 487 | C10H22 | 2,4,4-trimethylheptane | 6.86062 | 1418.400 | 205.400 | 37 | 180 | Y3 | 0 |
| 488 | C10H22 | 2,4,5-trimethylheptane | 6.87583 | 1437.300 | 203.300 | 41 | 185 | Y3 | 0 |
| 489 | C10H22 | 2,4,6-trimethylheptane | 6.91395 | 1411.300 | 202.300 | 36 | 175 | Y3 | 0 |
| 490 | C10H22 | 2,5,5-trimethylheptane | 6.88204 | 1429.090 | 204.360 | 39 | 181 | Y3 | 0 |
| 491 | C10H22 | 3,3,4-trimethylheptane | 6.86861 | 1466.800 | 205.900 | 44 | 191 | Y3 | 0 |
| 492 | C10H22 | 3,3,5-trimethylheptane | 6.85524 | 1435.430 | 205.490 | 40 | 185 | Y3 | 0 |
| 493 | C10H22 | 3,4,4-trimethylheptane | 6.86721 | 1464.100 | 206.200 | 43 | 190 | Y3 | 0 |
| 494 | C10H22 | 3,4,5-trimethylheptane | 6.87113 | 1463.400 | 204.200 | 45 | 192 | Y3 | 0 |
| 495 | C10H22 | 3-isopropyl-2-methylhexane | 6.76103 | 1441.000 | 204.700 | 45 | 197 | Y3 | 0 |
| 496 | C10H22 | 3,3-diethylhexane | 6.88355 | 1490.900 | 206.200 | 47 | 196 | Y3 | 0 |
| 497 | C10H22 | 3,4-diethylhexane | 6.88347 | 1473.200 | 204.200 | 46 | 193 | Y3 | 0 |
| 498 | C10H22 | 3-ethyl-2,2-dimethylhexane | 6.86594 | 1444.400 | 206.400 | 40 | 185 | Y3 | 0 |
| 499 | C10H22 | 4-ethyl-2,2-dimethylhexane | 6.89526 | 1416.000 | 206.000 | 34 | 175 | Y3 | 0 |
| 500 | C10H22 | 3-ethyl-2,3-dimethylhexane | 6.86128 | 1475.800 | 206.800 | 45 | 194 | Y3 | 0 |
| 501 | C10H22 | 4-ethyl-2,3-dimethylhexane | 6.86823 | 1458.000 | 204.700 | 44 | 190 | Y3 | 0 |
| 502 | C10H22 | 3-ethyl-2,4-dimethylhexane | 6.86682 | 1455.300 | 205.000 | 43 | 189 | Y3 | 0 |
| 503 | C10H22 | 4-ethyl-2,4-dimethylhexane | 6.86721 | 1464.100 | 206.200 | 43 | 190 | Y3 | 0 |
| 504 | C10H22 | 3-ethyl-2,5-dimethylhexane | 6.87155 | 1429.300 | 204.100 | 39 | 183 | Y3 | 0 |

505 C10H22 4-ethyl-3,3-dimethylhexane 6.86288 1473.100 207.000 44 193 Y3 0

506 C10H22 3-ethyl-3,4-dimethylhexane 6.86148 1470.400 207.300 44 192 Y3 0

507 C10H22 2,2,3,3-tetramethylhexane 6.84438 1464.030 209.060 41 190 Y3 0

508 C10H22 2,2,3,4-tetramethylhexane 6.82410 1443.600 207.300 41 188 Y3 0

509 C10H22 2,2,3,5-tetramethylhexane 6.87685 1417.600 206.300 35 177 Y3 0

510 C10H22 2,2,4,4-tetramethylhexane 6.73151 1396.000 208.700 35 184 Y3 0

511 C10H22 2,2,4,5-tetramethylhexane 6.83561 1400.550 206.260 34 176 Y3 0

512 C10H22 2,2,5,5-tetramethylhexane 6.88124 1377.980 207.000 27 165 Y3 0

513 C10H22 2,3,3,4-tetramethylhexane 6.84243 1474.940 207.720 45 195 Y3 0

514 C10H22 2,3,3,5-tetramethylhexane 6.85043 1429.200 206.900 37 182 Y3 0

515 C10H22 2,3,4,4-tetramethylhexane 6.82940 1457.900 207.600 42 191 Y3 0

516 C10H22 2,3,4,5-tetramethylhexane 6.87156 1442.800 205.300 40 185 Y3 0

517 C10H22 3,3,4,4-tetramethylhexane 6.81164 1492.700 209.700 47 201 Y3 0

518 C10H22 24dimethyl3isopropylpentane 6.82154 1432.150 206.380 40 186 Y3 0

519 C10H22 33-diethyl-2-methylpentane 6.85984 1501.800 207.700 49 200 Y3 0

520 C10H22 3ethyl-223trimethylpentane 6.80710 1490.100 210.000 47 200 Y3 0

521 C10H22 3ethyl-224trimethylpentane 6.83149 1435.600 208.100 38 185 Y3 0

522 C10H22 3ethyl-234trimethylpentane 6.81616 1486.620 208.320 47 200 Y3 0

523 C10H22 22334-pentamethylpentane 6.79659 1474.890 210.600 44 197 Y3 0

524 C10H22 22344-pentamethylpentane 6.73273 1423.830 210.350 38 190 Y3 0

525 C10H22O decyl-alcohol 6.92240 1472.010 134.160 103 230 Y2 0

526 C10H22S butyl-hexyl-sulfide 6.06898 1421.32 205.81 143 285 N 282

527 C10H22S ethyl-octyl-sulfide 6.06898 1421.32 205.81 143 285 N 282

528 C10H22S heptyl-propyl-sulfide 6.06898 1421.32 205.81 143 285 N 282

529 C10H22S methyl-nonyl-sulfide 6.06898 1421.32 205.81 143 285 N 282

530 C10H22S pentyl-sulfide 6.06898 1421.32 205.81 143 285 N 282

531 C10H22S 1-decanethiol 6.99810 1713.600 177.000 109 271 Y3 0

532 C10H22S2 pentyl-disulfide 6.95810 1756.000 166.800 128 298 Y3 0

533 C11H10 1-methylnaphthalene 7.03592 1826.948 195.002 108 278 Y3 0

534 C11H10 2-methylnaphthalene 7.06850 1840.268 198.395 105 274 Y3 0

535 C11H16 pentylbenzene 6.97833 1639.910 194.760 80 237 Y3 0

536 C11H16 pentamethylbenzene 7.13760 1833.800 198.960 125 270 Y1 0

537 C11H20 1-undecyne 7.13064 1687.200 202.000 80 267 Y9 0

538 C11H22 1-undecene 6.96662 1562.469 189.743 72 222 Y3 0

539 C11H22 1-cyclopentylhexane 6.95480 1608.000 191.600 78 234 Y3 0

540 C11H22 pentylcyclohexane 6.94667 1619.110 194.510 78 235 Y3 0

541 C11H24 undecane 6.97220 1569.570 187.700 75 226 Y3 0

542 C11H24O undecyl-alcohol 6.52710 1250.000 100.000 120 243 Y11 0

543 C11H24S butyl-heptyl-sulfide 5.9321 1421.32 205.81 155 309 N 282

544 C11H24S decyl-methyl-sulfide 5.9321 1421.32 205.81 155 309 N 282

545 C11H24S ethyl-nonyl-sulfide 5.9321 1421.32 205.81 155 309 N 282

546 C11H24S octyl-propyl-sulfide 5.9321 1421.32 205.81 155 309 N 282

547 C11H24S 1-undecanethiol 7.01220 1767.400 170.400 124 290 Y3 0

548 C12H10 biphenyl 7.24540 1998.720 202.740 70 272 Y2 0

549 C12H12 1-ethylnaphthalene 7.03159 1841.320 185.280 120 292 Y3 0

550 C12H12 2-ethylnaphthalene 7.07566 1880.730 191.410 118 291 Y3 0

551 C12H12 1,2-dimethylnaphthalene 7.00605 1805.310 171.370 129 269 Y3 0

552 C12H12 1,3-dimethylnaphthalene 7.26980 2076.000 210.000 148 310 Y4 0

553 C12H12 1,4-dimethylnaphthalene 7.26980 2076.000 210.000 148 310 Y4 0

554 C12H12 1,5-dimethylnaphthalene 7.04930 1855.000 180.000 150 313 Y8 0

555 C12H12 1,6-dimethylnaphthalene 7.26980 2076.000 210.000 148 310 Y4 0

556 C12H12 1,7-dimethylnaphthalene 7.05640 1879.000 180.000 150 320 Y4 0

557 C12H12 2,3-dimethylnaphthalene 7.05270 1869.000 180.000 155 315 Y4 0

558 C12H12 2,6-dimethylnaphthalene 7.04600 1841.000 180.000 150 310 Y8 0

559 C12H12 2,7-dimethylnaphthalene 7.04780 1846.000 180.000 150 310 Y4 0

560 C12H18 hexylbenzene 6.98530 1700.500 188.200 96 258 Y3 0

561 C12H18 1,2,3-triethylbenzene 7.58877 2133.55 235.68 146 247 N 562

562 C12H18 1,2,4-triethylbenzene 7.57869 2133.558 235.681 46 218 Y6 0

563 C12H18 1,3,5-triethylbenzene 7.6044 2133.55 235.68 145 246 N 562

564 C12H18 hexamethylbenzene 7.15544 2133.55 235.68 178 300 N 562

565 C12H22 1-dodecyne 7.16929 1771.100 198.000 113 288 Y9 0

566 C12H24 1-dodecene 6.97522 1619.862 182.271 89 244 Y3 0

567 C12H24 1-cyclopentylheptane 6.97430 1672.200 184.400 95 256 Y3 0

568 C12H24 1-cyclohexylhexane 6.95550 1681.000 187.800 94 257 Y3 0

569 C12H26 dodecane 6.99795 1639.270 181.835 91 247 Y3 0

570 C12H26O dodecyl-alcohol 7.53986 2003.290 168.130 138 214 Y4 0

571 C12H26S butyl-octyl-sulfide 6.62900 1408.000 116.060 134 307 Y1 0

572 C12H26S decyl-ethyl-sulfide 5.81251 1421.32 205.81 166 333 N 282

573 C12H26S hexyl-sulfide 5.81251 1421.32 205.81 166 333 N 282

574 C12H26S methyl-undecyl-sulfide 5.81251 1421.32 205.81 166 333 N 282

575 C12H26S nonyl-propyl-sulfide 5.81251 1421.32 205.81 166 333 N 282

576 C12H26S 1-dodecanethiol 7.02440 1817.800 164.100 138 308 Y3 0

577 C12H26S2 hexyl-disulfide 6.96320 1824.900 153.500 153 328 Y3 0

578 C13H14 1-propylnaphthalene 7.05940 1890.800 180.000 155 335 Y8 0

579 C13H14 2-propylnaphthalene 7.06050 1895.500 180.000 160 335 Y8 0

580 C13H14 2ethyl-3-methylnaphthalene 7.02851 1895.5 180. 196 312 N 579

581 C13H14 2ethyl-6-methylnaphthalene 7.09303 1895.5 180. 192 303 N 579

582 C13H14 2ethyl-7-methylnaphthalene 7.09303 1895.5 180. 192 303 N 579

583 C13H20 1-phenylheptane 7.00060 1761.200 181.500 112 279 Y3 0

584 C13H24 1-tridecyne 7.15674 1834.400 195.000 120 308 Y9 0

585 C13H26 1-tridecene 6.98563 1674.741 175.214 105 264 Y3 0

586 C13H26 1-cyclopentyloctane 6.98960 1729.800 177.300 112 276 Y3 0

587 C13H26 1-cyclohexylheptane 6.97430 1743.000 180.900 111 278 Y3 0

588 C13H28 tridecane 7.00756 1690.670 174.220 107 267 Y3 0

589 C13H28O 1-tridecanol 7.41181 2003.29 168.13 202 304 N 570

590 C13H28S butyl-nonyl-sulfide 5.70756 1421.32 205.81 177 355 N 282

591 C13H28S decyl-propyl-sulfide 5.70756 1421.32 205.81 177 355 N 282

592 C13H28S dodecyl-methyl-sulfide 5.70756 1421.32 205.81 177 355 N 282

593 C13H28S ethyl-undecyl-sulfide 5.70756 1421.32 205.81 177 355 N 282

594 C13H28S 1-tridecanethiol 7.03700 1864.900 157.900 151 325 Y3 0

595 C14H16 1-butylnaphthalene 4.96310 656.800 26.000 139 292 Y3 0

596 C14H16 2-butylnaphthalene 6.61170 1591.400 138.500 145 291 Y3 0

597 C14H22 1-phenyloctane 7.00860 1812.200 174.600 127 298 Y3 0

598 C14H22 1,2,3,4-tetraethylbenzene 7.65632 2312.864 236.261 66 248 Y6 0

599 C14H22 1,2,3,5-tetraethylbenzene 7.63235 2312.86 236.26 174 282 N 598

600 C14H22 1,2,4,5-tetraethylbenzene 7.63723 2312.86 236.26 174 282 N 598

601 C14H26 1-tetradecyne 7.23227 1927.700 191.000 145 326 Y9 0

602 C14H28 1-tetradecene 7.02005 1745.001 170.475 119 283 Y3 0

603 C14H28 1-cyclopentylnonane 6.99600 1779.000 170.200 126 296 Y3 0

604 C14H28 1-cyclohexyloctane 6.98970 1799.300 174.300 126 298 Y3 0

605 C14H30 tetradecane 7.01300 1740.880 167.720 122 286 Y3 0

606 C14H30O 1-tetradecanol 6.67410 1204.500 54.000 130 264 Y4 0

607 C14H30S butyl-decyl-sulfide 5.61512 1421.32 205.81 187 376 N 282

608 C14H30S dodecyl-ethyl-sulfide 5.61512 1421.32 205.81 187 376 N 282

609 C14H30S heptyl-sulfide 5.61512 1421.32 205.81 187 376 N 282

610 C14H30S methyl-tridecyl-sulfide 5.61512 1421.32 205.81 187 376 N 282

611 C14H30S propyl-undecyl-sulfide 5.61512 1421.32 205.81 187 376 N 282

612 C14H30S 1-tetradecanethiol 7.04850 1909.200 151.900 164 341 Y3 0

613 C14H30S2 heptyl-disulfide 6.96020 1878.600 139.800 175 357 Y3 0

614 C15H18 1-pentylnaphthalene 7.07430 2000.000 170.000 185 360 Y8 0

615 C15H18 2-pentylnaphthalene 7.06000 2005.900 170.000 190 370 Y8 0

616 C15H24 1-phenylnonane 7.02450 1862.600 167.500 142 316 Y3 0

617 C15H28 1-pentadecyne 7.20553 1972.070 188.000 140 349 Y9 0

618 C15H30 1-pentadecene 7.01555 1781.974 162.582 134 302 Y3 0

619 C15H30 1-cyclopentyldecane 7.00349 1825.748 163.479 141 314 Y3 0

620 C15H30 1-cyclohexylnonane 7.00060 1850.200 167.600 141 316 Y3 0

621 C15H32 pentadecane 7.02359 1789.950 161.380 136 304 Y3 0

622 C15H32O 1-pentadecanol 6.23737 1204.5 54. 230 339 N 606

623 C15H32S butyl-undecyl-sulfide 5.53347 1421.32 205.81 196 397 N 282

624 C15H32S dodecyl-propyl-sulfide 5.53347 1421.32 205.81 196 397 N 282

625 C15H32S ethyl-tridecyl-sulfide 5.53347 1421.32 205.81 196 397 N 282

626 C15H32S methyl-tetradecyl-sulfide 5.53347 1421.32 205.81 196 397 N 282

627 C15H32S 1-pentadecanethiol 7.06120 1951.000 146.000 176 356 Y3 0

628 C16H26 1-phenyldecane 7.03642 1904.132 160.318 155 333 Y3 0

629 C16H26 pentaethylbenzene 8.29495 2972.770 272.052 86 277 Y6 0

630 C16H30 1-hexadecyne 7.47511 2154.700 185.000 172 367 Y9 0

631 C16H32 1-hexadecene 7.04437 1843.581 157.917 147 319 Y3 0

632 C16H32 1-cyclopentylundecane 7.02000 1869.200 156.000 154 330 Y3 0

633 C16H32 1-cyclohexyldecane 7.01852 1899.242 161.348 154 333 Y3 0

634 C16H34 hexadecane 7.02867 1830.510 154.450 149 321 Y3 0

635 C16H34O 1-hexadecanol 6.15860 1380.000 91.000 145 190 Y4 0

636 C16H34S butyl-dodecyl-sulfide 5.46123 1421.32 205.81 204 416 N 282

637 C16H34S ethyl-tetradecyl-sulfide 5.46123 1421.32 205.81 204 416 N 282

638 C16H34S methyl-pentadecyl-sulfide 5.46123 1421.32 205.81 204 416 N 282

639 C16H34S octyl-sulfide 5.46123 1421.32 205.81 204 416 N 282

640 C16H34S propyl-tridecyl-sulfide 5.46123 1421.32 205.81 204 416 N 282

641 C16H34S 1-hexadecanethiol 7.07500 1990.000 140.000 188 370 Y3 0

642 C16H34S2 octyl-disulfide 6.95790 1935.600 129.000 196 383 Y3 0

643 C17H28 1-phenylundecane 7.05090 1944.100 153.000 168 349 Y3 0

644 C17H32 1-heptadecyne 7.48829 2216.200 182.000 184 384 Y9 0

645 C17H34 1-heptadecene 7.03925 1877.910 151.530 159 335 Y3 0

646 C17H34 1-cyclopentyldodecane 7.03190 1909.100 149.000 168 346 Y3 0

647 C17H34 1-cyclohexylundecane 7.02900 1939.700 154.500 167 349 Y3 0

648 C17H36 heptadecane 7.01430 1865.100 149.200 161 337 Y3 0

649 C17H36O 1-heptadecanol 6.78200 1595.000 85.060 191 383 Y1 0

650 C17H36S butyl-tridecyl-sulfide 5.39727 1421.32 205.81 212 434 N 282

651 C17H36S ethyl-pentadecyl-sulfide 5.39727 1421.32 205.81 212 434 N 282

652 C17H36S hexadecyl-methyl-sulfide 5.39727 1421.32 205.81 212 434 N 282

653 C17H36S propyl-tetradecyl-sulfide 5.39727 1421.32 205.81 212 434 N 282

654 C17H36S 1-heptadecanethiol 7.08100 2027.000 135.000 198 384 Y3 0

655 C18H30 1-phenyldodecane 7.06930 1981.600 145.500 181 363 Y3 0

656 C18H30 hexaethylbenzene 7.50288 2360.733 212.652 134 298 Y6 0

657 C18H34 1-octadecyne 7.50787 2281.100 180.000 196 400 Y9 0

658 C18H36 1-octadecene 7.04518 1917.900 145.900 171 350 Y3 0

659 C18H36 1-cycopentyltridecane 7.04730 1947.000 141.900 180 361 Y3 0

660 C18H36 1-cyclohexyldodecane 7.03620 1976.700 148.000 179 364 Y3 0

661 C18H38 octadecane 7.00220 1894.300 143.300 172 352 Y3 0

662 C18H38O 1-octadecanol 6.81400 1632.000 80.060 201 385 Y1 0

663 C18H38S butyl-tetradecyl-sulfide 5.3364 1421.32 205.81 220 452 N 282

664 C18H38S ethyl-hexadecyl-sulfide 5.3364 1421.32 205.81 220 452 N 282

665 C18H38S heptadecyl-methyl-sulfide 5.3364 1421.32 205.81 220 452 N 282

666 C18H38S nonyl-sulfide 5.3364 1421.32 205.81 220 452 N 282

667 C18H38S pentadecyl-propyl-sulfide 5.3364 1421.32 205.81 220 452 N 282

668 C18H38S 1-octadecanethiol 7.09600 2061.000 129.000 209 397 Y3 0

669 C18H38S2 nonyl-disulfide 6.96050 1981.500 117.000 215 407 Y3 0

670 C19H32 1-phenyltridecane 7.08430 2013.900 137.900 193 377 Y3 0

671 C19H36 1-nonadecyne 7.51711 2336.700 177.000 208 416 Y9 0

672 C19H38 1-nonadecene 7.05710 1961.600 141.200 183 364 Y3 0

673 C19H38 1-cyclopentyltetradecane 7.06300 1982.000 135.000 192 375 Y3 0

674 C19H38 1-cyclohexyltridecane 7.04690 2012.200 141.500 191 378 Y3 0

675 C19H40 nonadecane 7.01530 1932.800 137.600 184 366 Y3 0

676 C19H40O 1-nonadecanol 6.60769 1632 80.06 274 395 N 662

677 C19H40S butyl-pentadecyl-sulfide 5.28246 1421.32 205.81 227 468 N 282

678 C19H40S ethyl-heptadecyl-sulfide 5.28246 1421.32 205.81 227 468 N 282

679 C19H40S hexadecyl-propyl-sulfide 5.28246 1421.32 205.81 227 468 N 282

680 C19H40S methyl-octadecyl-sulfide 5.28246 1421.32 205.81 227 468 N 282

681 C19H40S 1-nonadecanethiol 7.10500 2094.000 124.000 219 409 Y3 0

682 C20H34 1-phenyltetradecane 7.10100 2042.000 130.000 205 390 Y3 0

683 C20H38 1-eicosyne 7.52336 2386.300 174.000 219 431 Y9 0

684 C20H40 1-eicosene 7.05770 1995.300 136.000 193 378 Y3 0

685 C20H40 1-cyclopentylpentadecane 7.08300 2016.000 128.000 203 388 Y3 0

686 C20H40 1-cyclohexyltetradecane 7.06100 2046.000 135.000 203 392 Y3 0

687 C20H42 eicosane 7.15220 2032.700 132.100 198 379 Y3 0

688 C20H42O 1-eicosanol 6.87200 1699.000 70.060 219 406 Y1 0

689 C20H42S butyl-hexadecyl-sulfide 5.23473 1421.32 205.81 233 484 N 282

690 C20H42S decyl-sulfide 5.23473 1421.32 205.81 233 484 N 282

691 C20H42S ethyl-octadecyl-sulfide 5.23473 1421.32 205.81 233 484 N 282

692 C20H42S heptadecyl-propyl-sulfide 5.23473 1421.32 205.81 233 484 N 282

693 C20H42S methyl-nonadecyl-sulfide 5.23473 1421.32 205.81 233 484 N 282

694 C20H42S 1-eicosanethiol 7.11400 2125.000 119.000 229 421 Y3 0

695 C20H42S2 decyl-disulfide 6.97200 2019.000 103.100 235 429 Y3 0

696 C21H36 1-phenylpentadecane 7.11400 2067.000 122.000 216 403 Y3 0

697 C21H42 1-cyclopentylhexadecane 7.10300 2048.000 121.000 215 401 Y3 0

698 C21H42 1-cyclohexylpentadecane 7.07200 2078.000 129.000 213 404 Y3 0

699 C22H38 1-phenylhexadecane 7.14000 2095.000 114.000 227 415 Y3 0

700 C22H44 1-cyclohexylhexadecane 7.07400 2099.000 122.000 224 416 Y3 0