

ماده ۵۰۰۰

# ضرایب معادله آنتوان برای محاسبه فشار بخار

( ANTOINE COEFFICIENTS FOR VAPOR PRESSURE )

Collected By :

Iranian Chemical Engineers Website ([www.IrChe.com](http://www.IrChe.com))

\* Antoine Equation:  $\log_{10}(P^*) = A - \frac{B}{T + C}$

\* where P is in mmHg and T is in Celsius

\* Where  $T_{\min} < T < T_{\max}$

$$\log(P^*) = A - \frac{B}{(T + C)}$$

## ANTOINE COEFFICIENTS FOR VAPOR PRESSURE

No.	material or substance name	mol.formula	A	B	C	T_min (°C)	T_max (°C)
1	abietic acid	C20H30O2	7.06195	1850.91	66.1306	173.5	558.85
2	acenaphthene	C12H10	7.16063	2033.35	197.714	93.41	530
3	acetal	C6H14O2	7.28439	1445.63	224.685	-100	267.85
4	acetaldehyde	C2H4O	7.25504	1110.4	233.451	-123	187.85
5	acetamide	C2H5NO	7.40993	1808.24	178.098	81	487.85
6	acetanilide	C8H9NO	7.49658	2229.78	179.279	113.5	551.85
7	acetic acid	C2H4O2	7.8152	1800.03	246.894	16.66	319.56
8	acetic anhydride	C4H6O3	8.81453	2394.8	264.961	-73	296
9	acetone	C3H6O	7.31414	1315.67	240.479	-94.7	235.05
10	acetone cyanohydrin	C4H7NO	8.91995	3024.38	310.947	-20	373.85
11	acetonitrile	C2H3N	7.54662	1583.98	257.887	-43.83	272.35
12	acetophenone	C8H8O	7.39996	1901.19	218.697	19.65	427.85
13	acetylacetone	C5H8O2	7.43842	1599.97	210.655	-23.2	328.85
14	acetyl chloride	C2H3ClO	7.34554	1271.26	233.984	-112.85	234.85
15	acetylene	C2H2	7.31465	790.209	262.859	-80.75	35.17
16	acrolein	C3H4O	7.38041	1343.54	245.902	-87.7	232.85
17	acrylamide	C3H5NO	6.4374	894.333	58.8579	84.5	436.85
18	acrylic acid	C3H4O2	7.82557	1817.73	226.609	13.5	341.85
19	acrylonitrile	C3H3N	7.4321	1482.76	248.44	-83.52	261.85
20	adipic acid	C6H10O4	8.52199	2969.1	188.477	152.35	535.85
21	adiponitrile	C6H8N2	7.61843	2295.33	189.49	2.49	507.85

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22	allene	C3H4	6.92395	833.311	240.605	-136.28	120
23	allyl acetate	C5H8O2	7.45775	1609.44	247.641	-135.15	285.85
24	allyl alcohol	C3H6O	7.96765	1704.51	238.003	-129	271.9
25	allylamine	C3H7N	7.32854	1274.12	233.166	-88.2	231.85
26	3-amino-1-propanol	C3H9NO	8.07048	1946.9	187.65	11	375.85
27	1-amino-2,2-dimethylbutane	C6H15N	6.87335	1182.53	182.684	36.4553	296.401
28	1-amino-2,3-dimethylbutane	C6H15N	6.94084	1180.99	185.882	30.269	279.568
29	2-amino-2,3-dimethylbutane	C6H15N	6.95778	1218.6	194.398	26.4667	283.732
30	1-amino-2-ethylbutane	C6H15N	6.98809	1289.13	178.246	55.6757	319.761
31	1-amino-2-methylpentane	C6H15N	6.9913	1264.03	180.662	48.5695	307.041
32	2-amino-2-methylpentane	C6H15N	6.87708	1156.29	185.343	28.7867	282.407
33	3-amino-2-methylpentane	C6H15N	6.9294	1265.92	177.501	54.6801	323.68
34	1-amino-2-propanol	C3H9NO	8.01915	1807.96	192.396	1.74	340.85
35	1-amino-3,3-dimethylbutane	C6H15N	6.86631	1235.92	177.274	52.0589	324.875
36	2-amino-3,3-dimethyl butane	C6H15N	6.82011	1130.77	185.049	26.5876	283.954
37	1-amino-3-methylpentane	C6H15N	7.05717	1264.03	180.662	48.5695	307.041
38	2-amino-3-methylpentane	C6H15N	6.9294	1265.92	177.501	54.6801	323.68
39	3-amino-3-methylpentane	C6H15N	6.86897	1215.12	179.381	45.9805	313.783
40	1-amino-4-methylpentane	C6H15N	6.99241	1255.58	181.475	46.1791	302.762
41	2-amino-4-methylpentane	C6H15N	6.93942	1190.84	184.91	33.1	284.684
42	p-aminoazobenzene	C12H11N3	7.47943	2420.19	166.437	127.85	603.85
43	p-aminodiphenyl	C12H11N	7.44251	2227.77	186.514	52.85	543.85
44	p-aminodiphenylamine	C12H12N2	7.66753	2520.35	172.53	68	593.85

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45	2-aminoethoxyethanol	C4H11NO2	8.14609	2165.16	170.364	0	425.85
46	N-aminoethyl ethanolamine	C4H12N2O	8.46342	2421.58	189.922	20	424.85
47	N-aminoethyl piperazine	C6H15N3	7.57065	1980.02	201.794	-19	434.85
48	2-aminohexane	C6H15N	6.99013	1273.04	179.794	51.1219	311.61
49	3-aminohexane	C6H15N	6.98809	1289.13	178.246	55.6757	319.761
50	6-aminohexanol	C6H15NO	8.26771	2347.46	200.922	57.85	407.85
51	p-tert-amylphenol	C11H16O	7.38313	2007.72	183.931	92.85	477.85
52	anethole	C10H12O	7.29113	1918.63	199.732	21.35	449.85
53	aniline	C6H7N	7.29291	1668.15	193.636	-6.02	425.85
54	anisole	C7H8O	7.32615	1674.45	223.096	-37.5	368.5
55	anthracene	C14H10	7.62455	2759.81	239.75	215.78	599.85
56	anthraquinone	C14H8O2	8.49022	3820.73	301.228	286	626.85
57	ascorbic acid	C6H8O6	10.2475	3536.95	116.281	192	509.85
58	azelaic acid	C9H16O4	8.35296	2820.61	155.238	106.5	537.85
59	azulene	C10H8	7.71999	2566.46	288.342	160	500.33
60	benzaldehyde	C7H6O	7.25411	1734.8	217.931	-26	421.85
61	benzene	C6H6	7.06437	1296.93	229.916	5.53	289.01
62	1,2,3-benzenetriol	C6H6O3	9.38415	3798.12	275.326	133.85	556.85
63	benzoic acid	C7H6O2	7.41844	1824.74	152.886	122.37	477.85
64	benzonitrile	C7H5N	7.36682	1868.3	225.472	-12.75	426.2
65	benzophenone	C13H10O	7.64336	2518.51	222.727	48.2	542.85
66	benzothiophene	C8H6S	7.16508	1854.63	212.993	31.35	480.85
67	benzotrichloride	C7H5Cl3	7.03224	1802.94	220.794	-4.75	463.85

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68	benzotrifluoride	C7H5F3	7.03951	1363.9	225.913	-29.01	291.85
69	benoyl chloride	C7H5ClO	7.54146	2017.05	235.784	-0.5	423.85
70	benzyl acetate	C9H10O2	7.3784	1914.89	212.258	-51.5	425.85
71	benzyl alcohol	C7H8O	7.92338	2060.53	203.928	-15.3	403.85
72	benzylamine	C7H9N	7.40339	1813.01	216.379	-46	410.35
73	benzyl benzoate	C14H12O2	7.49894	2356.69	186.813	19.4	546.85
74	benzyl chloride	C7H7Cl	7.195	1731.66	221.989	-39	412.85
75	benzyl dichloride	C7H6Cl2	7.34379	2033.3	241.742	-16.15	457.85
76	benzyl ethyl ether	C9H12O	7.32289	1799.43	220.087	2.5	388.85
77	biacetylene	C4H2	6.5326	761.685	198.268	-78	204.87
78	bicyclohexyl	C12H22	7.27281	2010.95	218.827	3.63	453.85
79	bis(chloromethyl) ether	C2H4Cl2O	7.25172	1441.52	224.949	-41.5	305.85
80	bis(cyanoethyl) ether	C6H8N2O	7.85429	2474.89	191.768	-26.3	509.85
81	bisphenol a	C15H16O2	7.13999	1756.42	51.8844	153	575.85
82	cis-1-bromo-1-butene	C4H7Br	6.83966	1075.86	185.61	15.0145	281.002
83	trans-1-bromo-1-butene	C4H7Br	6.83616	1098.81	183.104	21.9348	294.189
84	2-bromo-1-butene	C4H7Br	6.80854	1051.64	186.748	10.5053	275.009
85	3-bromo-1-butene	C4H7Br	6.791	1112.47	179.505	29.8464	313.133
86	4-bromo-1-butene	C4H7Br	6.85069	1116.09	182.341	25.3599	298.207
87	cis-1-bromo-1-decene	C10H19Br	7.09388	1626.22	160.994	128.536	410.561
88	trans-1-bromo-1-decene	C10H19Br	7.09388	1626.22	160.994	128.536	410.561
89	cis-1-bromo-1-dodecene	C12H23Br	7.18345	1792.1	155.513	190.223	439.41
90	trans-1-bromo-1-dodecene	C12H23Br	7.18345	1792.1	155.513	190.223	439.41

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91	cis-1-bromo-1-eicosene	C20H39Br	7.30086	2267.25	137.947	289.767	531.863
92	trans-1-bromo-1-eicosene	C20H39Br	7.30086	2267.25	137.947	289.767	531.863
93	cis-1-bromo-1-heptadecene	C17H33Br	7.32559	2138.36	144.095	257.43	499.505
94	trans-1-bromo-1-heptadecene	C17H33Br	7.32559	2138.36	144.095	257.43	499.505
95	cis-1-bromo-1-heptene	C7H13Br	6.95558	1361.36	171.095	77.398	357.396
96	trans-1-bromo-1-heptene	C7H13Br	6.95558	1361.36	171.095	77.398	357.396
97	cis-1-bromo-1-hexadecene	C16H31Br	7.31197	2079.35	146.257	245.189	488.122
98	trans-1-bromo-1-hexadecene	C16H31Br	7.31197	2079.35	146.257	245.189	488.122
99	cis-1-bromo-1-hexene	C6H11Br	6.91272	1270.51	175.115	58.6245	336.238
100	trans-1-bromo-1-hexene	C6H11Br	6.91272	1270.51	175.115	58.6245	336.238
101	cis-1-bromo-1-nonadecene	C19H37Br	7.32122	2233.28	139.946	279.748	521.34
102	trans-1-bromo-1-nonadecene	C19H37Br	7.32122	2233.28	139.946	279.748	521.34
103	cis-1-bromo-1-nonene	C9H17Br	7.04732	1538.25	164.195	111.963	393.713
104	trans-1-bromo-1-nonene	C9H17Br	7.04732	1538.25	164.195	111.963	393.713
105	cis-1-bromo-1-octadecene	C18H35Br	7.32915	2188.91	142.073	268.669	510.146
106	trans-1-bromo-1-octadecene	C18H35Br	7.32915	2188.91	142.073	268.669	510.146
107	cis-1-bromo-1-octene	C8H15Br	7.00217	1437.21	168.724	91.4033	369.876
108	trans-1-bromo-1-octene	C8H15Br	7.00217	1437.21	168.724	91.4033	369.876
109	cis-1-bromo-1-pentadecene	C15H29Br	7.28944	2016.18	148.326	232.845	477.237
110	trans-1-bromo-1-pentadecene	C15H29Br	7.28944	2016.18	148.326	232.845	477.237
111	cis-1-bromo-1-pentene	C5H9Br	6.87345	1176.84	179.754	38.3287	311.824
112	trans-1-bromo-1-pentene	C5H9Br	6.87345	1176.84	179.754	38.3287	311.824
113	2-bromo-1-pentene	C5H9Br	6.84283	1146.59	181.395	32.293	303.185

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114	3-bromo-1-pentene	C5H9Br	6.83395	1148.98	180.649	33.8389	307.11
115	4-bromo-1-pentene	C5H9Br	6.83358	1151.68	180.361	34.647	308.625
116	5-bromo-1-pentene	C5H9Br	6.8853	1219.21	176.462	48.9771	329.151
117	cis-1-bromo-1-propene	C3H5Br	6.81089	979.705	191.484	-7.80429	250.085
118	trans-1-bromo-1-propene	C3H5Br	6.80835	993.911	189.862	-3.4302	258.622
119	2-bromo-1-propene	C3H5Br	6.78209	945.427	193.938	-15.7225	237.169
120	3-bromo-1-propene	C3H5Br	7.35721	1433.47	250.22	17	267.05
121	cis-1-bromo-1-tetradecene	C14H27Br	7.25959	1946.58	150.55	219.552	465.53
122	trans-1-bromo-1-tetradecene	C14H27Br	7.25959	1946.58	150.55	219.552	465.53
123	cis-1-bromo-1-tridecene	C13H25Br	7.22381	1871.57	152.941	205.337	452.943
124	trans-1-bromo-1-tridecene	C13H25Br	7.22381	1871.57	152.941	205.337	452.943
125	cis-1-bromo-1-undecene	C11H21Br	7.13956	1712.11	158.021	175.102	426.205
126	trans-1-bromo-1-undecene	C11H21Br	7.13956	1712.11	158.021	175.102	426.205
127	1-bromo-2,2-dimethylbutane	C6H13Br	6.89916	1259.49	176.585	55.706	328.503
128	1-bromo-2,2-dimethylpropane	C5H11Br	6.74106	1108.06	181.044	29.4561	305.03
129	1-bromo-2,3-dimethylbutane	C6H13Br	6.77746	1222.91	173.837	56.8863	342.962
130	2-bromo-2,3-dimethylbutane	C6H13Br	7.10497	1411.09	201.053	45.9849	322.77
131	1-bromo-cis-2-butene	C4H7Br	6.83254	1123.79	180.379	29.4623	308.532
132	1-bromo-trans-2-butene	C4H7Br	6.83254	1123.79	180.379	29.4623	308.532
133	2-bromo-cis-2-butene	C4H7Br	6.79053	1058.37	184.901	14.2863	284.731
134	2-bromo-trans-2-butene	C4H7Br	6.78692	1082.16	182.244	21.561	298.718
135	3-bromo-2-ethyl-1-propene	C5H9Br	6.84461	1134.02	182.725	28.5512	296.184
136	1-bromo-2-ethylbutane	C6H13Br	6.71999	1210.12	171.902	58.9098	353.147

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137	cis-1-bromo-2-methyl-1-butene	C5H9Br	6.8231	1164.47	178.378	39.4427	319.063
138	trans-1-bromo-2-methyl-1-butene	C5H9Br	6.8231	1164.47	178.378	39.4427	319.063
139	3-bromo-2-methyl-1-butene	C5H9Br	6.78741	1112.69	181.894	27.6412	300.559
140	4-bromo-2-methyl-1-butene	C5H9Br	6.84461	1134.02	182.725	28.5512	296.184
141	1-bromo-2-methyl-1-propene	C4H7Br	6.78842	1072.11	183.366	18.4895	292.812
142	3-bromo-2-methyl-1-propene	C4H7Br	6.8028	1088.87	182.631	21.8245	296.678
143	1-bromo-2-methyl-cis-2-butene	C5H9Br	6.82062	1183.36	176.359	45.0982	329.688
144	1-bromo-2-methyl-trans-2-butene	C5H9Br	6.82062	1183.36	176.359	45.0982	329.688
145	1-bromo-2-methylbutane	C5H11Br	6.85575	1189.69	178.797	42.3908	316.86
146	2-bromo-2-methylbutane	C5H11Br	6.74032	1113.33	180.465	31.0665	308.08
147	1-bromo-2-methylpentane	C6H13Br	6.89674	1279.44	174.591	61.4843	338.995
148	2-bromo-2-methylpentane	C6H13Br	7.68278	1850.66	242.895	45.9849	322.77
149	3-bromo-2-methylpentane	C6H13Br	6.84404	1215.67	177.927	48.5844	321.438
150	1-bromo-2-methylpropane	C4H9Br	6.82042	1088.09	184.662	18.974	285.992
151	2-bromo-2-methylpropane	C4H9Br	6.70881	1000.45	188.099	3.1285	267.899
152	1-bromo-cis-2-pentene	C5H9Br	6.87054	1198.76	177.463	44.8014	323.88
153	1-bromo-trans-2-pentene	C5H9Br	6.87054	1198.76	177.463	44.8014	323.88
154	2-bromo-cis-2-pentene	C5H9Br	6.82493	1150.97	179.82	35.4031	311.474
155	2-bromo-trans-2-pentene	C5H9Br	6.82493	1150.97	179.82	35.4031	311.474
156	3-bromo-cis-2-pentene	C5H9Br	6.82567	1145.58	180.397	33.7872	308.438
157	3-bromo-trans-2-pentene	C5H9Br	6.82567	1145.58	180.397	33.7872	308.438
158	4-bromo-cis-2-pentene	C5H9Br	6.81521	1160.04	178.345	38.9681	319.235
159	4-bromo-trans-2-pentene	C5H9Br	6.81521	1160.04	178.345	38.9681	319.235

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160	5-bromo-cis-2-pentene	C5H9Br	6.86983	1204.24	176.89	46.4196	326.895
161	5-bromo-trans-2-pentene	C5H9Br	6.86983	1204.24	176.89	46.4196	326.895
162	1-bromo-3,3-dimethylbutane	C6H13Br	6.84123	1238.13	175.625	55.1915	333.553
163	2-bromo-3,3-dimethylbutane	C6H13Br	6.72361	1180.24	175.131	49.8274	336.153
164	cis-1-bromo-3-methyl-1-butene	C5H9Br	6.81759	1142.54	180.223	33.7176	309.353
165	trans-1-bromo-3-methyl-1-butene	C5H9Br	6.81759	1142.54	180.223	33.7176	309.353
166	2-bromo-3-methyl-1-butene	C5H9Br	6.78815	1107.55	182.453	26.0839	297.615
167	3-bromo-3-methyl-1-butene	C5H9Br	6.71815	1081.27	181.517	24.7925	302.545
168	4-bromo-3-methyl-1-butene	C5H9Br	6.83661	1130.17	182.649	28.2232	296.585
169	1-bromo-3-methyl-2-butene	C5H9Br	6.82536	1147.87	180.152	34.474	309.728
170	2-bromo-3-methyl-2-butene	C5H9Br	6.7737	1149.42	177.261	39.7503	324.944
171	1-bromo-3-methylbutane	C5H11Br	6.85579	1189.41	178.825	42.31	316.71
172	2-bromo-3-methylbutane	C5H11Br	6.80014	1154.73	179.324	37.6069	314.084
173	1-bromo-3-methylpentane	C6H13Br	6.89542	1290.6	173.476	64.7169	344.865
174	2-bromo-3-methylpentane	C6H13Br	6.84404	1215.67	177.927	48.5844	321.438
175	3-bromo-3-methylpentane	C6H13Br	6.95052	1301.81	189.878	45.9849	322.77
176	1-bromo-4-methylpentane	C6H13Br	6.89575	1287.81	173.755	63.9087	343.398
177	2-bromo-4-methylpentane	C6H13Br	6.84328	1221.67	177.311	50.3511	324.677
178	bromobenzene	C6H5Br	7.13213	1615.76	223.972	-30.72	397
179	1-bromobutane	C4H9Br	7.25188	1456.01	231.502	-112.4	303.85
180	2-bromobutane	C4H9Br	7.23919	1435.76	238.205	-111.9	293.85
181	bromochlorodifluoromethane	CBrClF2	7.04234	1021.9	249.569	-159.15	153
182	bromochloromethane	CH2BrCl	7.30547	1357.06	238.654	-87.95	283.85

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183	1-bromodecane	C10H21Br	7.55047	2129.17	215.358	109.682	425.277
184	1-bromodocosane	C22H45Br	7.37833	2563.59	162.001	342.911	564.241
185	1-bromododecane	C12H25Br	7.59557	2268.78	205.309	138.677	453.396
186	1-bromodotriacontane	C32H65Br	6.64653	2423	147.437	424.64	546
187	1-bromoeicosane	C20H41Br	7.32284	2339.51	140.677	229.333	543.044
188	bromoethane	C2H5Br	7.31438	1260.42	245.939	-118.6	230.65
189	bromoform	CHBr3	7.04365	1526.6	217.523	8.05	422.85
190	1-bromoheneicosane	C21H43Br	7.44003	2557.73	164.001	333.708	553.316
191	1-bromohentriacontane	C31H63Br	6.70862	2441.39	149.803	420.363	538
192	1-bromoheptacosane	C27H55Br	6.73458	2252.5	128.493	378.601	620.977
193	1-bromoheptadecane	C17H35Br	7.5757	2467.11	176.488	198.697	510.919
194	1-bromoheptane	C7H15Br	7.36161	1802.33	223.334	-56.1	377.85
195	1-bromoheptatriacontane	C37H75Br	6.39519	2350.69	137.88	435.686	581
196	1-bromohexacosane	C26H53Br	6.98574	2467.06	154.001	372.62	608.843
197	1-bromohexadecane	C16H33Br	7.59139	2437.36	181.422	188.357	500.512
198	1-bromohexane	C6H13Br	7.45417	1793.95	236.962	40.9906	350.709
199	2-bromohexane	C6H13Br	6.89677	1279.16	174.619	61.4035	338.849
200	3-bromohexane	C6H13Br	6.89764	1271.9	175.344	59.3023	335.033
201	1-bromohexatriacontane	C36H73Br	6.44305	2364.26	139.702	434.31	574
202	1-bromonaphthalene	C10H7Br	7.26796	2139.41	206.554	6.2	550.85
203	1-bromononacosane	C29H59Br	6.18881	1785.33	66.7022	388.578	646.529
204	1-bromononadecane	C19H39Br	7.41975	2391.59	152.906	219.631	532.159
205	1-bromononane	C9H19Br	7.52501	2052.39	220.525	94.0166	409.505

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206	1-bromononatriacontane	C39H79Br	6.31696	2330.12	135.12	435.366	593
207	1-bromooctacosane	C28H57Br	6.45576	2006.26	97.1988	383.338	632.708
208	1-bromooctadecane	C18H37Br	7.49757	2427.7	163.844	209.787	521.877
209	1-bromooctane	C8H17Br	7.49972	1970.73	225.866	77.3363	391.944
210	1-bromooctatriacontane	C38H77Br	6.35562	2340.18	136.469	435.75	587
211	1-bromopentacosane	C25H51Br	7.10362	2504.13	156.001	365.411	596.275
212	1-bromopentadecane	C15H31Br	7.62504	2431.01	190.413	176.529	489.358
213	1-bromopentane	C5H11Br	9.01055	2883.39	340.804	41	291.61
214	2-bromopentane	C5H11Br	6.85688	1181.21	179.68	39.8857	312.214
215	3-bromopentane	C5H11Br	6.85644	1184.49	179.338	40.8554	314.012
216	1-bromopentatriacontane	C35H71Br	6.49209	2378.29	141.574	432.5	567
217	1-bromopropane	C3H7Br	7.33043	1403.41	244.4	-110	270.85
218	2-bromopropane	C3H7Br	7.27146	1339.77	245.732	-89	258.85
219	1-bromotetracontane	C40H81Br	6.27921	2320.55	133.835	434.525	599
220	1-bromotetracosane	C24H49Br	7.20969	2536.72	158.001	358.785	585.692
221	1-bromotetradecane	C14H29Br	7.62292	2383.07	195.534	164.288	477.408
222	1-bromotetratriacontane	C34H69Br	6.54234	2392.77	143.49	430.274	560
223	p-bromotoluene	C7H7Br	7.3498	1871.14	234.343	26.8	425.85
224	1-bromotriacontane	C30H61Br	6.78193	2481.09	154.995	392.532	531
225	bromotrichloromethane	CBrCl3	7.1184	1455.22	238.507	-21	332.85
226	1-bromotricosane	C23H47Br	7.30114	2554.95	160.001	350.978	574.615
227	1-bromotridecane	C13H27Br	7.63156	2352.16	203.114	151.578	465.912
228	bromotrifluoroethylene	C2BrF3	7.018	1010.75	246.808	-100.15	158.85

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229	bromotrifluoromethane	CBrF <sub>3</sub>	6.9716	800.838	253.656	-168	67
230	1-bromotritriacontane	C <sub>33</sub> H <sub>67</sub> Br	6.59381	2407.68	145.446	427.647	553
231	1-bromoundecane	C <sub>11</sub> H <sub>23</sub> Br	7.57362	2200.78	210.169	124.621	439.923
232	1,2-butadiene	C <sub>4</sub> H <sub>6</sub>	7.27134	1169.61	255.545	-136.2	170.85
233	butadiene (1,3 butadiene)	C <sub>4</sub> H <sub>6</sub>	7.02238	998.751	245.563	-108.9	152.22
234	butane	C <sub>4</sub> H <sub>10</sub>	7.00961	1022.48	248.145	-138.29	152.03
235	1,2-butanediol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	9.55708	3097.79	273	110.391	348.993
236	1,3-butanediol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	8.97864	2583.12	216.613	-77	369.85
237	1,4-butanediol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	9.37541	3080.18	246.268	19.9	393.85
238	butanol	C <sub>4</sub> H <sub>10</sub> O	7.62121	1543.89	208.029	-89.3	289.78
239	sec-butanol	C <sub>4</sub> H <sub>10</sub> O	7.56142	1448.35	209.886	-114.7	262.86
240	tert-butanol	C <sub>4</sub> H <sub>10</sub> O	7.13278	1068.74	168.931	25.82	233.05
241	1-butene	C <sub>4</sub> H <sub>8</sub>	7.0342	1013.6	250.292	-185.35	146.44
242	cis-2-butene	C <sub>4</sub> H <sub>8</sub>	7.02701	1028.06	244.234	-138.89	162.43
243	trans-2-butene	C <sub>4</sub> H <sub>8</sub>	7.06654	1038.12	247.135	-105.53	155.48
244	cis-2-butene-1,4-diol	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	9.40227	3113.76	242.464	11	404.73
245	trans-2-butene-1,4-diol	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	9.49439	3242.29	253.397	27.3	407.85
246	cis-2-butenoic acid	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	7.60698	1752.54	198.917	15.5	373.85
247	trans-2-butenoic acid	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	7.49988	1701.16	183.292	71.4	392.85
248	cis-(1-butenyl)benzene	C <sub>10</sub> H <sub>12</sub>	7.05973	1638.51	203.09	90.4128	405.397
249	trans-(1-butenyl)benzene	C <sub>10</sub> H <sub>12</sub>	7.05723	1670.28	201.251	98.0763	419.61
250	2-butoxyethanol	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	8.29012	2182.89	232.223	-70	326.85
251	2-sec-butyl-1,3-propanediol	C <sub>7</sub> H <sub>16</sub> O <sub>2</sub>	9.56529	3396.12	273	146.887	386.957

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252	1-butyl-[1,2,3,4-tetrahydronaphthalene]	C <sub>14</sub> H <sub>20</sub>	7.19432	1985.24	187.105	218.601	483.598
253	2-butyl-[1,2,3,4-tetrahydronaphthalene]	C <sub>14</sub> H <sub>20</sub>	7.19321	2003.48	186.085	223.441	491.035
254	butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	7.23548	1515.76	222.077	-73.5	306.5
255	sec-butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	7.32351	1539.86	234.604	-99	287.85
256	tert-butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	7.07055	1327.54	220.856	10	271.85
257	butyl acrylate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	7.32729	1687.45	231.652	-64.6	324.85
258	butylamine	C <sub>4</sub> H <sub>11</sub> N	7.21033	1316.41	226.655	-49.1	258.75
259	sec-butylamine	C <sub>4</sub> H <sub>11</sub> N	7.17241	1290.85	237.787	-104.5	241.15
260	tert-butylamine	C <sub>4</sub> H <sub>11</sub> N	7.15888	1216.94	240.061	-66.96	210.75
261	butylbenzene	C <sub>10</sub> H <sub>14</sub>	7.18472	1720.37	216.413	-87.85	387.4
262	sec-butylbenzene	C <sub>10</sub> H <sub>14</sub>	6.90771	1536.8	208.305	-75.43	391.39
263	tert-butylbenzene	C <sub>10</sub> H <sub>14</sub>	6.88707	1509.57	207.654	-57.88	386.85
264	butyl benzoate	C <sub>11</sub> H <sub>14</sub> O <sub>2</sub>	7.59592	2225.32	221.955	-21.5	450.85
265	butyl butanoate	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	7.32431	1719.58	221.989	-92	342.85
266	sec-butyl butanoate	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	6.98455	1352.83	177.659	67.9791	322.85
267	tert-butyl butanoate	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	6.94196	1290.79	181.839	54.3603	300.85
268	p-tert-butylcatechol	C <sub>10</sub> H <sub>14</sub> O <sub>2</sub>	7.78202	2265.73	177.43	51.85	502.85
269	butylcyclohexane	C <sub>10</sub> H <sub>20</sub>	6.87773	1570.94	212.057	-74.73	393.85
270	butylcyclopentane	C <sub>9</sub> H <sub>18</sub>	7.05154	1551.44	215.372	41	351.9
271	sec-butylcyclopentane	C <sub>9</sub> H <sub>18</sub>	6.95241	1482.16	209.674	39.3276	353.44
272	tert-butylcyclopentane	C <sub>9</sub> H <sub>18</sub>	6.8417	1411.38	211.479	30.1252	349.414
273	1-butylcyclopentene	C <sub>9</sub> H <sub>16</sub>	7.02187	1512.98	209.36	63.5064	353.379
274	butyl decyl sulfide	C <sub>14</sub> H <sub>30</sub> S	7.78265	2485.95	211.297	245.85	345.85

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275	butyl dodecyl sulfide	C16H34S	7.22342	2014.32	140	273.85	373.85
276	butyl ethyl sulfate	C6H14O4S	---	---	---	---	---
277	butyl ethyl sulfite	C6H14O3S	---	---	---	---	---
278	tert-butylformamide	C5H11NO	7.31893	1800.86	203.771	16	418.85
279	butyl formate	C5H10O2	7.3709	1546.73	238.376	-91.9	285.85
280	sec-butyl formate	C5H10O2	6.82272	1125.4	195.097	-1.81906	273.85
281	tert-butyl formate	C5H10O2	6.75103	1054.36	189.629	10.291	259.85
282	sec-butyl glycolate	C6H12O3	7.92251	2068.51	232.782	28.3	177.5
283	4-tert-butylheptane	C11H24	6.83947	1431.85	187.7	57.5012	349.059
284	butyl heptyl sulfide	C11H24S	7.09661	1759.04	170.4	196.85	296.85
285	butyl hexadecyl sulfide	C20H42S	7.18259	2111.53	119.001	321.85	421.85
286	butyl hexyl sulfide	C10H22S	7.16824	1809.06	195.094	176.85	276.85
287	butyl isocyanate	C5H9NO	7.30431	1503.29	224.841	-80.15	294.85
288	butyl isocyanide	C5H9N	6.95055	1242.13	180.713	46.2265	306.777
289	sec-butyl isocyanide	C5H9N	6.89682	1185.65	183.38	35.3858	292.735
290	tert-butyl isocyanide	C5H9N	6.78399	1088.6	187.402	17.7291	271.57
291	butyl mercaptan	C4H10S	7.14944	1415.11	233.055	-115.69	295.85
292	sec-butyl mercaptan	C4H10S	7.15048	1391.49	240.922	-140.13	280.85
293	tert-butyl mercaptan	C4H10S	6.92597	1187.37	229.308	1.11	256.85
294	butyl methacrylate	C8H14O2	7.19482	1609.88	212.325	-50.15	342.85
295	butyl methyl sulfate	C5H12O4S	---	---	---	---	---
296	butyl methyl sulfite	C5H12O3S	---	---	---	---	---

ANTOINE COEFFICIENTS FOR VAPOR PRESSURE

297	1-butyl-naphthalene	C14H16	7.32328	2164.31	197.795	-19.72	518.85
298	2-butyl-naphthalene	C14H16	7.59916	2467.29	233.904	139	507.81
299	1-sec-butyl-naphthalene	C14H16	6.73898	1854.71	207.724	135	545.337
300	2-sec-butyl-naphthalene	C14H16	8.51736	3993.45	396.231	135	545.337
301	1-tert-butyl-naphthalene	C14H16	7.15868	2021.32	194.207	134	508.18
302	2-tert-butyl-naphthalene	C14H16	7.20867	2087.26	202.184	134	510.73
303	butyl nonanoate	C13H26O2	7.6466	2030.51	196.21	-38	378.85
304	butyl nonyl sulfide	C13H28S	7.13871	1863.9	157.9	229.85	329.85
305	4-tert-butyl-octane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
306	butyl octyl sulfide	C12H26S	7.61843	2223.04	205.383	213.85	313.85
307	butyl pentadecyl sulfide	C19H40S	7.20937	2103.03	124	311.85	411.85
308	butyl pentyl sulfide	C9H20S	7.15298	1737.33	199.813	156.85	256.85
309	2-butylphenol	C10H14O	7.13364	1701.13	165	143.094	440.537
310	3-butylphenol	C10H14O	7.25024	1800.2	165	159.287	469.075
311	4-butylphenol	C10H14O	7.25167	1805.16	165	160.096	470.502
312	2-sec-butylphenol	C10H14O	7.16713	1684.52	165	143.06	447.129
313	3-sec-butylphenol	C10H14O	7.18027	1727.74	165	150.206	459.849
314	4-sec-butylphenol	C10H14O	7.18785	1753.4	165	154.445	467.394
315	2-tert-butylphenol	C10H14O	7.04719	1621.06	165	138.102	452.233
316	3-tert-butylphenol	C10H14O	7.06984	1696.56	165	150.881	475.458
317	4-tert-butylphenol	C10H14O	7.06947	1695.28	165	150.664	475.064
318	butyl propanoate	C7H14O2	7.39996	1681.36	225.452	-89.52	320.85
319	sec-butyl propanoate	C7H14O2	7.38037	1412.36	180.889	64.809	305.85

## ANTOINE COEFFICIENTS FOR VAPOR PRESSURE

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320	tert-butyl propanoate	C7H14O2	7.58433	1535.55	185.069	66.3638	283.85
321	butyl propyl sulfite	C7H16O3S	---	---	---	---	---
322	butyl stearate	C22H44O2	7.76507	2544.16	170.889	26.3	490.85
323	butyl tetradecyl sulfide	C18H38S	7.13143	2069.41	135	301.85	401.85
324	butyl tridecyl sulfide	C17H36S	7.25728	2069.41	135	287.85	387.85
325	butyl undecyl sulfide	C15H32S	7.22529	1980.43	146	259.85	359.85
326	butyl valerate	C9H18O2	7.58116	1951.79	228.743	-92.8	355.85
327	butyl vinyl ether	C6H12O	7.21206	1398.28	229.015	-92	262.85
328	"2-butyne-1,4-diol "	C4H6O2	8.51955	2280.56	166.445	57.85	421.85
329	butyraldehyde	C4H8O	7.21736	1317.94	229.115	-96.4	251.85
330	butyric acid	C4H8O2	7.68706	1778.18	206.702	-5.2	354.85
331	butyric anhydride	C8H14O3	7.66787	1931.49	208.482	-73.3	365.85
332	gamma-butyrolactone	C4H6O2	7.67415	2147.61	244.041	-43.37	465.85
333	butyronitrile	C4H7N	7.36921	1593.17	237.353	-111.9	309.1
334	camphene	C10H16	6.99704	1573.98	221.884	47	364.85
335	camphor	C10H16O	6.94819	1641.75	196.218	180.1	435.85
336	carbon dioxide	CO2	7.58828	861.82	271.883	-56.57	31.04
337	carbon disulfide	CS2	7.2179	1303.79	254.394	-111.57	278.85
338	carbon monoxide	CO	6.72527	295.228	268.243	-205	-140.23
339	carbon tetrabromide	CBr4	8.4814	2690.19	290.841	91	451.762
340	carbon tetrachloride	CCl4	7.01144	1278.54	232.888	-22.82	283.2
341	carbon tetrafluoride	CF4	6.95192	536.118	259.748	-183.59	-45.65
342	carbon tetraiodide	CI4	6.57159	1575.05	108.292	200.876	687.936

## ANTOINE COEFFICIENTS FOR VAPOR PRESSURE

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343	carbonyl fluoride	CF <sub>2</sub> O	7.01104	623.786	234.03	-111.26	23.85
344	carbonyl sulfide	COS	7.00667	833.067	252.064	-138.8	105.65
345	2-chloro-1,1,1,2-tetrafluoroethane	C <sub>2</sub> HClF <sub>4</sub>	6.96877	895.337	230.978	-15.41	122.7
346	2-chloro-1,1,1-trifluoroethane	C <sub>2</sub> H <sub>2</sub> ClF <sub>3</sub>	7.38732	1244.22	269.993	-32.56	159.02
347	1-chloro-1,1,2,2-tetrafluoroethane	C <sub>2</sub> HClF <sub>4</sub>	7.06944	968.741	243.018	-15.41	126.85
348	1-chloro-1,1,2-trifluoroethane	C <sub>2</sub> H <sub>2</sub> ClF <sub>3</sub>	7.28251	1101.48	238.24	-32.56	155.803
349	1-chloro-1,1-difluoroethane	C <sub>2</sub> H <sub>3</sub> ClF <sub>2</sub>	7.30141	1135.31	266.834	-130.8	137.05
350	2-chloro-1,1-difluoroethane	C <sub>2</sub> H <sub>3</sub> ClF <sub>2</sub>	7.29712	1286.52	256.21	-46.0294	204.76
351	2-chloro-1,1-difluoroethylene	C <sub>2</sub> HClF <sub>2</sub>	7.10734	969.906	248.08	-138.5	127.4
352	1-chloro-1,2,2-trifluoroethane	C <sub>2</sub> H <sub>2</sub> ClF <sub>3</sub>	7.56641	1246.19	248.963	-50.4648	155.528
353	1-chloro-1,2-difluoroethane	C <sub>2</sub> H <sub>3</sub> ClF <sub>2</sub>	6.77633	840.473	208.214	-49.6106	162.031
354	cis-1-chloro-1-butene	C <sub>4</sub> H <sub>7</sub> Cl	6.68017	970.337	191.895	-5.4011	247.922
355	trans-1-chloro-1-butene	C <sub>4</sub> H <sub>7</sub> Cl	6.67811	982.14	190.542	-1.70487	255.042
356	2-chloro-1-butene	C <sub>4</sub> H <sub>7</sub> Cl	6.65068	948.171	193.014	-9.74085	242.034
357	3-chloro-1-butene	C <sub>4</sub> H <sub>7</sub> Cl	6.64036	959.521	191.223	-5.38551	251.461
358	4-chloro-1-butene	C <sub>4</sub> H <sub>7</sub> Cl	6.69151	1003.06	189.222	3.14174	261.992
359	cis-1-chloro-1-decene	C <sub>10</sub> H <sub>19</sub> Cl	6.93471	1557.58	161.218	124.179	409.381
360	trans-1-chloro-1-decene	C <sub>10</sub> H <sub>19</sub> Cl	6.93471	1557.58	161.218	124.179	409.381
361	cis-1-chloro-1-dodecene	C <sub>12</sub> H <sub>23</sub> Cl	7.02519	1731.27	154.741	157.309	443.473
362	trans-1-chloro-1-dodecene	C <sub>12</sub> H <sub>23</sub> Cl	7.02519	1731.27	154.741	157.309	443.473
363	cis-1-chloro-1-eicosene	C <sub>20</sub> H <sub>39</sub> Cl	7.15787	2219.54	135.941	254.772	542.42
364	trans-1-chloro-1-eicosene	C <sub>20</sub> H <sub>39</sub> Cl	7.15787	2219.54	135.941	254.772	542.42
365	1-chloro-1-fluoroethane	C <sub>2</sub> H <sub>4</sub> ClF	7.20144	1178.58	256.631	-61.0254	184.92

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366	cis-1-chloro-1-heptadecene	C17H33Cl	7.17402	2087.51	142.235	224.194	509.291
367	trans-1-chloro-1-heptadecene	C17H33Cl	7.17402	2087.51	142.235	224.194	509.291
368	cis-1-chloro-1-heptene	C7H13Cl	6.79657	1270	174.331	64.4159	340.365
369	trans-1-chloro-1-heptene	C7H13Cl	6.79657	1270	174.331	64.4159	340.365
370	cis-1-chloro-1-hexadecene	C16H31Cl	7.15828	2029.08	144.365	212.795	498.081
371	trans-1-chloro-1-hexadecene	C16H31Cl	7.15828	2029.08	144.365	212.795	498.081
372	cis-1-chloro-1-hexene	C6H11Cl	6.75445	1167.18	180.013	41.1551	310.459
373	trans-1-chloro-1-hexene	C6H11Cl	6.75445	1167.18	180.013	41.1551	310.459
374	cis-1-chloro-1-nonadecene	C19H37Cl	7.17489	2185.3	137.91	245.626	532.053
375	trans-1-chloro-1-nonadecene	C19H37Cl	7.17489	2185.3	137.91	245.626	532.053
376	cis-1-chloro-1-nonene	C9H17Cl	6.88774	1466.3	164.942	106.062	389.778
377	trans-1-chloro-1-nonene	C9H17Cl	6.88774	1466.3	164.942	106.062	389.778
378	cis-1-chloro-1-octadecene	C18H35Cl	7.17991	2140.97	140.006	235.42	521.025
379	trans-1-chloro-1-octadecene	C18H35Cl	7.17991	2140.97	140.006	235.42	521.025
380	cis-1-chloro-1-octene	C8H15Cl	6.84124	1371.13	169.208	86.4037	367.33
381	trans-1-chloro-1-octene	C8H15Cl	6.84124	1371.13	169.208	86.4037	367.33
382	cis-1-chloro-1-pentadecene	C15H29Cl	7.13437	1960.42	146.889	199.643	484.797
383	trans-1-chloro-1-pentadecene	C15H29Cl	7.13437	1960.42	146.889	199.643	484.797
384	cis-1-chloro-1-pentene	C5H9Cl	6.71693	1056.84	186.997	14.6971	273.699
385	trans-1-chloro-1-pentene	C5H9Cl	6.71693	1056.84	186.997	14.6971	273.699
386	2-chloro-1-pentene	C5H9Cl	6.68534	1045.45	186.792	13.9394	274.779
387	3-chloro-1-pentene	C5H9Cl	6.67542	1055.6	185.185	17.882	283.238
388	4-chloro-1-pentene	C5H9Cl	6.67387	1065.96	184.03	21.091	289.316

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389	5-chloro-1-pentene	C5H9Cl	6.72754	1101.09	183.241	26.474	293.471
390	cis-1-chloro-1-propene	C3H5Cl	6.65084	872.543	198.642	-29.993	212.411
391	trans-1-chloro-1-propene	C3H5Cl	6.64843	884.09	197.255	-26.2943	219.712
392	2-chloro-1-propene	C3H5Cl	7.04889	1139.05	250.63	-137.4	204.85
393	3-chloro-1-propene	C3H5Cl	7.05562	1230.85	249.869	-134.5	241
394	cis-1-chloro-1-tetradecene	C14H27Cl	7.10323	1888.81	149.33	186.393	471.951
395	trans-1-chloro-1-tetradecene	C14H27Cl	7.10323	1888.81	149.33	186.393	471.951
396	cis-1-chloro-1-tridecene	C13H25Cl	7.06641	1812.12	151.942	172.271	458.2
397	trans-1-chloro-1-tridecene	C13H25Cl	7.06641	1812.12	151.942	172.271	458.2
398	cis-1-chloro-1-undecene	C11H21Cl	6.98081	1647.13	157.739	141.538	427.689
399	trans-1-chloro-1-undecene	C11H21Cl	6.98081	1647.13	157.739	141.538	427.689
400	1-chloro-2,2-dimethylbutane	C6H13Cl	6.62688	1112.58	179.999	36.0458	310.534
401	1-chloro-2,2-dimethylpropane	C5H11Cl	6.58927	1006.01	186.974	9.81352	273.82
402	1-chloro-2,3-dimethylbutane	C6H13Cl	6.68568	1147.14	179.493	40.7484	313.194
403	2-chloro-2,3-dimethylbutane	C6H13Cl	6.57399	1080.19	180.482	31.4495	307.989
404	1-chloro-2,4-dinitrobenzene	C6H3ClN2O4	7.75735	2391.91	175.644	53.4	540.62
405	1-chloro-cis-2-butene	C4H7Cl	6.67129	1023.46	185.807	11.2322	279.962
406	1-chloro-trans-2-butene	C4H7Cl	6.67093	1025.77	185.543	11.9554	281.355
407	2-chloro-cis-2-butene	C4H7Cl	6.63112	963.625	190.146	-3.17917	257.129
408	2-chloro-trans-2-butene	C4H7Cl	6.63298	953.015	191.39	-6.54934	250.578
409	3-chloro-2-ethyl-1-propene	C5H9Cl	6.68453	1050.65	186.216	15.5443	277.814
410	1-chloro-2-ethylbutane	C6H13Cl	6.74026	1178.18	179.271	44.5834	314.364
411	1-chloro-2-fluoroethane	C2H4ClF	6.72621	949.078	193.809	-22.8063	237.85

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412	cis-1-chloro-2-methyl-1-butene	C5H9Cl	6.66837	1044.64	185.809	15.4224	279.955
413	trans-1-chloro-2-methyl-1-butene	C5H9Cl	6.66837	1044.64	185.809	15.4224	279.955
414	3-chloro-2-methyl-1-butene	C5H9Cl	6.62763	1041.51	184.173	18.0427	288.565
415	4-chloro-2-methyl-1-butene	C5H9Cl	6.67988	1081.81	182.756	25.1734	296.02
416	1-chloro-2-methyl-1-propene	C4H7Cl	6.63055	966.909	189.76	-2.13602	259.157
417	3-chloro-2-methyl-1-propene	C4H7Cl	6.64457	982.982	188.97	1.25547	263.316
418	1-chloro-2-methyl-cis-2-butene	C5H9Cl	6.66155	1091.12	180.6	29.8612	307.37
419	1-chloro-2-methyl-trans-2-butene	C5H9Cl	6.66264	1083.37	181.468	27.4547	302.801
420	1-chloro-2-methylbutane	C5H11Cl	7.07153	1386.46	230.301	4.87564	288.775
421	2-chloro-2-methylbutane	C5H11Cl	6.81907	1185.1	215.309	7	275.82
422	1-chloro-2-methylpentane	C6H13Cl	6.74238	1162.13	180.949	39.7684	305.533
423	2-chloro-2-methylpentane	C6H13Cl	6.62882	1098.4	181.562	31.6489	302.305
424	3-chloro-2-methylpentane	C6H13Cl	6.6893	1120.48	182.355	32.6176	298.133
425	1-chloro-2-methylpropane	C4H9Cl	6.66332	982.579	190.919	-1.4589	253.057
426	2-chloro-2-methylpropane	C4H9Cl	6.96058	1176.32	237.729	-25.4	233.85
427	1-chloro-cis-2-pentene	C5H9Cl	6.709	1110.59	181.108	31.1653	304.697
428	1-chloro-trans-2-pentene	C5H9Cl	6.70864	1113.21	180.82	31.9687	306.21
429	2-chloro-cis-2-pentene	C5H9Cl	6.66758	1049.8	185.23	17.0267	283.001
430	2-chloro-trans-2-pentene	C5H9Cl	6.66758	1049.8	185.23	17.0267	283.001
431	3-chloro-cis-2-pentene	C5H9Cl	6.66837	1044.64	185.809	15.4224	279.955
432	3-chloro-trans-2-pentene	C5H9Cl	6.66837	1044.64	185.809	15.4224	279.955
433	4-chloro-cis-2-pentene	C5H9Cl	6.65776	1059.86	183.613	20.968	291.513
434	4-chloro-trans-2-pentene	C5H9Cl	6.65776	1059.86	183.613	20.968	291.513

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435	5-chloro-cis-2-pentene	C5H9Cl	6.70937	1107.97	181.395	30.362	303.185
436	5-chloro-trans-2-pentene	C5H9Cl	6.70937	1107.97	181.395	30.362	303.185
437	1-chloro-3,3-dimethylbutane	C6H13Cl	6.62688	1112.58	179.999	36.0458	310.534
438	2-chloro-3,3-dimethylbutane	C6H13Cl	6.57433	1077.65	180.769	30.6514	306.48
439	cis-1-chloro-3-methyl-1-butene	C5H9Cl	6.6593	1049.56	184.772	17.7601	285.411
440	trans-1-chloro-3-methyl-1-butene	C5H9Cl	6.6593	1049.56	184.772	17.7601	285.411
441	2-chloro-3-methyl-1-butene	C5H9Cl	6.6291	1031.82	185.278	14.9986	282.748
442	3-chloro-3-methyl-1-butene	C5H9Cl	6.5653	984.061	187.082	6.31908	273.251
443	4-chloro-3-methyl-1-butene	C5H9Cl	6.67581	1053.01	185.474	17.0797	281.719
444	1-chloro-3-methyl-2-butene	C5H9Cl	6.66083	1096.29	180.021	31.4655	310.416
445	2-chloro-3-methyl-2-butene	C5H9Cl	6.61941	1038.81	183.862	18.1519	290.2
446	1-chloro-3-methylbutane	C5H11Cl	7.26558	1547.55	254.428	39	285.72
447	2-chloro-3-methylbutane	C5H11Cl	6.64617	1047.65	185.434	17.2436	281.928
448	1-chloro-3-methylpentane	C6H13Cl	6.73922	1186.2	178.432	46.991	318.78
449	2-chloro-3-methylpentane	C6H13Cl	6.69115	1107.34	183.765	28.6123	290.713
450	3-chloro-3-methylpentane	C6H13Cl	6.62723	1110	180.283	35.2464	309.038
451	4-chloro-3-nitrobenzotrifluoride	C7H3ClF3NO2	7.4342	1894.16	193.989	20	412.85
452	1-chloro-4-methylpentane	C6H13Cl	6.74061	1175.5	179.551	43.7809	312.892
453	2-chloro-4-methylpentane	C6H13Cl	6.68888	1123.5	182.031	33.5388	299.839
454	chloroacetaldehyde	C2H3ClO	7.27707	1342.1	220.432	19.85	281.85
455	chloroacetic acid	C2H3ClO2	7.6413	1820.08	192.982	60	412.85
456	chloroacetyl chloride	C2H2Cl2O	7.29542	1419.24	215.487	-22	307.85
457	m-chloroaniline	C6H6ClN	7.40372	1952.27	203.141	-10.4	477.85

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458	p-chloroaniline	C6H6ClN	7.40172	1957.87	202.57	69.9	480.85
459	chlorobenzene	C6H5Cl	7.18342	1574.53	234.229	-45.2	359.2
460	p-chlorobenzotrifluoride	C7H4ClF3	7.16969	1548.6	222.073	-36	327.85
461	m-chlorobenzoyl chloride	C7H4Cl2O	7.54675	2099.23	225.056	6.85	450.85
462	1-chlorobutane	C4H9Cl	7.12193	1329.37	235.017	-123.1	263.85
463	2-chlorobutane	C4H9Cl	7.25318	1378.58	247.194	-131.3	247.45
464	1-chlorodecane	C10H21Cl	7.25952	1868.3	200.808	106.306	406.735
465	chlorodifluoromethane	CHClF2	7.07154	848.817	243.376	-157.42	96.15
466	1-chlorodocosane	C22H45Cl	6.95946	2092.35	118.001	303.89	548.597
467	1-chlorododecane	C12H25Cl	7.30956	2009.02	190.451	137.101	437.874
468	1-chlorodotriacontane	C32H65Cl	6.19739	1888.14	85.3027	390.215	534
469	1-chloroeicosane	C20H41Cl	6.97391	1979.91	110.718	230.775	527.487
470	2-chloroethanol	C2H5ClO	8.36278	2112.72	256.794	-67.5	311.85
471	chlorofluoromethane	CH2ClF	7.92235	1587.64	324.003	-55	151.76
472	chloroform	CHCl3	7.11148	1232.79	230.213	-63.52	263.25
473	1-chloroheneicosane	C21H43Cl	7.02818	2102.72	123.001	295.186	537.724
474	1-chlorohentriacontane	C31H63Cl	6.26814	1913.53	88.909	386.658	526
475	1-chloroheptacosane	C27H55Cl	6.37004	1826.23	80.3899	336.53	604.825
476	1-chloroheptadecane	C17H35Cl	7.35256	2271.12	167.883	199.825	500.418
477	1-chloroheptane	C7H15Cl	7.16071	1608.42	215.369	53.3923	347.927
478	1-chloroheptatriacontane	C37H75Cl	5.91505	1790.07	70.9567	397.661	569
479	1-chlorohexacosane	C26H53Cl	6.54067	1933.42	94.2759	331.25	592.826
480	1-chlorohexadecane	C16H33Cl	7.30623	2172.24	164.256	190.1	489.511

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481	1-chlorohexane	C6H13Cl	7.12663	1508.6	220.224	33.3003	323.041
482	2-chlorohexane	C6H13Cl	6.74096	1172.83	179.83	42.9784	311.42
483	3-chlorohexane	C6H13Cl	6.74131	1170.15	180.11	42.1759	309.949
484	1-chlorohexatriacontane	C36H73Cl	5.96841	1808.33	73.6764	396.995	562
485	1-chloronaphthalene	C10H7Cl	7.14388	1931.55	193.79	-4	511.85
486	m-chloronitrobenzene	C6H4ClNO2	7.42076	1956.77	195.411	44.5	468.85
487	p-chloronitrobenzene	C6H4ClNO2	7.39602	1951.27	190.155	83.5	477.85
488	1-chlorononacosane	C29H59Cl	5.97308	1554.22	42.6146	344.993	630.053
489	1-chlorononadecane	C19H39Cl	7.11701	2092.1	130.862	221.29	519.113
490	1-chlorononane	C9H19Cl	7.20883	1767.2	203.096	89.8404	388.733
491	1-chlorononatriacontane	C39H79Cl	5.82882	1762.61	66.8986	396.16	581
492	1-chlorooctacosane	C28H57Cl	6.18126	1701.23	63.4531	341.392	617.631
493	1-chlorooctadecane	C18H37Cl	7.18475	2122.15	141.072	212.112	510.102
494	1-chlorooctane	C8H17Cl	7.17727	1682.87	208.218	72.2071	369.261
495	1-chlorooctatriacontane	C38H77Cl	5.87137	1776.04	68.8827	397.106	575
496	1-chloropentacosane	C25H51Cl	6.68545	2014.23	104.414	325.575	581.601
497	1-chloropentadecane	C15H31Cl	7.33542	2161.98	173.335	177.676	477.58
498	chloropentafluoroethane	C2ClF5	7.01458	870.384	249.665	-99.44	80
499	1-chloropentane	C5H11Cl	7.21236	1494.95	236.74	-99	294.85
500	2-chloropentane	C5H11Cl	7.05365	1356.55	228.571	2.23227	282.73
501	3-chloropentane	C5H11Cl	6.69986	1079.68	184.919	21.8077	284.639
502	1-chloropentatriacontane	C35H71Cl	6.02329	1827.27	76.4757	395.913	555
503	m-chlorophenol	C6H5ClO	7.95713	2396.76	258.295	32.85	455.85

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504	p-chlorophenol	C6H5ClO	7.88595	2340.65	247.69	42.85	464.85
505	chloroprene	C4H5Cl	7.0847	1285.63	246.42	-130	251.85
506	1-chloropropane	C3H7Cl	7.11195	1208.24	239.039	-122.8	230
507	2-chloropropane	C3H7Cl	6.85852	1009.5	218.091	-117.18	215.85
508	1-chlorotetracontane	C40H81Cl	5.78738	1749.77	65.0064	394.834	587
509	1-chlorotetracosane	C24H49Cl	6.78302	2040.86	108.001	318.687	569.894
510	1-chlorotetradecane	C14H29Cl	7.34738	2134.36	181.012	164.843	465.392
511	1-chlorotetratriacontane	C34H69Cl	6.07972	1846.89	79.35	394.419	548
512	p-chlorotoluene	C7H7Cl	7.13594	1605.85	214.891	7.5	386.85
513	m-chlorotoluene	C7H7Cl	7.1374	1620.34	218.365	53.4449	387.029
514	1-chlorotriacontane	C30H61Cl	6.38297	1989.1	99.9644	348.149	518
515	1-chlorotricosane	C23H47Cl	6.87717	2070.11	113.001	311.449	558.901
516	1-chlorotridecane	C13H27Cl	7.3403	2082.9	187.071	150.833	451.438
517	chlorotrifluoroethylene	C2ClF3	7.02751	881.594	240.451	-158.15	106
518	chlorotrifluoromethane	CClF3	7.05316	746.56	260.34	-181	28.81
519	1-chlorotritriacontane	C33H67Cl	6.13774	1867.18	82.2942	392.517	541
520	1-chloroundecane	C11H23Cl	7.29439	1951.07	196.722	122.172	423.278
521	chrysene	C18H12	7.30847	2609.83	148.439	258	705.85
522	citraconic acid	C5H6O4	8.11441	2587.85	160.618	83	555.85
523	citric acid	C6H8O7	9.37143	3305.17	123.373	153	548.85
524	m-cresol	C7H8O	7.26723	1670.93	178.653	12.24	432.7
525	p-cresol	C7H8O	7.45834	1768.27	184.313	34.78	431.5
526	trans-crotonaldehyde	C4H6O	7.28193	1460.08	227.652	-76.5	297.85

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527	trans-crotonitrile	C4H5N	7.45169	1653.01	240.409	-51.15	312.85
528	cis-crotonitrile	C4H5N	7.47046	1633.44	248.446	-72.6	294.85
529	cumene	C9H12	7.10691	1577.97	220.977	-96.01	358
530	cumene hydroperoxide	C9H12O2	6.95989	1116.91	104.264	-8.89	331.85
531	p-cumylphenol	C15H16O	7.52176	2371.68	176.035	72.85	560.85
532	cyanogen	C2N2	7.24606	947.481	238.201	-27.9	127
533	cyanogen chloride	CClN	7.5797	1265.43	256.454	-6.5	175.85
534	cyclobutane	C4H8	7.11632	1109.64	249.476	-90.67	186.78
535	cyclobutene	C4H6	7.17769	1102.63	254.012	-77	173.18
536	cyclodecane	C10H20	6.90113	1618.66	200.62	129.642	435.85
537	cyclododecane	C12H24	6.85731	1720.19	193.59	160.555	474.078
538	cycloeicosane	C20H40	6.83775	2061.09	172.88	253.163	569.659
539	cycloheptadecane	C17H34	6.84231	1951.16	179.53	223.409	541.909
540	cycloheptane	C7H14	7.0113	1417.93	224.495	-8.03	331.15
541	1,3,5-cycloheptatriene	C7H8	7.33889	1585.78	240.209	0	320.75
542	cyclohexadecane	C16H32	6.84404	1910.28	182	212.356	530.932
543	1,3-cyclohexadiene	C6H8	7.14886	1359.07	238.088	-112.15	284.85
544	cyclohexane	C6H12	7.00854	1296.23	233.309	6.54	280.39
545	1,4-cyclohexanedicarboxylic acid	C8H12O4	8.034	2688.93	125.95	312.5	615.85
546	cyclohexanol	C6H12O	7.14994	1405.48	168.37	23.45	352
547	cyclohexanone	C6H10O	7.60652	1884.55	243.036	-31.15	356
548	cyclohexanone oxime	C6H11NO	7.41015	1821.35	194.123	90	441.85
549	cyclohexene	C6H10	7.0229	1300.39	230.976	-103.48	287.25

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550	cyclohexylamine	C6H13N	7.36494	1647.76	232.966	-17.7	341.85
551	cyclohexylbenzene	C12H16	7.00955	1753.02	184.47	6.99	470.85
552	cyclohexyl isocyanate	C7H11NO	7.52412	1795.14	217.608	-80.15	359.85
553	cyclohexyl peroxide	C6H12O2	7.91206	2068.6	194.3	-20	411.85
554	cyclononadecane	C19H38	6.83935	2026.65	174.97	243.816	561.243
555	cyclononane	C9H18	6.92639	1551.5	205.104	109.831	408.85
556	cyclooctadecane	C18H36	6.84087	1988.94	177.25	233.614	551.543
557	1,5-cyclooctadiene	C8H12	7.14156	1594.32	224.067	-69.17	371.85
558	cyclooctane	C8H16	6.99639	1527.08	219.9	94	374.05
559	1,3,5,7-cyclooctatetraene	C8H8	6.96737	1439.91	212.343	0	369.4
560	cyclopentadecane	C15H30	6.84622	1866.36	184.66	200.456	518.567
561	cyclopentadiene	C5H6	7.26828	1326.36	260.807	-85	233.85
562	cyclopentane	C5H10	7.04267	1202.53	239.69	-93.87	238.61
563	cyclopentanethiol	C5H10S	7.10422	1510.95	225.577	81	355.85
564	cyclopentanone	C5H8O	7.56585	1727.86	238.153	-51.3	352.85
565	cyclopentene	C5H8	7.09158	1209.22	242.943	-135.02	233.85
566	cyclopropane	C3H6	7.0298	904.465	250.776	-127.56	124.76
567	cyclotetradecane	C14H28	6.84906	1819.48	187.51	187.713	504.763
568	cyclotridecane	C13H26	6.85256	1772.83	190.36	174.979	490.91
569	cycloundecane	C11H22	6.86335	1664.74	197.01	145.293	455.631
570	m-cymene	C10H14	7.11317	1675.81	220.871	-63.71	383.85
571	p-cymene	C10H14	7.13238	1671.47	216.013	-67.9	380
572	D-limonene	C10H16	7.06744	1691.15	227.441	-74.15	386.85

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573	decafluorobutane	C4F10	7.06833	1002.58	241.421	-128.2	113.2
574	cis-decahydronaphthalene	C10H18	7.02551	1695.68	213.301	-42.95	429.1
575	trans-decahydronaphthalene	C10H18	6.82768	1544.81	204.091	-30.36	413.9
576	decanal	C10H20O	7.45314	1888.66	198.063	-6	383.85
577	decane	C10H22	7.21745	1693.93	216.459	-29.66	345.3
578	1,2-decanediol	C10H22O2	9.65155	3744.22	273.001	185.04	423.934
579	1,3-decanediol	C10H22O2	7.60016	2182.89	232.223	180.318	280.318
580	1,4-decanediol	C10H22O2	9.65163	3960.93	273.001	211.546	464.261
581	1,10-decanediol	C10H22O2	9.70657	3904.34	273.001	201.434	445.908
582	decanenitrile	C10H19N	7.17122	1726.02	159.298	143.827	419.486
583	2-decanethiol	C10H22S	7.15356	1809.06	195.094	98.891	416.85
584	decanoic acid	C10H20O2	7.3443	1755.03	123.197	31.6	439.85
585	1-decanol	C10H22O	7.03752	1579.82	149.864	6.9	416.85
586	2-decanol	C10H22O	6.80298	1341.69	125.078	126.841	400.05
587	3-decanol	C10H22O	8.61878	2770.58	273	114.946	359.7
588	4-decanol	C10H22O	8.61878	2771.44	273	115.066	359.897
589	5-decanol	C10H22O	8.61876	2719.79	273	107.835	348.104
590	2-decanone	C10H20O	7.40209	1852.35	199.497	89.8387	383.442
591	1-decene	C10H20	7.17365	1656.67	215.316	-66.26	343.9
592	1-decyl-[1,2,3,4-tetrahydronaphthalene]	C20H32	7.39501	2398.89	170.411	300.516	541.013
593	2-decyl-[1,2,3,4-tetrahydronaphthalene]	C20H32	7.39466	2406.02	170.031	302.328	543.581
594	decyl acetate	C12H24O2	6.87474	1609.86	159.077	139.177	420.65
595	decylamine	C10H23N	7.654	2086.71	216.674	15.7	389.85

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596	decylbenzene	C16H26	7.4989	2283.54	196.586	-14.38	479.85
597	decyl butanoate	C14H28O2	6.34862	1187.08	62.3129	148.735	447.05
598	decylcyclohexane	C16H32	7.31408	2127.35	182.262	-1.73	478.1
599	decylcyclopentane	C15H30	7.17072	1953.27	175.928	141	457.49
600	1-decylcyclopentene	C15H28	7.25553	1998.77	187.89	158.012	445.447
601	decyl formate	C11H22O2	7.00261	1632.58	160.635	134.829	412.45
602	decyl mercaptan	C10H22S	7.35259	1955.29	198.051	-25.59	422.85
603	1-declynaphthalene	C20H28	7.4838	2513.19	166.991	317.921	565.518
604	2-declynaphthalene	C20H28	7.48312	2527.73	166.231	321.551	570.662
605	decyl propanoate	C13H26O2	7.42575	1992.34	156.455	178.469	434.45
606	1-decyne	C10H18	7.07163	1583.08	203.739	78	359.34
607	2-decyne	C10H18	7.07436	1643.12	207.222	71.3569	377.706
608	3-decyne	C10H18	7.07535	1625.05	208.122	67.3474	370.17
609	dehydroabietylamine	C20H31N	7.49099	2586.95	174.289	44.5	589.85
610	2,6-di-tert-butyl-p-cresol	C15H24O	7.41286	2010.21	178.703	70.85	446.85
611	di-sec-butyl ether	C8H18O	7.23165	1515.43	227.258	-100	285.85
612	di-tert-butyl ether	C8H18O	7.04933	1401.98	229.075	-78.15	276.85
613	di-pentyl ether	C10H22O	7.6263	2007.96	236.38	-69.43	348.85
614	di-propylamine	C6H15N	7.36576	1469.89	218.887	-63	282.65
615	di-t-butyl peroxide	C8H18O2	7.09393	1395.39	220.201	-40	273.85
616	diacetone alcohol	C6H12O2	8.63179	2570.51	279.12	-44	332.85
617	diallyl maleate	C10H12O4	7.7475	2167.26	198.476	-47	419.85
618	dibenzofuran	C12H8O	7.20786	2284.28	243.198	82.5	564.65

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619	dibenzopyrrole	C12H9N	7.47115	2545.26	199.771	244.8	625.85
620	dibenzyl ether	C14H14O	7.33137	2084.84	180.145	3.6	503.85
621	1,1-dibromo-2,2-dimethylpropane	C5H10Br2	7.10828	1456.13	164.444	94.1396	392.399
622	1,3-dibromo-2,2-dimethylpropane	C5H10Br2	6.92256	1388.08	160.436	94.4711	413.496
623	1,3-dibromo-2-(bromomethyl)propane	C4H7Br3	7.34427	1665.6	153.163	130.722	451.776
624	1,3-dibromo-2-ethylpropane	C5H10Br2	6.98518	1375.11	165.296	84.3582	387.915
625	1,1-dibromo-2-methylbutane	C5H10Br2	7.05033	1408.22	165.652	87.0249	386.045
626	1,2-dibromo-2-methylbutane	C5H10Br2	6.98422	1384.37	164.372	87.008	392.781
627	1,3-dibromo-2-methylbutane	C5H10Br2	7.05033	1408.22	165.652	87.0249	386.045
628	1,4-dibromo-2-methylbutane	C5H10Br2	7.11054	1434.13	166.529	88.0459	381.428
629	2,3-dibromo-2-methylbutane	C5H10Br2	7.12314	1535.82	191.164	81	395.22
630	1,1-dibromo-2-methylpropane	C4H8Br2	7.01369	1310.55	170.104	66.6043	362.612
631	1,2-dibromo-2-methylpropane	C4H8Br2	6.94749	1291.03	168.466	67.5385	371.234
632	1,3-dibromo-2-methylpropane	C4H8Br2	7.06487	1414.87	163.158	90.0518	399.17
633	1,1-dibromo-3-methylbutane	C5H10Br2	7.05033	1408.22	165.652	87.0249	386.045
634	1,2-dibromo-3-methylbutane	C5H10Br2	7.05033	1408.22	165.652	87.0249	386.045
635	1,3-dibromo-3-methylbutane	C5H10Br2	6.98518	1375.11	165.296	84.3582	387.915
636	2,2-dibromo-3-methylbutane	C5H10Br2	6.92643	1349.84	164.354	83.3536	392.873
637	m-dibromobenzene	C6H4Br2	7.22786	1893.89	217.673	-6.9	487.85
638	1,1-dibromobutane	C4H8Br2	7.48829	1751.2	222.079	47.8236	373.666
639	1,2-dibromobutane	C4H8Br2	7.82182	2131.34	265.048	8	386.13
640	1,3-dibromobutane	C4H8Br2	7.06487	1414.87	163.158	90.0518	399.17
641	1,4-dibromobutane	C4H8Br2	7.11908	1504.6	158.005	108.677	426.293

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642	2,2-dibromobutane	C4H8Br2	6.94909	1277.1	169.916	63.473	363.602
643	1,1-dibromodecane	C10H20Br2	7.71055	2317.8	202.903	142.494	468.671
644	dibromodifluoromethane	CBr2F2	7.22244	1203.61	254.436	-110.1	204.85
645	1,1-dibromodocosane	C22H44Br2	7.53655	2781.22	163.374	340.366	594.988
646	1,1-dibromododecane	C12H24Br2	7.6433	2324.1	178	233.832	493.224
647	1,1-dibromodotriacontane	C32H64Br2	6.59384	2356.08	115.546	421.21	569
648	1,1-dibromoeicosane	C20H40Br2	7.53283	2600.48	146.001	324.008	574.423
649	1,1-dibromoethane	C2H4Br2	6.98532	1330.25	216.095	-63	354.85
650	1,2-dibromoethane	C2H4Br2	7.22206	1605.23	238.402	9.79	377
651	1,1-dibromoheneicosane	C21H42Br2	7.56668	2728.29	158.238	332.764	584.975
652	1,1-dibromohentriacontane	C31H62Br2	6.65053	2374.47	117.881	418.951	562
653	1,1-dibromoheptacosane	C27H54Br2	6.67224	2194.39	98.7768	369.561	651.428
654	1,1-dibromoheptadecane	C17H34Br2	7.65768	2565.18	158.001	295.397	545.444
655	1,1-dibromoheptane	C7H14Br2	7.58699	2038.68	211.193	98.3083	426.895
656	1,1-dibromoheptatriacontane	C37H74Br2	6.33918	2276.46	105.247	425.083	603
657	1,1-dibromohexacosane	C26H52Br2	6.90972	2386.09	121.242	364.701	638.786
658	1,1-dibromohexadecane	C16H32Br2	7.67336	2530.47	162.001	284.026	534.929
659	1,1-dibromohexane	C6H12Br2	7.55575	1950.86	215.302	82.2781	411.064
660	1,1-dibromohexatriacontane	C36H72Br2	6.3891	2291.79	107.251	425.045	596
661	dibromomethane	CH2Br2	7.23867	1423.39	229.675	-52.55	337.85
662	1,1-dibromonacosane	C29H58Br2	6.15884	1771.66	44.4654	376.23	676.889
663	1,1-dibromononadecane	C19H38Br2	7.58772	2598.21	150.001	314.986	564.537
664	1,1-dibromononane	C9H18Br2	7.68389	2245.16	207.441	128.464	456.295

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665	1,1-dibromonatriacontane	C39H78Br2	6.2583	2253.98	102.356	422.162	615
666	1,1-dibromooctacosane	C28H56Br2	6.41436	1978.79	72.0012	373.13	663.707
667	1,1-dibromooctadecane	C18H36Br2	7.62948	2588.02	154.001	305.727	555.301
668	1,1-dibromooctane	C8H16Br2	7.63062	2140.01	208.547	114.2	442.871
669	1,1-dibromooctatriacontane	C38H76Br2	6.29823	2264.92	103.759	423.844	609
670	1,1-dibromopentacosane	C25H50Br2	7.142	2581.09	142.721	360.259	628.2
671	1,1-dibromopentadecane	C15H30Br2	7.67889	2490.2	166.001	272.501	524.987
672	1,1-dibromopentane	C5H10Br2	7.5111	1840.56	217.504	65.176	392.399
673	1,2-dibromopentane	C5H10Br2	7.1071	1467.91	163.328	97.4026	398.274
674	1,3-dibromopentane	C5H10Br2	7.10537	1485.58	161.654	102.297	407.086
675	1,4-dibromopentane	C5H10Br2	7.10259	1515.04	158.863	110.455	421.773
676	1,5-dibromopentane	C5H10Br2	7.15749	1608.09	153.714	129.382	448.874
677	2,2-dibromopentane	C5H10Br2	6.9851	1375.85	165.223	84.5695	388.303
678	2,3-dibromopentane	C5H10Br2	7.04842	1426.77	163.849	92.2451	395.535
679	2,4-dibromopentane	C5H10Br2	7.04741	1436.91	162.864	95.0955	400.717
680	3,3-dibromopentane	C5H10Br2	6.986	1367.33	166.073	82.1311	383.826
681	1,1-dibromopentatriacontane	C35H70Br2	6.43227	2304.53	108.896	425.387	590
682	1,1-dibromopropane	C3H6Br2	7.48574	1668.45	228.819	28.4302	350.964
683	1,2-dibromopropane	C3H6Br2	7.73989	1946.68	260.617	50	360.96
684	1,3-dibromopropane	C3H6Br2	7.08608	1391.56	163.61	84.4869	396.791
685	2,2-dibromopropane	C3H6Br2	6.91913	1173.91	175.592	40.12	333.903
686	1,1-dibromotetracontane	C40H80Br2	6.21935	2243.63	101.039	420.042	621
687	1,1-dibromotetracosane	C24H48Br2	7.31207	2691.2	154.323	353.715	615.962

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688	1,1-dibromotetradecane	C14H28Br2	7.6744	2439.94	170.001	259.99	514.319
689	1,2-dibromotetrafluoroethane	C2Br2F4	7.04279	1204.83	242.224	-110.5	214.65
690	1,1-dibromotetratriacontane	C34H68Br2	6.48474	2321.1	111.048	424.44	583
691	1,1-dibromotriacontane	C30H60Br2	6.75259	2442.52	126.853	378.842	554
692	1,1-dibromotricosane	C23H46Br2	7.45698	2778.32	163.13	347.643	605.717
693	1,1-dibromotridecane	C13H26Br2	7.66246	2386.04	174.001	247.379	504.173
694	1,1-dibromotritriacontane	C33H66Br2	6.53858	2338.29	113.266	423.044	576
695	1,1-dibromoundecane	C11H22Br2	7.61835	2255.07	182	219.375	481.412
696	dibutylamine	C8H19N	7.48571	1694.45	209.117	-62	334.35
697	dibutyl disulfide	C8H18S2	7.44733	2035.74	214.588	101	431.01
698	dibutyl ether	C8H18O	7.2781	1602.15	224.059	-95.2	307.85
699	dibutyl maleate	C12H20O4	7.77306	2265.01	182.978	1.85	442.85
700	dibutyl phthalate	C16H22O4	7.96819	2657.06	182.284	-35	507.85
901	4,4-diethyloctane	C12H26	6.92555	1544.42	181.835	78.8026	371.135
902	4,5-diethyloctane	C12H26	6.97693	1551.75	181.835	77.7886	363.511
903	diethyloctylamine	C12H27N	7.06936	1557.06	158.743	118.577	372.728
904	diethyl oxalate	C6H10O4	7.4848	1811.09	207.673	-40.6	372.85
905	diethylpentacosylamine	C29H61N	6.2713	1450	9.66667	308.724	468
906	diethylpentadecylamine	C19H41N	6.90998	1687.7	101.872	203.403	462.524
907	3,3-diethylpentane	C9H20	7.09525	1578.99	228.471	-33.03	336.9
908	diethylpentatriacontylamine	C39H81N	9.17719	4805.08	273.15	359.103	540
909	diethylpentylamine	C9H21N	7.01117	1378.6	177.771	71.3401	322.256
910	2,3-diethylphenol	C10H14O	7.21813	1721.27	165	146.871	446.549

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911	2,4-diethylphenol	C10H14O	7.21224	1702.25	165	143.755	441.063
912	2,5-diethylphenol	C10H14O	7.21046	1696.57	165	142.825	439.424
913	2,6-diethylphenol	C10H14O	7.1965	1652.91	165	135.664	426.811
914	3,4-diethylphenol	C10H14O	7.27815	1933.6	165	181.574	507.646
915	3,5-diethylphenol	C10H14O	7.2419	1801.13	165	159.942	469.566
916	diethyl phthalate	C12H14O4	7.68399	2304.78	185.845	-4	483.85
917	diethylpropylamine	C7H17N	6.92101	1202.94	185.744	35.2276	280.297
918	diethyl succinate	C8H14O4	7.64782	1958.15	194.271	-20.8	386.85
919	diethyl sulfate	C4H10O4S	7.17299	1780.2	204.905	-25.15	518.85
920	diethyl sulfide	C4H10S	7.20449	1423.41	237.112	-103.95	284
921	diethyl sulfite	C4H10O3S	---	---	---	---	---
922	diethyltetracosylamine	C28H59N	6.21945	1400	9.33333	305.161	460
923	diethyltetradecylamine	C18H39N	7.03065	1759.49	119.991	193.239	450.765
924	diethyltetratriacontylamine	C38H79N	9.26604	4828.19	273.15	359.342	533
925	diethyltriacontylamine	C34H71N	9.25679	4655.42	273.15	357.752	507
926	diethyltricosylamine	C27H57N	6.1735	1350	9	300.317	451
927	diethyltridecylamine	C17H37N	6.98254	1669.94	116.132	182.867	439.502
928	diethyltritriacontylamine	C37H77N	9.26487	4789	273.15	360.002	527
929	diethylundecylamine	C15H33N	7.07943	1685.38	138.412	160.021	415.817
930	1,1-difluoro-2,2-dimethylpropane	C5H10F2	6.63839	893.081	202.155	-29.1196	193.923
931	1,3-difluoro-2,2-dimethylpropane	C5H10F2	6.69398	910.394	202.79	-28.28	190.581
932	1,3-difluoro-2-(fluoromethyl)-propane	C4H7F3	6.86451	896.064	209.793	-43.4667	153.722
933	1,3-difluoro-2-ethylpropane	C5H10F2	6.8116	952.003	203.442	-24.9794	187.149

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934	1,1-difluoro-2-methylbutane	C5H10F2	6.7546	934.204	202.85	-25.8333	190.262
935	1,2-difluoro-2-methylbutane	C5H10F2	6.69398	910.394	202.79	-28.28	190.581
936	1,3-difluoro-2-methylbutane	C5H10F2	6.7546	934.204	202.85	-25.8333	190.262
937	1,4-difluoro-2-methylbutane	C5H10F2	6.8116	952.003	203.442	-24.9794	187.149
938	2,3-difluoro-2-methylbutane	C5H10F2	6.63839	893.081	202.155	-29.1196	193.923
939	1,1-difluoro-2-methylpropane	C4H8F2	6.70691	900.707	202.411	-30.1851	192.572
940	1,2-difluoro-2-methylpropane	C4H8F2	6.64441	888.36	201.04	-29.1202	199.789
941	1,3-difluoro-2-methylpropane	C4H8F2	6.74794	996.121	194.587	-5.5989	233.755
942	1,1-difluoro-3-methylbutane	C5H10F2	6.7546	934.204	202.85	-25.8333	190.262
943	1,2-difluoro-3-methylbutane	C5H10F2	6.7546	934.204	202.85	-25.8333	190.262
944	1,3-difluoro-3-methylbutane	C5H10F2	6.69398	910.394	202.79	-28.28	190.581
945	2,2-difluoro-3-methylbutane	C5H10F2	6.63839	893.081	202.155	-29.1196	193.923
946	m-difluorobenzene	C6H4F2	7.21033	1393.09	231.255	36	279.79
947	p-difluorobenzene	C6H4F2	7.20567	1376.63	229.456	34	282.85
948	1,1-difluorobutane	C4H8F2	7.20361	1204.08	237.542	-43.4484	190.15
949	1,2-difluorobutane	C4H8F2	6.75439	961.853	198.311	-16.048	214.151
950	1,3-difluorobutane	C4H8F2	6.74938	988.212	195.446	-8.01025	229.231
951	1,4-difluorobutane	C4H8F2	6.79812	1053.75	191.199	6.83748	251.586
952	2,2-difluorobutane	C4H8F2	6.64666	877.953	202.236	-32.4037	193.496
953	2,3-difluorobutane	C4H8F2	6.6994	936.946	198.365	-18.9515	213.87
954	1,1-difluorodecane	C10H20F2	6.90744	1436.98	173.868	69.3802	348.85
955	1,1-difluorodocosane	C22H44F2	7.11168	2145.05	156.001	289.896	493.503
956	1,1-difluorododecane	C12H24F2	7.14499	1769.63	196	147.953	383.75

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957	1,1-difluorodotriacontane	C32H64F2	6.38015	2005.62	135.142	345.873	488
958	1,1-difluoroeicosane	C20H40F2	7.07461	2071.74	164.001	244.255	480.85
959	1,1-difluoroethane	C2H4F2	7.11973	928.549	244.854	-117	113.45
960	1,2-difluoroethane	C2H4F2	7.0601	1124.53	238.572	-58.15	202.85
961	cis-1,2-difluoroethene	C2H2F2	10.4281	3891.37	540.888	-78	121.52
962	trans-1,2-difluoroethene	C2H2F2	10.4281	3891.37	540.888	-78	121.52
963	1,1-difluoroethylene	C2H2F2	6.95654	695.51	256.297	-144	29.65
964	1,1-difluoroheneicosane	C21H42F2	7.18764	2157.72	160.001	281.557	483.371
965	1,1-difluorohentriacontane	C31H62F2	6.4392	2022.78	137.453	343.348	481
966	1,1-difluoroheptacosane	C27H54F2	6.39469	1778.61	107.166	325.972	551.591
967	1,1-difluoroheptadecane	C17H34F2	7.10809	1982.59	176.001	212.128	450.45
968	1,1-difluoroheptane	C7H14F2	7.01248	1339.88	204.595	18.2545	282.95
969	1,1-difluoroheptatriacontane	C37H74F2	6.11596	1930.86	124.839	351.404	522
970	1,1-difluorohexacosane	C26H52F2	6.60627	1923.45	126.3	319.874	539.295
971	1,1-difluorohexadecane	C16H32F2	7.12991	1954.59	180.001	201.017	438.95
972	1,1-difluorohexane	C6H12F2	7.04305	1289.56	214.824	-1.42843	255.85
973	1,1-difluorohexatriacontane	C36H72F2	6.15946	1942.37	126.432	351.817	516
974	difluoromethane	CH2F2	7.2902	863.592	247.503	-136.15	78.45
975	1,1-difluorononacosane	C29H58F2	5.91489	1431.73	56.8851	335.394	576.076
976	1,1-difluorononadecane	C19H38F2	7.07972	2040.67	168.001	233.729	471.35
977	1,1-difluorononane	C9H18F2	6.9346	1406.14	183.872	53.0682	329.05
978	1,1-difluorononatriacontane	C39H78F2	6.02457	1906.53	121.449	350.11	535
979	1,1-difluorooctacosane	C28H56F2	6.15544	1603.66	82.7232	330.857	563.431

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980	1,1-difluorooctadecane	C18H36F2	7.10524	2019.28	172.001	223.53	461.25
981	1,1-difluorooctane	C8H16F2	6.96837	1374.27	194.208	36.0509	307.15
982	1,1-difluorooctatriacontane	C38H76F2	6.07358	1919.87	123.319	350.569	528
983	1,1-difluoropentacosane	C25H50F2	6.79163	2042.2	141.192	313.464	527.737
984	1,1-difluoropentadecane	C15H30F2	7.14335	1918.14	184	188.936	426.65
985	1,1-difluoropentane	C5H10F2	7.11549	1252.09	226.677	-21.9351	225.25
986	1,2-difluoropentane	C5H10F2	6.793	1049.55	193.277	4.15964	240.647
987	1,3-difluoropentane	C5H10F2	6.79073	1063.01	191.875	8.17895	248.026
988	1,4-difluoropentane	C5H10F2	6.7881	1079.16	190.193	13.0022	256.88
989	1,5-difluoropentane	C5H10F2	6.8373	1151.59	185.564	29.278	281.245
990	2,2-difluoropentane	C5H10F2	6.68171	971.977	196.023	-9.26918	226.196
991	2,3-difluoropentane	C5H10F2	6.74477	983.22	197.609	-10.9568	217.847
992	2,4-difluoropentane	C5H10F2	6.74477	983.22	197.609	-10.9568	217.847
993	3,3-difluoropentane	C5H10F2	6.68142	973.534	195.852	-8.7887	227.096
994	1,1-difluoropentatriacontane	C35H70F2	6.21238	1957.36	128.519	350.974	509
995	1,1-difluoropropane	C3H6F2	7.0471	1026.09	238.284	-68.6011	156.85
996	1,2-difluoropropane	C3H6F2	6.72245	851.585	206.672	-44.3212	170.147
997	1,3-difluoropropane	C3H6F2	6.76734	936.002	199.533	-22.6018	207.724
998	2,2-difluoropropane	C3H6F2	6.61827	781.114	209.396	-57.4625	155.809
999	1,1-difluorotetracontane	C40H80F2	5.99205	1899.45	120.514	347.646	540
1000	1,1-difluorotetracosane	C24H48F2	6.9213	2097.01	148.001	305.872	515.66
1001	1,1-difluorotetradecane	C14H28F2	7.13713	1868.53	188	175.729	413.45
1002	1,1-difluorotetratriacontane	C34H68F2	6.26678	1972.9	130.67	349.697	502

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1003	1,1-difluorotriacontane	C30H60F2	6.50907	2043.5	140.217	339.564	473
1004	1,1-difluorotricosane	C23H46F2	7.02396	2129.58	152.001	298.902	505.484
1005	1,1-difluorotridecane	C13H26F2	7.16291	1832.74	192	162.981	399.15
1006	1,1-difluorotritriacontane	C33H66F2	6.32269	1988.99	132.879	347.993	495
1007	1,1-difluoroundecane	C11H22F2	7.15715	1719.09	200	133.34	367.05
1008	diglycolic acid	C4H6O5	8.28041	2600.1	144.686	148	546.85
1009	diheptadecylamine	C34H71N	8.91081	4583.71	273.15	380.931	537
1010	diheptylamine	C14H31N	7.14619	1733.21	134.344	168.909	433.25
1011	diheptyl disulfide	C14H30S2	7.57764	2385.29	187.141	175	492.81
1012	diheptyl ether	C14H30O	7.55861	2207.92	210	153.056	419.68
1013	diheptyl sulfide	C14H30S	7.76195	2485.95	211.297	169.505	489.08
1014	dihexadecylamine	C32H67N	8.91541	4502.71	273.15	377.651	523
1015	dihexyl adipate	C18H34O4	8.01511	2699.82	177.84	-13.8	493.85
1016	dihexylamine	C12H27N	6.77993	1339.93	103.849	141.68	405.05
1017	dihexyl disulfide	C12H26S2	7.56669	2305.32	198.461	153	473.95
1018	dihexyl ether	C12H26O	7.5023	1976.43	201.962	-43	384.85
1019	dihexyl sulfide	C12H26S	7.98677	2223.04	205.383	200	460.53
1020	2,5-dihydrofuran	C4H6O	7.15647	1271.44	231.516	-0.15	268.85
1021	1,3-dihydroxy-2-methylbenzene	C7H8O2	7.39139	1820.36	138.576	181.211	528.547
1022	1,4-dihydroxy-2-methylbenzene	C7H8O2	7.38751	1876.95	133.482	196.472	555.362
1023	1,2-dihydroxy-3-methylbenzene	C7H8O2	7.39531	1766.92	143.388	166.797	503.221
1024	1,2-dihydroxy-4-methylbenzene	C7H8O2	7.39297	1798.36	140.558	175.276	518.118
1025	1,3-dihydroxy-4-methylbenzene	C7H8O2	7.39029	1836.08	137.161	185.45	535.995

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1026	1,3-dihydroxy-5-methylbenzene	C7H8O2	7.38668	1889.53	132.349	199.864	561.32
1027	1,1-diiodo-2,2-dimethylpropane	C5H10I2	6.55572	1359.49	146.68	121.011	485.894
1028	1,3-diiodo-2,2-dimethylpropane	C5H10I2	6.60972	1385.4	147.83	122.092	479.845
1029	1,3-diiodo-2-(iodomethyl)-propane	C4H7I3	6.74014	1639.98	128.189	183.415	583.218
1030	1,3-diiodo-2-ethylpropane	C5H10I2	6.72484	1445.1	149.444	125.933	471.346
1031	1,1-diiodo-2-methylbutane	C5H10I2	6.66938	1418.53	148.374	124.827	476.979
1032	1,2-diiodo-2-methylbutane	C5H10I2	6.60972	1385.4	147.83	122.092	479.845
1033	1,3-diiodo-2-methylbutane	C5H10I2	6.66938	1418.53	148.374	124.827	476.979
1034	1,4-diiodo-2-methylbutane	C5H10I2	6.72484	1445.1	149.444	125.933	471.346
1035	2,3-diiodo-2-methylbutane	C5H10I2	6.55572	1359.49	146.68	121.011	485.894
1036	1,1-diiodo-2-methylpropane	C4H8I2	6.42355	1139.72	118.535	106.433	459.172
1037	1,2-diiodo-2-methylpropane	C4H8I2	6.33496	1081.84	112.38	103.769	462.259
1038	1,3-diiodo-2-methylpropane	C4H8I2	6.49535	1180.86	123.089	107.472	453.257
1039	1,1-diiodo-3-methylbutane	C5H10I2	6.66938	1418.53	148.374	124.827	476.979
1040	1,2-diiodo-3-methylbutane	C5H10I2	6.66938	1418.53	148.374	124.827	476.979
1041	1,3-diiodo-3-methylbutane	C5H10I2	6.60972	1385.4	147.83	122.092	479.845
1042	2,2-diiodo-3-methylbutane	C5H10I2	6.55572	1359.49	146.68	121.011	485.894
1043	1,1-diiodobutane	C4H8I2	6.49535	1180.86	123.089	107.472	453.257
1044	1,2-diiodobutane	C4H8I2	6.48855	1174.76	122.013	110	453.26
1045	1,3-diiodobutane	C4H8I2	6.49535	1180.86	123.089	107.472	453.257
1046	1,4-diiodobutane	C4H8I2	6.57085	1224.98	127.92	108.523	447.564
1047	2,2-diiodobutane	C4H8I2	6.33496	1081.84	112.38	103.769	462.259
1048	2,3-diiodobutane	C4H8I2	6.42355	1139.72	118.535	106.433	459.172

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1049	1,1-diiododecane	C10H20I2	6.96041	1929.29	132.021	219.827	563.049
1050	1,1-diiododocosane	C22H44I2	7.27561	3297.66	134.907	529.927	819.626
1051	1,1-diiodododecane	C12H24I2	7.04828	2131.33	124.77	297.419	601.214
1052	1,1-diiododotriacontane	C32H64I2	4.75234	1600	10.6667	740.301	894.25
1053	1,1-diiodoeicosane	C20H40I2	7.1311	2814.5	92.5013	456.017	771.05
1054	1,1-diiodoethane	C2H4I2	6.29573	965.122	103.62	87.9698	450.74
1055	1,2-diiodoethane	C2H4I2	6.50432	1174.16	124.031	98	476.76
1056	1,1-diiodoheneicosane	C21H42I2	7.09145	2865.46	87.9592	510.206	794.957
1057	1,1-diiodohentriacontane	C31H62I2	4.74446	1550	10.3333	723.727	871.37
1058	1,1-diiodoheptacosane	C27H54I2	7.46767	4746.74	305.006	622.872	956.554
1059	1,1-diiodoheptadecane	C17H34I2	7.17259	2602.58	105.36	397.788	703.374
1060	1,1-diiodoheptane	C7H14I2	6.81704	1632.75	142.552	163.212	507.622
1061	1,1-diiodoheptatriacontane	C37H74I2	4.7861	1850	12.3333	813.494	1008.65
1062	1,1-diiodohexacosane	C26H52I2	7.5666	4680.81	291.969	605.183	927.131
1063	1,1-diiodohexadecane	C16H32I2	7.16379	2516.64	109.421	377.942	681.999
1064	1,1-diiodohexane	C6H12I2	6.77004	1537.7	146.005	144.516	489.45
1065	1,1-diiodohexatriacontane	C36H72I2	4.78001	1800	12	800.249	985.77
1066	diiodomethane	CH2I2	6.56525	1211.8	146.897	6.1	473.85
1067	1,1-diiodononacosane	C29H58I2	7.0714	4446.18	285.383	656.59	1019
1068	1,1-diiodononadecane	C19H38I2	7.1573	2752.86	96.909	436.869	747.851
1069	1,1-diiodononane	C9H18I2	6.91314	1828.98	135.569	200.886	544.375
1070	1,1-diiodononatriacontane	C39H78I2	4.79745	1950	13	837.727	1054.41
1071	1,1-diiodooctacosane	C28H56I2	7.29829	4662.26	302.683	640.023	987.149

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1072	1,1-diiodooctadecane	C18H36I2	7.17081	2681.77	101.192	417.445	725.309
1073	1,1-diiodooctane	C8H16I2	6.86503	1729.97	139.076	182.008	525.915
1074	1,1-diiodooctatriacontane	C38H76I2	4.7919	1900	12.6667	825.993	1031.53
1075	1,1-diiodopentacosane	C25H50I2	7.58981	4469.38	265.025	586.999	898.8
1076	1,1-diiodopentadecane	C15H30I2	7.14565	2425.3	113.384	357.946	661.139
1077	1,1-diiodopentane	C5H10I2	6.72484	1445.1	149.444	125.933	471.346
1078	1,2-diiodopentane	C5H10I2	6.72484	1445.1	149.444	125.933	471.346
1079	1,3-diiodopentane	C5H10I2	6.72484	1445.1	149.444	125.933	471.346
1080	1,4-diiodopentane	C5H10I2	6.72484	1445.1	149.444	125.933	471.346
1081	1,5-diiodopentane	C5H10I2	6.78096	1471.93	150.475	127.048	465.924
1082	2,2-diiodopentane	C5H10I2	6.60972	1385.4	147.83	122.092	479.845
1083	2,3-diiodopentane	C5H10I2	6.66938	1418.53	148.374	124.827	476.979
1084	2,4-diiodopentane	C5H10I2	6.66938	1418.53	148.374	124.827	476.979
1085	3,3-diiodopentane	C5H10I2	6.60972	1385.4	147.83	122.092	479.845
1086	1,1-diiodopentatriacontane	C35H70I2	4.77361	1750	11.6667	786.279	962.89
1087	1,1-diiodopropane	C3H6I2	6.3189	983.738	105.399	89.1408	435.123
1088	1,2-diiodopropane	C3H6I2	6.63954	1393.87	143.825	125	507.34
1089	1,3-diiodopropane	C3H6I2	6.68429	1397.89	144.53	123.825	493.819
1090	2,2-diiodopropane	C3H6I2	6.15864	880.116	95.5061	81.6225	436.771
1091	1,1-diiodotetracontane	C40H80I2	4.80274	2000	13.3333	848.686	1077.29
1092	1,1-diiodotetracosane	C24H48I2	7.5409	4140.13	227.214	568.366	871.485
1093	1,1-diiodotetradecane	C14H28I2	7.11947	2329.85	117.258	337.839	640.75
1094	1,1-diiodotetratriacontane	C34H68I2	4.76689	1700	11.3333	771.61	940.01

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1095	1,1-diiodotriacontane	C30H60I2	5.78265	2356.23	13.4874	672.529	848.49
1096	1,1-diiodotricosane	C23H46I2	7.43097	3734.86	182.49	549.328	845.115
1097	1,1-diiodotridecane	C13H26I2	7.08658	2231.5	121.051	317.652	620.789
1098	1,1-diiodotritriacontane	C33H66I2	4.75981	1650	11	756.273	917.13
1099	1,1-diiodoundecane	C11H22I2	7.00583	2030.31	128.424	277.165	581.981
1100	diisobutylamine	C8H19N	7.43551	1714.21	237.261	-70	306.85
1101	diisobutyl ketone	C9H18O	7.34997	1720.84	216.788	-45.98	341.85
1102	diisodecyl phthalate	C28H46O4	7.915	3354.55	216.504	-40.15	613.85
1103	diisooctyl phthalate	C24H38O4	7.99481	3048.3	175.22	-13.15	577.85
1104	diisopropanolamine	C6H15NO2	8.69663	2401.26	164.134	45	398.85
1105	diisopropylamine	C6H15N	6.89567	1118.39	194.663	-96.3	249.95
1106	m-diisopropylbenzene	C12H18	7.01959	1711.81	210.423	-63.13	410.85
1107	p-diisopropylbenzene	C12H18	7.03004	1703.4	200.033	-17.07	415.85
1108	diisopropyl ether	C6H14O	7.20537	1354.97	245.019	-85.5	226.9
1109	diisopropyl sulfide	C6H14S	7.1154	1481.93	229.918	72.52	312.56
1110	diketene	C4H4O2	7.58867	1694.83	233.95	-6.5	342.85
1111	2,4'-dimethylbiphenyl	C14H14	7.21952	1999.88	186.94	219.665	515.05
1112	1,2-dimethoxyethane	C4H10O2	7.30039	1418.59	236.928	-58	263
1113	2,2-dimethyl,3,3-diethylhexane	C12H26	6.76997	1485.02	181.835	75.5347	382.739
1114	2,3-dimethyl-(1-thiaethyl)-benzene	C9H12S	7.1609	1846.63	193.858	163.954	470.686
1115	2,4-dimethyl-(1-thiaethyl)-benzene	C9H12S	7.1609	1846.63	193.858	163.954	470.686
1116	2,5-dimethyl-(1-thiaethyl)-benzene	C9H12S	7.1609	1846.63	193.858	163.954	470.686
1117	2,6-dimethyl-(1-thiaethyl)-benzene	C9H12S	7.1609	1846.63	193.858	163.954	470.686

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1118	3,4-dimethyl-(1-thiaethyl)-benzene	C9H12S	7.1609	1846.63	193.858	163.954	470.686
1119	3,5-dimethyl-(1-thiaethyl)-benzene	C9H12S	7.1609	1846.63	193.858	163.954	470.686
1120	dimethyl-1,1-dimethylpropylamine	C7H17N	6.74151	1156.86	181.651	38.1014	301.837
1121	2,3-dimethyl-1,2-butanediol	C6H14O2	9.37242	3115	273	121.538	363.196
1122	3,3-dimethyl-1,2-butanediol	C6H14O2	9.37241	3106.23	273	120.428	361.407
1123	dimethyl-1,2-dimethylpropylamine	C7H17N	6.86105	1197.42	183.491	38.9149	292.152
1124	4,4-dimethyl-1,2-pentanediol	C7H16O2	9.4059	3372.69	273	152.373	404.124
1125	2,3-dimethyl-1,3-butadiene	C6H10	6.91902	1204.77	229.562	-76	252.85
1126	2,2-dimethyl-1,3-butanediol	C6H14O2	9.3724	3086.1	273	117.879	357.297
1127	2,3-dimethyl-1,3-butanediol	C6H14O2	9.37242	3115	273	121.538	363.196
1128	2,2-dimethyl-1,3-pentanediol	C7H16O2	9.4058	3167.88	273	126.547	363.018
1129	2,3-dimethyl-1,3-pentanediol	C7H16O2	9.4059	3372.69	273	152.373	404.124
1130	2,2-dimethyl-1,3-propanediol	C5H12O2	9.44141	3122.83	272.997	130	365.351
1131	2,2-dimethyl-1,4-butanediol	C6H14O2	9.37242	3115	273	121.538	363.196
1132	3,4-dimethyl-1,4-pentanediol	C7H16O2	9.4059	3372.69	273	152.373	404.124
1133	2,2-dimethyl-1,5-pentanediol	C7H16O2	9.48101	3261.16	273	134.447	371.479
1134	3,3-dimethyl-1,5-pentanediol	C7H16O2	9.48101	3261.16	273	134.447	371.479
1135	2,2-dimethyl-1-butanol	C6H14O	7.0876	1303.25	172.996	41.0862	315.85
1136	2,3-dimethyl-1-butanol	C6H14O	7.23206	1412.38	175.592	51.0395	325.85
1137	3,3-dimethyl-1-butanol	C6H14O	7.35268	1458.46	183.141	46.4407	314.45
1138	2,3-dimethyl-1-butene	C6H12	6.996	1225.84	242.271	-157.26	226.85
1139	3,3-dimethyl-1-butene	C6H12	6.91634	1115.98	235.289	-115.2	206.85
1140	3,3-dimethyl-1-butyne	C6H10	6.73565	1009.76	224.226	-42.5991	218.005

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1141	1,cis-2-dimethyl-1-ethylcyclopentane	C9H18	6.88902	1425.48	211.64	51.7571	343.702
1142	1,trans-2-dimethyl-1-ethylcyclopentane	C9H18	6.88902	1425.48	211.64	51.7571	343.702
1143	1,cis-3-dimethyl-1-ethylcyclopentane	C9H18	6.89153	1400.38	213.16	45.4798	331.872
1144	1,trans-3-dimethyl-1-ethylcyclopentane	C9H18	6.89153	1400.38	213.16	45.4798	331.872
1145	2,4-dimethyl-1-ethylnaphthalene	C14H16	8.8486	4489.14	439.968	132	538.289
1146	4,6-dimethyl-1-ethylnaphthalene	C14H16	8.8486	4489.14	439.968	132	538.289
1147	2,2-dimethyl-1-heptanol	C9H20O	8.42447	2577.8	273	98.048	349.846
1148	4,6-dimethyl-1-heptanol	C9H20O	8.50271	2557.12	273	90.9722	333.196
1149	6,6-dimethyl-1-heptanol	C9H20O	8.42444	2521.52	273	89.9483	336.251
1150	2,2-dimethyl-1-hexanol	C8H18O	7.26728	1420.6	151.36	75.3095	332.136
1151	2,3-dimethyl-1-hexanol	C8H18O	8.4508	2488.95	273	61.0511	330.66
1152	2,4-dimethyl-1-hexanol	C8H18O	8.4508	2495.36	273	61.9109	332.214
1153	2,5-dimethyl-1-hexanol	C8H18O	8.45082	2517.64	273	64.9013	337.617
1154	3,3-dimethyl-1-hexanol	C8H18O	8.37088	2491.67	273	65.0419	343.477
1155	3,4-dimethyl-1-hexanol	C8H18O	8.45082	2527.95	273	66.2844	340.116
1156	3,5-dimethyl-1-hexanol	C8H18O	8.45083	2539.93	273	67.8918	343.02
1157	4,4-dimethyl-1-hexanol	C8H18O	8.37088	2497.16	273	65.7867	344.835
1158	4,5-dimethyl-1-hexanol	C8H18O	8.45083	2533.52	273	67.032	341.467
1159	5,5-dimethyl-1-hexanol	C8H18O	8.37088	2497.16	273	65.7867	344.835
1160	2,3-dimethyl-1-hexene	C8H16	6.943	1329.34	216.749	6.93388	286.893
1161	2,4-dimethyl-1-hexene	C8H16	6.94485	1333.31	216.875	7.40456	287.914
1162	2,5-dimethyl-1-hexene	C8H16	6.94625	1335.87	216.991	7.6659	288.498
1163	3,3-dimethyl-1-hexene	C8H16	6.80242	1225.62	208.531	2.69523	282.468

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1164	3,4-dimethyl-1-hexene	C8H16	6.93555	1332.21	216.557	7.88918	289.859
1165	3,5-dimethyl-1-hexene	C8H16	6.90587	1280.38	214.103	2.69523	278.165
1166	4,4-dimethyl-1-hexene	C8H16	6.81199	1243.79	209.191	4.8129	287.182
1167	4,5-dimethyl-1-hexene	C8H16	6.92458	1312.77	215.639	5.94028	285.474
1168	5,5-dimethyl-1-hexene	C8H16	6.79607	1215.67	207.996	1.74465	280.258
1169	2,2-dimethyl-1-octanol	C10H22O	8.47469	2690.66	273	111.513	363.048
1170	2,6-dimethyl-1-octanol	C10H22O	8.55073	2737.72	273	114.033	362.56
1171	3,7-dimethyl-1-octanol	C10H22O	8.55073	2749.91	273	115.756	365.389
1172	4,5-dimethyl-1-octanol	C10H22O	8.55073	2749.06	273	115.636	365.192
1173	4,6-dimethyl-1-octanol	C10H22O	8.55073	2749.06	273	115.636	365.192
1174	4,7-dimethyl-1-octanol	C10H22O	8.55073	2749.06	273	115.636	365.192
1175	7,7-dimethyl-1-octanol	C10H22O	8.4747	2712.2	273	114.59	368.138
1176	2,2-dimethyl-1-pentanol	C7H16O	8.31544	2315.15	273	43.4746	314.498
1177	2,3-dimethyl-1-pentanol	C7H16O	7.48948	1559.91	174.473	65.9021	326.108
1178	2,4-dimethyl-1-pentanol	C7H16O	8.39657	2382.81	273	49.1502	319.253
1179	3,3-dimethyl-1-pentanol	C7H16O	7.32804	1459.8	163.249	67.4381	331.046
1180	3,4-dimethyl-1-pentanol	C7H16O	7.89792	1925.12	218.712	60.3757	327.478
1181	4,4-dimethyl-1-pentanol	C7H16O	8.31547	2353.21	273	48.6752	324.151
1182	2,3-dimethyl-1-pentene	C7H14	6.89157	1219.03	219.659	-12.7489	259.565
1183	2,4-dimethyl-1-pentene	C7H14	6.96754	1269.66	229.068	-16.3076	255.586
1184	3,3-dimethyl-1-pentene	C7H14	6.75306	1120.95	212.002	-17.1587	254.594
1185	3,4-dimethyl-1-pentene	C7H14	6.86554	1190.58	217.986	-15.007	255.162
1186	4,4-dimethyl-1-pentene	C7H14	6.90795	1223.39	231.268	-24.193	247.126

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1187	3,3-dimethyl-1-pentyne	C7H12	6.7559	1113.24	217.282	-17.768	255.759
1188	3,4-dimethyl-1-pentyne	C7H12	6.81421	1163.29	215.748	-9.42012	266.308
1189	4,4-dimethyl-1-pentyne	C7H12	6.76015	1136.26	216.821	-13.3365	265.13
1190	2,2-dimethyl-1-propanethiol	C5H12S	7.03278	1380.49	228.809	0.0218883	296.85
1191	2,2-dimethyl-1-propanol	C5H12O	7.27679	1279.01	177.849	54	276.85
1192	dimethyl-2,2-dimethylpropylamine	C7H17N	6.74175	1155.13	181.833	37.5798	300.882
1193	2,3-dimethyl-2,3-butanediol	C6H14O2	9.20493	2819.3	273	91.8241	323.961
1194	2,3-dimethyl-2,3-diphenylbutane	C18H22	7.1468	2118.37	180.722	119	531.85
1195	2,3-dimethyl-2,3-pentanediol	C7H16O2	9.24416	3345.21	273	157.693	421.971
1196	2,4-dimethyl-2,3-pentanediol	C7H16O2	9.32983	2960.1	273	103.952	331.017
1197	2,4-dimethyl-2,4-pentanediol	C7H16O2	9.24399	2989.74	273	111.935	348.143
1198	2,3-dimethyl-2-butanol	C6H14O	7.02103	1216.83	175.305	26.7919	291.25
1199	3,3-dimethyl-2-butanol	C6H14O	6.9491	1166.75	166.791	29.3307	293.25
1200	3,3-dimethyl-2-butanone	C6H12O	6.91427	1312.9	219.202	2.78616	298.35
1201	2,3-dimethyl-2-butene	C6H12	6.88803	1197.57	225.653	-74.23	250.85
1202	2,3-dimethyl-2-tert-butyl-1-butanol	C10H22O	8.19111	2473.8	273	95.4547	355.623
1203	2,3-dimethyl-2-ethyl-1-butanol	C8H18O	8.29873	2415.58	273	57.9586	336.084
1204	3,3-dimethyl-2-ethyl-1-butanol	C8H18O	8.29873	2415.58	273	57.9586	336.084
1205	3,3-dimethyl-2-ethyl-1-butene	C8H16	6.74521	1220.64	205.869	6.59367	295.069
1206	5,5-dimethyl-2-ethyl-1-hexanol	C10H22O	8.40589	2684.36	273	114.422	372.572
1207	2,4-dimethyl-2-ethyl-1-pentanol	C9H20O	8.35371	2523.01	273	93.8977	347.749
1208	1,1-dimethyl-2-ethylcyclopentane	C9H18	6.89089	1406.66	212.78	47.0491	334.83
1209	1,cis-3-dimethyl-cis-2-ethylcyclopentane	C9H18	6.87726	1447.19	210.12	57.8718	348.596

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1210	1,cis-3-dimethyl-trans-2-ethylcyclopentane	C9H18	6.8819	1400.26	212.97	46.1081	326.66
1211	1,trans-3-dimethyl-cis-2-ethylcyclopentane	C9H18	6.87969	1422.16	211.64	51.5978	336.897
1212	3,4-dimethyl-2-ethylphenol	C10H14O	7.22336	1766.77	165	154.812	459.881
1213	3,5-dimethyl-2-ethylphenol	C10H14O	7.25145	1865.61	165	170.995	488.348
1214	2,3-dimethyl-2-heptanol	C9H20O	8.35369	2489.34	273	89.0029	339.469
1215	2,4-dimethyl-2-heptanol	C9H20O	8.35369	2489.34	273	89.0029	339.469
1216	2,5-dimethyl-2-heptanol	C9H20O	8.35369	2489.34	273	89.0029	339.469
1217	2,6-dimethyl-2-heptanol	C9H20O	8.35366	2429.95	273	80.3672	324.86
1218	4,6-dimethyl-2-heptanol	C9H20O	8.43202	2592.41	273	99.7463	352.569
1219	5,6-dimethyl-2-heptanol	C9H20O	8.43201	2581.31	273	98.1499	349.89
1220	2,3-dimethyl-2-hexanol	C8H18O	7.39364	1508.47	174.163	61.77	318.667
1221	2,4-dimethyl-2-hexanol	C8H18O	7.59421	1642.33	197.739	51.3176	305.827
1222	2,5-dimethyl-2-hexanol	C8H18O	7.28676	1396.39	164.432	57.6832	308.286
1223	3,3-dimethyl-2-hexanol	C8H18O	8.29869	2345.13	273	48.3079	318.326
1224	3,4-dimethyl-2-hexanol	C8H18O	8.37846	2440.96	273	57.8216	330.145
1225	3,5-dimethyl-2-hexanol	C8H18O	8.37842	2380.47	273	49.6251	315.204
1226	4,4-dimethyl-2-hexanol	C8H18O	8.29869	2355.97	273	49.7926	321.058
1227	4,5-dimethyl-2-hexanol	C8H18O	8.37843	2390.64	273	51.0036	317.716
1228	5,5-dimethyl-2-hexanol	C8H18O	8.29871	2378.46	273	52.8734	326.727
1229	2,3-dimethyl-2-hexene	C8H16	6.96827	1394.27	219.34	14.2742	304.51
1230	2,4-dimethyl-2-hexene	C8H16	6.91471	1314.01	215.141	7.01775	288.953
1231	2,5-dimethyl-2-hexene	C8H16	6.88619	1295.82	211.321	8.82538	291.297
1232	3,4-dimethyl-cis-2-hexene	C8H16	6.93583	1350.33	217.002	10.4858	296.863

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1233	3,4-dimethyl-trans-2-hexene	C8H16	6.93583	1350.33	217.002	10.4858	296.863
1234	3,5-dimethyl-cis-2-hexene	C8H16	6.92147	1324.44	215.778	7.88918	291.004
1235	3,5-dimethyl-trans-2-hexene	C8H16	6.92147	1324.44	215.778	7.88918	291.004
1236	4,4-dimethyl-cis-2-hexene	C8H16	6.78348	1224.11	207.66	3.99635	287.386
1237	4,4-dimethyl-trans-2-hexene	C8H16	6.78348	1224.11	207.66	3.99635	287.386
1238	4,5-dimethyl-cis-2-hexene	C8H16	6.9005	1304.02	214.407	6.59367	288.86
1239	4,5-dimethyl-trans-2-hexene	C8H16	6.9005	1304.02	214.407	6.59367	288.86
1240	5,5-dimethyl-cis-2-hexene	C8H16	6.78586	1228.95	207.807	4.59788	288.717
1241	5,5-dimethyl-trans-2-hexene	C8H16	6.77618	1212.11	207.067	2.77923	284.577
1242	1,3-dimethyl-2-isopropylbenzene	C11H16	7.06822	1675.76	201.19	110.913	401.634
1243	1,4-dimethyl-2-isopropylbenzene	C11H16	7.06895	1666.55	201.722	108.624	397.632
1244	dimethyl-2-methylbutylamine	C7H17N	6.862	1190.49	184.179	36.9013	288.533
1245	2,4-dimethyl-2-octanol	C10H22O	8.40589	2678.83	273	113.625	371.244
1246	2,7-dimethyl-2-octanol	C10H22O	8.40589	2678.83	273	113.625	371.244
1247	3,7-dimethyl-2-octanol	C10H22O	8.4822	2715.83	273	114.695	368.18
1248	2,3-dimethyl-2-pentanol	C7H16O	7.43628	1485.28	187.043	43.7235	298.72
1249	2,4-dimethyl-2-pentanol	C7H16O	7.50626	1520.15	195.65	37.9947	290.394
1250	3,3-dimethyl-2-pentanol	C7H16O	8.36084	2372.16	285.873	36.3938	309.82
1251	3,4-dimethyl-2-pentanol	C7H16O	8.32314	2318.43	273	43.5896	314.547
1252	4,4-dimethyl-2-pentanol	C7H16O	7.43087	1477.3	186.677	43.043	297.332
253	3,3-dimethyl-2-pentanone	C7H14O	7.58364	1898.06	273	37.8253	315.922
1254	3,4-dimethyl-2-pentanone	C7H14O	7.65753	1934.57	273	40.0165	313.541
1255	4,4-dimethyl-2-pentanone	C7H14O	7.58363	1871.72	273	33.5123	307.752

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256	2,3-dimethyl-2-pentene	C7H14	6.92461	1294.65	222.757	-4.23648	280.32
1257	2,4-dimethyl-2-pentene	C7H14	6.85493	1194.33	217.228	-13.2405	260.055
1258	3,4-dimethyl-cis-2-pentene	C7H14	6.88277	1236.38	219.695	-9.52445	268.956
1259	3,4-dimethyl-trans-2-pentene	C7H14	6.89068	1250.42	220.335	-8.06459	272.321
1260	4,4-dimethyl-cis-2-pentene	C7H14	6.87142	1224.24	226.35	-17.842	261.816
1261	4,4-dimethyl-trans-2-pentene	C7H14	6.78414	1149.06	217.64	-18.9829	255.476
1262	dimethyl-2-pentylamine	C7H17N	6.86429	1174.28	185.788	32.1894	280.064
1263	4,4-dimethyl-2-pentyne	C7H12	6.69985	1126.39	211.941	3.52	279.664
1264	1,4-dimethyl-2-phenyl benzene	C14H14	7.0217	1885.22	188.27	211.085	522.85
1265	1,3-dimethyl-2-propylbenzene	C11H16	7.12179	1726.74	199.556	118.865	409.105
1266	1,4-dimethyl-2-propylbenzene	C11H16	7.12264	1715.75	200.183	116.161	404.422
1267	3,3-dimethyl-2-thiabutane	C5H12S	6.48522	1045.71	191.221	61.949	311.85
1268	3,3-dimethyl-2-thiapentane	C6H14S	6.8912	1345.4	207.478	76.5	329.362
1269	3,4-dimethyl-2-thiapentane	C6H14S	6.95135	1365.93	207.565	76.5	324.386
1270	4,4-dimethyl-2-thiapentane	C6H14S	6.8912	1345.4	207.478	76.5	329.362
1271	2,4-dimethyl-3,3-diethylhexane	C12H26	6.82492	1506	181.835	76.7089	378.766
1272	2,5-dimethyl-3,3-diethylhexane	C12H26	6.81105	1461.4	181.835	69.6513	364.988
1273	2,2-dimethyl-3,3-diethylpentane	C11H24	6.75303	1458.67	187.7	65.847	378.359
1274	2,4-dimethyl-3,3-diethylpentane	C11H24	6.8088	1479.67	187.7	67.0294	374.099
1275	2,2-dimethyl-3,4-diethylhexane	C12H26	6.81105	1461.4	181.835	69.6513	364.988
1276	2,3-dimethyl-3,4-diethylhexane	C12H26	6.83031	1523.85	181.835	79.5325	384.278
1277	2,4-dimethyl-3,4-diethylhexane	C12H26	6.82492	1506	181.835	76.7089	378.766
1278	2,5-dimethyl-3,4-diethylhexane	C12H26	6.86607	1481.86	181.835	70.7801	361.236

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1279	3,4-dimethyl-3,4-diethylhexane	C12H26	6.78299	1529.01	181.835	82.5626	396.601
1280	2,2-dimethyl-3-tert-butylhexane	C12H26	6.71504	1448.7	181.835	71.6548	381.334
1281	2,2-dimethyl-3-ethyl-1-pentanol	C9H20O	8.35371	2522.19	273	93.7783	347.547
1282	2,3-dimethyl-3-ethyl-2-pentanol	C9H20O	8.20499	2453.65	273	91.6989	354.394
1283	4,4-dimethyl-3-ethyl-2-pentanol	C9H20O	8.28294	2489.57	273	92.8001	350.931
1284	5,5-dimethyl-3-ethyl-3-hexanol	C10H22O	8.26031	2473.76	273	91.69	344.226
1285	2,4-dimethyl-3-ethyl-3-isopropylpentane	C12H26	6.7828	1513.33	181.835	79.8595	391.113
1286	2,2-dimethyl-3-ethyl-3-pentanol	C9H20O	8.20495	2379.89	273	80.738	335.541
1287	2,4-dimethyl-3-ethyl-3-pentanol	C9H20O	8.28291	2435.81	273	84.9019	337.461
1288	1,1-dimethyl-3-ethylcyclopentane	C9H18	6.89217	1394.11	213.54	43.9104	328.915
1289	1,cis-2-dimethyl-cis-3-ethylcyclopentane	C9H18	6.87726	1447.19	210.12	57.8718	348.596
1290	1,cis-2-dimethyl-trans-3-ethylcyclopentane	C9H18	6.87938	1425.29	211.45	52.3821	338.359
1291	1,trans-2-dimethyl-cis-3-ethylcyclopentane	C9H18	6.88158	1403.39	212.78	46.8924	328.122
1292	1,trans-2-dimethyl-trans-3-ethylcyclopentane	C9H18	6.87938	1425.29	211.45	52.3821	338.359
1293	2,2-dimethyl-3-ethylheptane	C11H24	6.84227	1440.78	187.7	58.9133	351.842
1294	2,3-dimethyl-3-ethylheptane	C11H24	6.84781	1458.67	187.7	61.7377	357.408
1295	2,4-dimethyl-3-ethylheptane	C11H24	6.90276	1474.85	187.7	62.1573	352.136
1296	2,5-dimethyl-3-ethylheptane	C11H24	6.89851	1461.24	187.7	60.0297	347.987
1297	2,6-dimethyl-3-ethylheptane	C11H24	6.89851	1461.24	187.7	60.0297	347.987
1298	3,4-dimethyl-3-ethylheptane	C11H24	6.8546	1481.03	187.7	65.2685	364.365
1299	3,5-dimethyl-3-ethylheptane	C11H24	6.84781	1458.67	187.7	61.7377	357.408
1300	4,4-dimethyl-3-ethylheptane	C11H24	6.84227	1440.78	187.7	58.9133	351.842
1301	2,5-dimethyl-3-ethylnaphthalene	C14H16	8.8486	4489.14	439.968	132	538.289

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1302	2,2-dimethyl-3-ethyloctane	C12H26	6.86956	1507.09	181.835	74.9284	369.403
1303	2,3-dimethyl-3-ethyloctane	C12H26	6.87791	1534.23	181.835	79.1803	377.62
1304	2,4-dimethyl-3-ethyloctane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
1305	2,5-dimethyl-3-ethyloctane	C12H26	6.92211	1518.86	181.835	74.6378	363.015
1306	2,6-dimethyl-3-ethyloctane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
1307	2,7-dimethyl-3-ethyloctane	C12H26	6.925	1528.04	181.835	76.0611	365.738
1308	3,4-dimethyl-3-ethyloctane	C12H26	6.87515	1525.18	181.835	77.763	374.881
1309	3,5-dimethyl-3-ethyloctane	C12H26	6.86956	1507.09	181.835	74.9284	369.403
1310	3,6-dimethyl-3-ethyloctane	C12H26	6.87376	1520.66	181.835	77.0543	373.511
1311	4,4-dimethyl-3-ethyloctane	C12H26	6.87237	1516.13	181.835	76.3456	372.142
1312	4,5-dimethyl-3-ethyloctane	C12H26	6.92928	1541.8	181.835	78.1962	369.824
1313	2,2-dimethyl-3-ethylpentane	C9H20	7.09332	1541.78	232.161	-99.47	316.85
1314	2,3-dimethyl-3-ethylpentane	C9H20	7.12831	1592.54	230.225	30	333.65
1315	2,4-dimethyl-3-ethylpentane	C9H20	7.1514	1590.45	235.7	-122.36	317.85
1316	2,4-dimethyl-3-ethylphenol	C10H14O	7.22336	1766.77	165	154.812	459.881
1317	2,5-dimethyl-3-ethylphenol	C10H14O	7.20081	1692.79	165	142.677	438.531
1318	2,6-dimethyl-3-ethylphenol	C10H14O	7.20081	1692.79	165	142.677	438.531
1319	2,2-dimethyl-3-heptanol	C9H20O	8.35368	2467.44	273	85.8192	334.083
1320	2,3-dimethyl-3-heptanol	C9H20O	8.35367	2446.37	273	82.7549	328.899
1321	2,6-dimethyl-3-heptanol	C9H20O	8.43196	2486.92	273	84.5803	327.12
1322	3,5-dimethyl-3-heptanol	C9H20O	8.35368	2461.97	273	85.0233	332.736
1323	3,6-dimethyl-3-heptanol	C9H20O	7.98299	2137.4	245.92	85.0233	332.736
1324	2,2-dimethyl-3-hexanol	C8H18O	8.59057	2630.39	304.583	41.9506	313.203

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1325	2,3-dimethyl-3-hexanol	C8H18O	7.96787	2010.57	237.032	51.5164	316.072
1326	2,4-dimethyl-3-hexanol	C8H18O	8.54694	2555.59	291.03	47.5963	315.204
1327	2,5-dimethyl-3-hexanol	C8H18O	7.72056	1750.91	202.777	57.7533	313.845
1328	3,4-dimethyl-3-hexanol	C8H18O	7.66079	1704.75	204.643	51.2944	307.603
1329	3,5-dimethyl-3-hexanol	C8H18O	8.25371	2257.6	268.183	43.0508	307.603
1330	4,4-dimethyl-3-hexanol	C8H18O	7.85366	1907.2	224.524	53.7516	317.165
1331	4,5-dimethyl-3-hexanol	C8H18O	8.37841	2357.65	273	46.5327	309.567
1332	5,5-dimethyl-3-hexanol	C8H18O	7.80664	1838.07	220.149	49.8914	308.969
1333	2,2-dimethyl-cis-3-hexene	C8H16	6.86383	1287.97	217.935	1.71106	286.543
1334	2,2-dimethyl-trans-3-hexene	C8H16	6.79688	1218.2	210.227	-0.0797104	279.772
1335	2,3-dimethyl-cis-3-hexene	C8H16	6.9288	1337.47	216.404	9.18486	293.933
1336	2,3-dimethyl-trans-3-hexene	C8H16	6.9288	1337.47	216.404	9.18486	293.933
1337	2,4-dimethyl-cis-3-hexene	C8H16	6.90892	1303.75	214.662	5.97794	286.61
1338	2,4-dimethyl-trans-3-hexene	C8H16	6.90532	1296.02	214.431	5.03481	284.559
1339	2,5-dimethyl-cis-3-hexene	C8H16	6.97196	1335.33	224.394	-0.794681	277.125
1340	2,5-dimethyl-trans-3-hexene	C8H16	6.86734	1250.05	211.568	1.48366	277.125
1341	3,4-dimethyl-cis-3-hexene	C8H16	6.97114	1397.57	219.676	14.3774	304.847
1342	3,4-dimethyl-trans-3-hexene	C8H16	6.97114	1397.57	219.676	14.3774	304.847
1343	4,4-dimethyl-3-isopropyl-1-pentanol	C10H22O	8.33673	2487.08	273	89.5687	335.748
1344	3,4-dimethyl-3-isopropyl-2-pentanol	C10H22O	8.26245	2453.22	273	88.5475	337.808
1345	2,4-dimethyl-3-isopropyl-3-pentanol	C10H22O	8.26249	2515.93	273	97.7879	353.417
1346	1,2-dimethyl-3-isopropylbenzene	C11H16	7.06728	1687.59	200.506	113.855	406.779
1347	2,2-dimethyl-3-isopropylheptane	C12H26	6.81105	1461.4	181.835	69.6513	364.988

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1348	2,3-dimethyl-3-isopropylheptane	C12H26	6.82628	1510.46	181.835	77.4148	380.144
1349	2,4-dimethyl-3-isopropylheptane	C12H26	6.86895	1490.91	181.835	72.1977	363.975
1350	2,5-dimethyl-3-isopropylheptane	C12H26	6.86607	1481.86	181.835	70.7801	361.236
1351	2,6-dimethyl-3-isopropylheptane	C12H26	6.86723	1485.48	181.835	71.3471	362.332
1352	2,2-dimethyl-3-isopropylhexane	C11H24	6.78598	1404.69	187.7	55.0745	350.29
1353	2,3-dimethyl-3-isopropylhexane	C11H24	6.79693	1439.96	187.7	60.6998	361.494
1354	2,4-dimethyl-3-isopropylhexane	C11H24	6.84598	1438.17	187.7	58.3093	350.505
1355	2,5-dimethyl-3-isopropylhexane	C11H24	6.83888	1415.8	187.7	54.7779	343.547
1356	2,4-dimethyl-3-isopropylpentane	C10H22	7.03264	1563.62	219.559	40	341.25
1357	dimethyl-3-methylbutylamine	C7H17N	6.86253	1186.75	184.55	35.8139	286.579
1358	2,2-dimethyl-3-octanol	C10H22O	8.40584	2579.36	273	99.2706	347.328
1359	2,3-dimethyl-3-octanol	C10H22O	8.40583	2553.11	273	95.4827	341.017
1360	2,7-dimethyl-3-octanol	C10H22O	8.48215	2615.82	273	100.421	344.576
1361	3,5-dimethyl-3-octanol	C10H22O	8.40584	2573.83	273	98.4731	346
1362	3,6-dimethyl-3-octanol	C10H22O	8.40583	2569.14	273	97.7953	344.87
1363	3,7-dimethyl-3-octanol	C10H22O	8.40585	2591.24	273	100.985	350.185
1364	2,2-dimethyl-3-pentanol	C7H16O	7.60402	1612.63	205.427	38.7624	294.557
1365	2,3-dimethyl-3-pentanol	C7H16O	7.56959	1599.26	201.083	42.3509	300.107
1366	2,4-dimethyl-3-pentanol	C7H16O	7.71085	1680.4	209.106	41.2942	294.964
1367	2,2-dimethyl-3-pentanone	C7H14O	7.58363	1871.72	273	33.5123	307.752
1368	2,4-dimethyl-3-pentanone	C7H14O	7.22513	1509.18	222.992	-68.34	302.85
1369	dimethyl-3-pentylamine	C7H17N	6.86156	1193.68	183.863	37.8276	290.198
1370	2,4-dimethyl-3-propyl-3-pentanol	C10H22O	8.33674	2493.36	273	90.4834	337.284

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1371	1,2-dimethyl-3-propylbenzene	C11H16	7.12099	1737.06	198.967	121.404	413.505
1372	2,2-dimethyl-3-thiapentane	C6H14S	6.91504	1340.42	211.851	72.705	317.962
1373	2,2-dimethyl-4,4-diethylhexane	C12H26	6.76997	1485.02	181.835	75.5347	382.739
1374	2,3-dimethyl-4,4-diethylhexane	C12H26	6.83031	1523.85	181.835	79.5325	384.278
1375	3,3-dimethyl-4,4-diethylhexane	C12H26	6.78299	1529.01	181.835	82.5626	396.601
1376	2,2-dimethyl-4-ethyl-3-hexanol	C10H22O	8.33675	2509.73	273	92.8696	341.29
1377	2,4-dimethyl-4-ethyl-3-hexanol	C10H22O	8.33675	2508.91	273	92.7503	341.089
1378	1,cis-2-dimethyl-cis-4-ethylcyclopentane	C9H18	6.87877	1431.55	211.07	53.9505	341.284
1379	1,cis-2-dimethyl-trans-4-ethylcyclopentane	C9H18	6.87877	1431.55	211.07	53.9505	341.284
1380	1,trans-2-dimethyl-cis-4-ethylcyclopentane	C9H18	6.88095	1409.65	212.4	48.4609	331.047
1381	1,cis-3-dimethyl-cis-4-ethylcyclopentane	C9H18	6.87938	1425.29	211.45	52.3821	338.359
1382	1,cis-3-dimethyl-trans-4-ethylcyclopentane	C9H18	6.8819	1400.26	212.97	46.1081	326.66
1383	1,trans-3-dimethyl-cis-4-ethylcyclopentane	C9H18	6.86659	1569.24	202.71	88.4578	405.63
1384	1,trans-3-dimethyl-trans-4-ethylcyclopentane	C9H18	6.87938	1425.29	211.45	52.3821	338.359
1385	2,2-dimethyl-4-ethylheptane	C11H24	6.83089	1405.04	187.7	53.2653	340.71
1386	2,3-dimethyl-4-ethylheptane	C11H24	6.90276	1474.85	187.7	62.1573	352.136
1387	2,4-dimethyl-4-ethylheptane	C11H24	6.83378	1413.98	187.7	54.6772	343.493
1388	2,5-dimethyl-4-ethylheptane	C11H24	6.89708	1456.7	187.7	59.3205	346.604
1389	2,6-dimethyl-4-ethylheptane	C11H24	6.88983	1434.03	187.7	55.7748	339.69
1390	3,3-dimethyl-4-ethylheptane	C11H24	6.84781	1458.67	187.7	61.7377	357.408
1391	3,4-dimethyl-4-ethylheptane	C11H24	6.84918	1463.14	187.7	62.4438	358.799
1392	3,5-dimethyl-4-ethylheptane	C11H24	6.90557	1483.93	187.7	63.5758	354.902
1393	1,2-dimethyl-4-ethylnaphthalene	C14H16	8.8486	4489.14	439.968	132	538.289

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1394	2,2-dimethyl-4-ethyloctane	C12H26	6.85664	1466.42	181.835	68.5515	357.076
1395	2,3-dimethyl-4-ethyloctane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
1396	2,4-dimethyl-4-ethyloctane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
1397	2,5-dimethyl-4-ethyloctane	C12H26	6.9192	1509.69	181.835	73.2146	360.291
1398	2,6-dimethyl-4-ethyloctane	C12H26	6.91626	1500.52	181.835	71.7914	357.568
1399	2,7-dimethyl-4-ethyloctane	C12H26	6.91626	1500.52	181.835	71.7914	357.568
1400	3,3-dimethyl-4-ethyloctane	C12H26	6.87237	1516.13	181.835	76.3456	372.142
1401	3,4-dimethyl-4-ethyloctane	C12H26	6.87653	1529.7	181.835	78.4716	376.251
1402	3,5-dimethyl-4-ethyloctane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
1403	3,6-dimethyl-4-ethyloctane	C12H26	6.925	1528.04	181.835	76.0611	365.738
1404	4,5-dimethyl-4-ethyloctane	C12H26	6.87515	1525.18	181.835	77.763	374.881
1405	2,3-dimethyl-4-ethylphenol	C10H14O	7.21599	1742.09	165	150.767	452.764
1406	2,5-dimethyl-4-ethylphenol	C10H14O	7.20081	1692.79	165	142.677	438.531
1407	2,6-dimethyl-4-ethylphenol	C10H14O	7.20259	1698.46	165	143.607	440.168
1408	3,5-dimethyl-4-ethylphenol	C10H14O	7.24758	1851.51	165	168.689	484.292
1409	2,2-dimethyl-4-heptanol	C9H20O	8.35367	2446.37	273	82.7549	328.899
1410	2,4-dimethyl-4-heptanol	C9H20O	8.35366	2432.14	273	80.6856	325.399
1411	2,6-dimethyl-4-heptanol	C9H20O	7.80665	1884.08	204.641	-65.15	329.85
1412	3,3-dimethyl-4-heptanol	C9H20O	8.35368	2457.32	273	84.3468	331.592
1413	3,5-dimethyl-4-heptanol	C9H20O	8.432	2553.55	273	94.1588	343.193
1414	1,2-dimethyl-4-isopropylbenzene	C11H16	7.06749	1684.96	200.658	113.202	405.636
1415	1,3-dimethyl-4-isopropylbenzene	C11H16	7.06819	1676.09	201.171	110.994	401.777
1416	2,2-dimethyl-4-isopropylheptane	C12H26	6.79952	1425.76	181.835	64.0063	353.966

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1417	2,3-dimethyl-4-isopropylheptane	C12H26	6.86895	1490.91	181.835	72.1977	363.975
1418	2,4-dimethyl-4-isopropylheptane	C12H26	6.81387	1470.32	181.835	71.0627	367.744
1419	2,5-dimethyl-4-isopropylheptane	C12H26	6.86462	1477.34	181.835	70.0713	359.866
1420	2,6-dimethyl-4-isopropylheptane	C12H26	6.85579	1450.21	181.835	65.8191	351.648
1421	3,3-dimethyl-4-isopropylheptane	C12H26	6.81667	1479.23	181.835	72.4741	370.499
1422	3,4-dimethyl-4-isopropylheptane	C12H26	6.82628	1510.46	181.835	77.4148	380.144
1423	3,5-dimethyl-4-isopropylheptane	C12H26	6.87181	1499.96	181.835	73.6153	366.715
1424	2,2-dimethyl-4-octanol	C10H22O	8.40583	2558.08	273	96.2004	342.213
1425	2,4-dimethyl-4-octanol	C10H22O	8.40583	2562.78	273	96.8782	343.342
1426	2,5-dimethyl-4-octanol	C10H22O	8.48214	2598.18	273	97.9018	340.411
1427	2,6-dimethyl-4-octanol	C10H22O	8.99464	3090.83	310.548	97.9018	340.411
1428	2,7-dimethyl-4-octanol	C10H22O	10.1122	4298.84	392.471	97.9018	340.411
1429	3,4-dimethyl-4-octanol	C10H22O	8.40583	2562.78	273	96.8782	343.342
1430	3,6-dimethyl-4-octanol	C10H22O	8.48214	2598.18	273	97.9018	340.411
1431	4,6-dimethyl-4-octanol	C10H22O	8.40583	2562.78	273	96.8782	343.342
1432	4,7-dimethyl-4-octanol	C10H22O	8.40583	2569.14	273	97.7953	344.87
1433	1,3-dimethyl-4-phenyl benzene	C14H14	7.19095	1972.75	187.7	215.732	510.05
1434	1,2-dimethyl-4-propylbenzene	C11H16	7.12145	1731.07	199.309	119.93	410.95
1435	1,3-dimethyl-4-propylbenzene	C11H16	7.12204	1723.41	199.746	118.045	407.686
1436	2,2-dimethyl-4-propylheptane	C12H26	6.85222	1452.88	181.835	66.4262	352.967
1437	2,3-dimethyl-4-propylheptane	C12H26	6.92211	1518.86	181.835	74.6378	363.015
1438	2,4-dimethyl-4-propylheptane	C12H26	6.85955	1475.46	181.835	69.9684	359.815
1439	2,5-dimethyl-4-propylheptane	C12H26	6.91626	1500.52	181.835	71.7914	357.568

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1440	2,6-dimethyl-4-propylheptane	C12H26	6.9082	1475.78	181.835	67.9492	350.214
1441	3,3-dimethyl-4-propylheptane	C12H26	6.86956	1507.09	181.835	74.9284	369.403
1442	3,4-dimethyl-4-propylheptane	C12H26	6.87237	1516.13	181.835	76.3456	372.142
1443	3,5-dimethyl-4-propylheptane	C12H26	6.925	1528.04	181.835	76.0611	365.738
1444	2,2-dimethyl-5-ethylheptane	C11H24	6.83663	1422.91	187.7	56.0892	346.276
1445	2,3-dimethyl-5-ethylheptane	C11H24	6.90135	1470.31	187.7	61.4481	350.753
1446	2,4-dimethyl-5-ethylheptane	C11H24	6.89851	1461.24	187.7	60.0297	347.987
1447	2,5-dimethyl-5-ethylheptane	C11H24	6.84505	1449.72	187.7	60.3255	354.625
1448	3,3-dimethyl-5-ethylheptane	C11H24	6.84087	1436.31	187.7	58.2073	350.45
1449	3,4-dimethyl-5-ethylheptane	C11H24	6.90696	1488.47	187.7	64.2851	356.285
1450	1,3-dimethyl-5-ethylnaphthalene	C14H16	8.8486	4489.14	439.968	132	538.289
1451	1,4-dimethyl-5-ethylnaphthalene	C14H16	7.83447	2902.8	273.73	151	538.289
1452	2,2-dimethyl-5-ethyloctane	C12H26	6.85955	1475.46	181.835	69.9684	359.815
1453	2,3-dimethyl-5-ethyloctane	C12H26	6.92211	1518.86	181.835	74.6378	363.015
1454	2,4-dimethyl-5-ethyloctane	C12H26	6.92066	1514.28	181.835	73.9262	361.653
1455	2,5-dimethyl-5-ethyloctane	C12H26	6.86531	1493.53	181.835	72.8026	365.294
1456	2,6-dimethyl-5-ethyloctane	C12H26	6.92356	1523.45	181.835	75.3495	364.377
1457	3,3-dimethyl-5-ethyloctane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
1458	3,4-dimethyl-5-ethyloctane	C12H26	6.92786	1537.21	181.835	77.4845	368.462
1459	3,5-dimethyl-5-ethyloctane	C12H26	6.861	1479.97	181.835	70.677	361.185
1460	4,4-dimethyl-5-ethyloctane	C12H26	6.86956	1507.09	181.835	74.9284	369.403
1461	2,3-dimethyl-5-ethylphenol	C10H14O	7.21599	1742.09	165	150.767	452.764
1462	2,4-dimethyl-5-ethylphenol	C10H14O	7.22358	1767.51	165	154.933	460.095

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1463	3,4-dimethyl-5-ethylphenol	C10H14O	7.22358	1767.51	165	154.933	460.095
1464	1,3-dimethyl-5-isopropylbenzene	C11H16	7.0694	1660.97	202.045	107.234	395.203
1465	1,3-dimethyl-5-phenyl benzene	C14H14	7.2545	2019.55	186.75	220.954	511.85
1466	1,3-dimethyl-5-propylbenzene	C11H16	7.12318	1708.89	200.575	114.474	401.499
1467	1,3-dimethyl-6-ethylnaphthalene	C14H16	7.92871	3036.01	289.177	149	538.289
1468	1,4-dimethyl-6-ethylnaphthalene	C14H16	8.33317	3640.75	355.478	141	538.289
1469	2,2-dimethyl-6-ethyloctane	C12H26	6.86531	1493.53	181.835	72.8026	365.294
1470	2,3-dimethyl-6-ethyloctane	C12H26	6.92928	1541.8	181.835	78.1962	369.824
1471	2,4-dimethyl-6-ethyloctane	C12H26	6.9192	1509.69	181.835	73.2146	360.291
1472	2,5-dimethyl-6-ethyloctane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
1473	2,6-dimethyl-6-ethyloctane	C12H26	6.87237	1516.13	181.835	76.3456	372.142
1474	3,3-dimethyl-6-ethyloctane	C12H26	6.86956	1507.09	181.835	74.9284	369.403
1475	3,4-dimethyl-6-ethyloctane	C12H26	6.92786	1537.21	181.835	77.4845	368.462
1476	3,5-dimethyl-6-ethyloctane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
1477	4,4-dimethyl-6-ethyloctane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
1478	2,3-dimethyl-6-ethylphenol	C10H14O	7.21599	1742.09	165	150.767	452.764
1479	2,4-dimethyl-6-ethylphenol	C10H14O	7.20104	1693.53	165	142.798	438.744
1480	2,5-dimethyl-6-ethylphenol	C10H14O	7.20081	1692.79	165	142.677	438.531
1481	3,4-dimethyl-6-ethylphenol	C10H14O	7.22336	1766.77	165	154.812	459.881
1482	1,2-dimethyl-7-ethylnaphthalene	C14H16	8.72789	4282.65	420.181	134	538.289
1483	dimethyl-sec-butylamine	C6H15N	6.81847	1109.86	187.859	19.9283	269.165
1484	dimethyl-tert-butylamine	C6H15N	6.7012	1059.35	187.29	15.4932	272.16
1485	1,4a-dimethyl-cis-decahydronaphthalene	C12H22	6.89242	1673.64	197.2	144.889	433.94

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1486	1,4a-dimethyl-trans-decahydronaphthalene	C12H22	6.89404	1651.57	198.53	138.934	423.90
1487	dimethyl-propylamine	C5H13N	6.46436	919.461	190.579	-6.21585	254.85
1488	dimethylacetylene	C4H6	6.86957	1009.54	226.118	-32.24	215
1489	dimethylaluminum chloride	C2H6AlCl	6.8335	1342.79	213.714	-21	345.85
1490	dimethylamine	C2H7N	7.16171	1005.33	227.96	-92.19	164.5
1491	p-dimethylaminobenzaldehyde	C9H11NO	7.76756	2740.88	246.031	74.85	558.85
1492	2,2'-dimethylbiphenyl	C14H14	7.26677	1964.82	189.98	205.695	488.45
1493	3,3'-dimethylbiphenyl	C14H14	7.32993	2094.02	184.66	231.737	522.95
1494	3,4'-dimethylbiphenyl	C14H14	7.13718	1992.96	185.23	226.866	535.15
1495	4,4'-dimethylbiphenyl	C14H14	7.19175	2053.43	183.33	236.532	544.55
1496	2,3-dimethylbiphenyl	C14H14	7.15097	1982.12	186.18	222.51	528.85
1497	3,4-dimethylbiphenyl	C14H14	7.22477	2030.46	185.42	226.96	528.05
1498	2,6-dimethylbiphenyl	C14H14	7.25343	1976.56	189.03	210.08	494.95
1499	2,2-dimethylbutanal	C6H12O	7.04624	1299.61	208	25.3605	285.67
1500	2,3-dimethylbutanal	C6H12O	7.12068	1361	208	33.1593	294.48
1501	3,3-dimethylbutanal	C6H12O	7.04624	1299.61	208	25.3605	285.67
1502	2,2-dimethylbutane	C6H14	6.93954	1169.51	238.418	-98.87	215.63
1503	2,3-dimethylbutane	C6H14	6.98947	1220.01	238.956	-127.96	226.83
1504	2,2-dimethylbutanenitrile	C6H11N	6.8205	1213.9	179.122	48.0572	315.15
1505	2,3-dimethylbutanenitrile	C6H11N	6.88393	1233.93	180.242	47.9755	309.25
1506	3,3-dimethylbutanenitrile	C6H11N	6.81808	1233.06	177.176	53.6921	325.39
1507	dimethylbutylamine	C6H15N	6.56108	1027.26	185.126	16.9328	283.55
1508	1,1-dimethylcyclobutane	C6H12	6.91449	1147.02	228.36	5.03476	240.88

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1509	1,cis-2-dimethylcyclobutane	C6H12	6.89337	1180.01	226.08	15.0651	252.67
1510	1,trans-2-dimethylcyclobutane	C6H12	6.89694	1155.04	227.6	8.26931	240.34
1511	1,cis-3-dimethylcyclobutane	C6H12	6.89671	1156.6	227.505	8.69405	241.11
1512	1,trans-3-dimethylcyclobutane	C6H12	6.89809	1147.24	228.075	6.14563	236.49
1513	1,1-dimethylcyclohexane	C8H16	6.86464	1363.21	222.636	-33.49	318
1514	cis-1,2-dimethylcyclohexane	C8H16	6.86433	1395.63	220.561	-49.99	333
1515	trans-1,2-dimethylcyclohexane	C8H16	6.92012	1420.58	228.259	-88.16	323
1516	cis-1,3-dimethylcyclohexane	C8H16	6.89241	1384.05	224.923	-75.57	318
1517	trans-1,3-dimethylcyclohexane	C8H16	6.89366	1402.52	225.047	-90.1	324.85
1518	cis-1,4-dimethylcyclohexane	C8H16	6.89096	1402.12	225.323	-87.43	325
1519	trans-1,4-dimethylcyclohexane	C8H16	6.87792	1369.34	223.224	-36.94	317
1520	1,2-dimethylcyclohexene	C8H14	6.87201	1399.97	212.784	46.7157	347.93
1521	1,3-dimethylcyclohexene	C8H14	6.87544	1365.97	214.851	38.1846	331.49
1522	1,4-dimethylcyclohexene	C8H14	6.86933	1368.78	214.68	38.8902	332.85
1523	1,5-dimethylcyclohexene	C8H14	6.87515	1368.78	214.68	38.8902	332.85
1524	1,6-dimethylcyclohexene	C8H14	6.87416	1378.47	214.091	41.3207	337.53
1525	3,3-dimethylcyclohexene	C8H14	6.89122	1345.05	216.39	32.0447	326.62
1526	3,cis-4-dimethylcyclohexene	C8H14	6.8769	1352.06	215.697	34.6956	324.77
1527	3,trans-4-dimethylcyclohexene	C8H14	6.8769	1352.06	215.697	34.6956	324.77
1528	3,cis-5-dimethylcyclohexene	C8H14	6.85517	1352.06	215.697	34.6956	324.77
1529	3,trans-5-dimethylcyclohexene	C8H14	6.8769	1352.06	215.697	34.6956	324.77
1530	3,cis-6-dimethylcyclohexene	C8H14	6.84934	1352.06	215.697	34.6956	324.77
1531	3,trans-6-dimethylcyclohexene	C8H14	6.8769	1352.06	215.697	34.6956	324.77

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1532	4,4-dimethylcyclohexene	C8H14	6.89181	1339.53	216.724	30.6645	323.93
1533	4,cis-5-dimethylcyclohexene	C8H14	6.87521	1368.19	214.716	38.7412	332.56
1534	4,trans-5-dimethylcyclohexene	C8H14	6.8769	1352.06	215.697	34.6956	324.76
1535	1,1-dimethylcyclopentane	C7H14	7.04515	1331.61	231.916	-69.79	273.85
1536	cis-1,2-dimethylcyclopentane	C7H14	7.03128	1366.11	229.616	-53.89	292
1537	trans-1,2-dimethylcyclopentane	C7H14	7.07143	1368.89	234.786	-117.57	280
1538	cis-1,3-dimethylcyclopentane	C7H14	7.14306	1421.81	242.813	-133.7	277.85
1539	trans-1,3-dimethylcyclopentane	C7H14	7.07206	1369.35	234.986	-133.97	279.85
1540	1,2-dimethylcyclopentene	C7H12	6.88821	1301.19	218.898	21.5699	306.29
1541	1,3-dimethylcyclopentene	C7H12	6.89333	1258	221.52	10.7464	285.19
1542	1,4-dimethylcyclopentene	C7H12	6.89286	1261.76	221.292	11.6876	287.02
1543	1,5-dimethylcyclopentene	C7H12	6.88958	1289.3	219.62	18.5895	300.48
1544	3,3-dimethylcyclopentene	C7H12	6.90975	1250.1	222.28	7.82922	286.20
1545	3,cis-4-dimethylcyclopentene	C7H12	6.89356	1256.13	221.634	10.2759	284.27
1546	3,cis-5-dimethylcyclopentene	C7H12	6.89356	1256.13	221.634	10.2759	284.27
1547	3,trans-5-dimethylcyclopentene	C7H12	6.89356	1256.13	221.634	10.2759	284.27
1548	4,4-dimethylcyclopentene	C7H12	6.90975	1250.1	222.28	7.82922	286.20
1549	1,1-dimethylcyclopropane	C5H10	6.94274	1038.68	235.08	-24.9385	191.82
1550	1,cis-2-dimethylcyclopropane	C5H10	6.92537	1087.96	231.964	-11.0748	212.54
1551	1,trans-2-dimethylcyclopropane	C5H10	6.93009	1060.31	233.64	-18.5723	198.73
1552	3,trans-4-dimethylcyclopentene	C7H12	6.89356	1256.13	221.634	10.2759	284.27
1553	2,2-dimethyldecane	C12H26	6.92696	1549.01	181.835	79.5141	372.49
1554	2,3-dimethyldecane	C12H26	6.98981	1593.62	181.835	84.219	375.69

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1555	2,4-dimethyldecane	C12H26	6.98128	1565.7	181.835	79.9319	367.57
1556	2,5-dimethyldecane	C12H26	6.97839	1556.4	181.835	78.503	364.86
1557	2,6-dimethyldecane	C12H26	6.97839	1556.4	181.835	78.503	364.865
1558	2,7-dimethyldecane	C12H26	6.98415	1575	181.835	81.3609	370.282
1559	2,8-dimethyldecane	C12H26	6.98699	1584.31	181.835	82.7899	372.99
1560	2,9-dimethyldecane	C12H26	6.98699	1584.31	181.835	82.7899	372.99
1561	3,3-dimethyldecane	C12H26	6.92976	1558.18	181.835	80.9371	375.22
1562	3,4-dimethyldecane	C12H26	6.98841	1588.96	181.835	83.5044	374.344
1563	3,5-dimethyldecane	C12H26	6.98128	1565.7	181.835	79.9319	367.573
1564	3,6-dimethyldecane	C12H26	6.98272	1570.35	181.835	80.6464	368.928
1565	3,7-dimethyldecane	C12H26	6.98415	1575	181.835	81.3609	370.282
1566	3,8-dimethyldecane	C12H26	6.98841	1588.96	181.835	83.5044	374.344
1567	4,4-dimethyldecane	C12H26	6.92413	1539.84	181.835	78.0911	369.773
1568	4,5-dimethyldecane	C12H26	6.98415	1575	181.835	81.3609	370.282
1569	4,6-dimethyldecane	C12H26	6.97839	1556.4	181.835	78.503	364.865
1570	4,7-dimethyldecane	C12H26	6.97984	1561.05	181.835	79.2174	366.219
1571	5,5-dimethyldecane	C12H26	6.92129	1530.67	181.835	76.6683	367.05
1572	5,6-dimethyldecane	C12H26	6.98272	1570.35	181.835	80.6464	368.928
1573	dimethyldecylamine	C12H27N	6.91902	1605.51	162.58	132.685	412.15
1574	2',3'-dimethyldiphenylmethane	C15H16	7.23532	2088.29	182.57	240.65	519.73
1575	2',4'-dimethyldiphenylmethane	C15H16	7.23552	2084.86	182.76	239.747	518.339
1576	2',5'-dimethyldiphenylmethane	C15H16	7.23571	2081.43	182.95	238.845	516.949
1577	2',6'-dimethyldiphenylmethane	C15H16	7.23532	2088.29	182.57	240.65	519.73

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1578	3',4'-dimethyldiphenylmethane	C15H16	7.23513	2091.73	182.38	241.553	521.121
1579	3',5'-dimethyldiphenylmethane	C15H16	7.23591	2077.99	183.14	237.942	515.558
1580	2',2"-dimethyldiphenylmethane	C15H16	7.23532	2088.29	182.57	240.65	519.73
1581	2',3"-dimethyldiphenylmethane	C15H16	7.23571	2081.43	182.95	238.845	516.949
1582	2',4"-dimethyldiphenylmethane	C15H16	7.23513	2091.73	182.38	241.553	521.121
1583	3',3"-dimethyldiphenylmethane	C15H16	7.23591	2077.99	183.14	237.942	515.558
1584	3',4"-dimethyldiphenylmethane	C15H16	7.23532	2088.29	182.57	240.65	519.73
1585	4',4"-dimethyldiphenylmethane	C15H16	7.23475	2098.6	182	243.358	523.902
1586	dimethyl disulfide	C2H6S2	7.25695	1502.73	233.641	-84.71	332.85
1587	dimethyldocosylamine	C24H51N	6.81139	1978.56	103.376	305.826	551.678
1588	2,2-dimethyldodecane	C14H30	6.95703	1661.96	167.72	111.27	406.829
1589	2,3-dimethyldodecane	C14H30	7.01979	1716.52	167.72	117.426	412.888
1590	2,4-dimethyldodecane	C14H30	7.00053	1654.97	167.72	116.424	395.742
1591	dimethyldodecylamine	C14H31N	6.93878	1699.65	147.842	162.477	441.35
1592	dimethyldotriacontylamine	C34H71N	8.93207	4587.76	273.15	381.991	535
1593	dimethyleicosylamine	C22H47N	6.7246	1737.14	72.9335	290.376	529.314
1594	dimethylethanolamine	C4H11NO	7.83644	1693.76	207.786	-59	298.67
1595	dimethyl ether	C2H6O	7.19658	984.579	252.976	-141.5	126.95
1596	dimethylethylamine	C4H11N	6.35036	808.052	195.899	-30.0844	226.85
1597	2,3-dimethylfuran	C6H8O	7.05959	1272.44	210	17.9345	286.264
1598	2,4-dimethylfuran	C6H8O	7.06031	1274.75	210	18.3187	287.024
1599	2,5-dimethylfuran	C6H8O	7.05741	1265.51	210	16.7819	283.981
1600	3,4-dimethylfuran	C6H8O	7.03543	1198.69	210	5.65725	261.949

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1601	dimethylheneicosylamine	C23H49N	6.57059	1640.53	54.6148	298.691	540.776
1602	dimethylhentriacontylamine	C33H69N	9.09343	4660.39	273.15	379.395	527
1603	dimethylheptacosylamine	C29H61N	6.06296	1450	9.66667	332.352	496
1604	2,2-dimethylheptadecane	C19H40	6.96397	1864.37	137.6	175.005	473.719
1605	2,3-dimethylheptadecane	C19H40	7.01361	1920.1	137.6	181.692	481.736
1606	2,4-dimethylheptadecane	C19H40	6.98404	1828.4	137.6	177.211	457.837
1607	dimethylheptadecylamine	C19H41N	6.92968	1866.1	116.896	222.304	497.45
1608	2,2-dimethylheptane	C9H20	7.09917	1506.94	224.544	-113	303.65
1609	2,3-dimethylheptane	C9H20	7.05755	1497.89	218.116	29	316.45
1610	2,4-dimethylheptane	C9H20	7.01462	1433.82	213.953	24	303.65
1611	2,5-dimethylheptane	C9H20	7.03511	1458.75	215.134	26.85	307.95
1612	2,6-dimethylheptane	C9H20	7.09083	1512.02	223.937	-102.9	305.85
1613	3,4-dimethylheptane	C9H20	7.06512	1505.63	219.218	29	318.75
1614	3,5-dimethylheptane	C9H20	7.03209	1459.3	215.521	26	310.05
1615	4,4-dimethylheptane	C9H20	7.0273	1471.25	219.607	24	312.25
1616	dimethylheptatriacontylamine	C39H81N	9.11753	4934.18	273.15	382.367	568
1617	dimethylheptylamine	C9H21N	6.75468	1328.99	171.066	80.7535	357.55
1618	dimethylhexacosylamine	C28H59N	6.01047	1400	9.33333	328.916	488
1619	2,2-dimethylhexadecane	C18H38	6.97664	1836.16	143.3	163.923	461.816
1620	2,3-dimethylhexadecane	C18H38	7.03013	1893.34	143.3	170.679	469.673
1621	2,4-dimethylhexadecane	C18H38	7.00229	1806.44	143.3	166.757	446.862
1622	dimethylhexadecylamine	C18H39N	6.83575	1740.69	110.132	210.563	487.75
1623	2,2-dimethylhexane	C8H18	7.05852	1411.47	231.017	-121.18	276.65

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1624	2,3-dimethylhexane	C8H18	7.04189	1411.43	223.588	-1.11	290.25
1625	2,4-dimethylhexane	C8H18	7.01809	1378.84	223.843	-1.11	280.35
1626	2,5-dimethylhexane	C8H18	7.05401	1400.91	226.581	-91.15	276.85
1627	3,3-dimethylhexane	C8H18	7.06105	1441.06	232.763	-126.1	288.85
1628	3,4-dimethylhexane	C8H18	7.03917	1420.61	223.898	-1.11	295.65
1629	dimethylhexatriacontylamine	C38H79N	8.9511	4760.01	273.15	382.824	561
1630	dimethylhexylamine	C8H19N	6.63591	1202.55	175.246	57.8621	335.55
1631	dimethylisobutylamine	C6H15N	6.82409	1074.57	191.507	9.46106	249.963
1632	dimethylisopropylamine	C5H13N	6.78089	1012.6	193.635	-2.71486	238.763
1633	dimethyl maleate	C6H8O4	7.53524	1922.72	208.096	-19	401.85
1634	1,2-dimethylnaphthalene	C12H12	7.15048	1913.6	181.875	129	502.19
1635	1,3-dimethylnaphthalene	C12H12	7.47479	2292.97	233.915	148	500.61
1636	1,4-dimethylnaphthalene	C12H12	7.56895	2419.97	248.881	148	503.63
1637	1,5-dimethylnaphthalene	C12H12	7.22357	1992.38	193.773	150	500.32
1638	1,6-dimethylnaphthalene	C12H12	7.38014	2168.76	219.008	148	497.45
1639	1,7-dimethylnaphthalene	C12H12	6.97776	1712.3	154.935	150	497.45
1640	1,8-dimethylnaphthalene	C12H12	7.09895	1930.64	187.7	214.691	518.85
1641	2,3-dimethylnaphthalene	C12H12	7.22831	2008.97	194.088	155	504.63
1642	2,6-dimethylnaphthalene	C12H12	7.26313	2046.22	204.926	110.17	503.85
1643	2,7-dimethylnaphthalene	C12H12	7.27802	2063.76	206.334	95.66	504.85
1644	dimethylnonacosylamine	C31H65N	8.91651	4437.14	273.15	373.796	512
1645	dimethylnonadecylamine	C21H45N	6.71797	1671.91	67.7167	281.774	518.49
1646	2,2-dimethylnonane	C11H24	6.89899	1477.48	187.7	62.7637	353.466

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1647	2,3-dimethylnonane	C11H24	6.96413	1525.94	187.7	68.1521	357.962
1648	2,4-dimethylnonane	C11H24	6.95279	1489.12	187.7	62.4553	346.966
1649	2,5-dimethylnonane	C11H24	6.95423	1493.72	187.7	63.1673	348.341
1650	2,6-dimethylnonane	C11H24	6.95423	1493.72	187.7	63.1673	348.341
1651	2,7-dimethylnonane	C11H24	6.95567	1498.32	187.7	63.8794	349.715
1652	2,8-dimethylnonane	C11H24	6.95993	1512.13	187.7	66.0157	353.839
1653	3,3-dimethylnonane	C11H24	6.90178	1486.55	187.7	64.1817	356.232
1654	3,4-dimethylnonane	C11H24	6.96274	1521.33	187.7	67.44	356.588
1655	3,5-dimethylnonane	C11H24	6.95567	1498.32	187.7	63.8794	349.715
1656	3,6-dimethylnonane	C11H24	6.95851	1507.53	187.7	65.3036	352.464
1657	3,7-dimethylnonane	C11H24	6.96134	1516.73	187.7	66.7278	355.213
1658	4,4-dimethylnonane	C11H24	6.89618	1468.42	187.7	61.3458	350.7
1659	4,5-dimethylnonane	C11H24	6.95851	1507.53	187.7	65.3036	352.464
1660	4,6-dimethylnonane	C11H24	6.95423	1493.72	187.7	63.1673	348.341
1661	5,5-dimethylnonane	C11H24	6.89476	1463.89	187.7	60.6368	349.318
1662	dimethylnonylamine	C11H25N	6.79505	1462.35	158.599	115.694	395.55
1663	dimethyloctacosylamine	C30H63N	8.47227	4065.83	273.15	335.324	504
1664	2,2-dimethyloctadecane	C20H42	6.94364	1889.62	132.1	185.823	486.115
1665	2,3-dimethyloctadecane	C20H42	6.98896	1943.57	132.1	192.424	494.305
1666	2,4-dimethyloctadecane	C20H42	6.95782	1847.29	132.1	187.407	469.312
1667	dimethyloctadecylamine	C20H43N	6.89407	1867.43	109.314	231.756	506.55
1668	2,2-dimethyloctane	C10H22	7.12586	1602.06	220.495	-48.15	328.85
1669	2,3-dimethyloctane	C10H22	7.06006	1565.51	210.271	48	340.05

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1670	2,4-dimethyloctane	C10H22	7.02287	1501.25	206.532	43	326.25
1671	2,5-dimethyloctane	C10H22	7.05764	1538.09	209.733	44	329.85
1672	2,6-dimethyloctane	C10H22	7.16267	1617.87	217.454	45	329.75
1673	2,7-dimethyloctane	C10H22	7.02337	1511.62	205.021	46	329.75
1674	3,3-dimethyloctane	C10H22	7.03178	1546.95	211.461	45	338.95
1675	3,4-dimethyloctane	C10H22	7.06886	1571.95	211.933	47	340.85
1676	3,5-dimethyloctane	C10H22	7.06509	1552.38	211.593	44	333.15
1677	3,6-dimethyloctane	C10H22	7.04102	1535.7	208.331	46	335.15
1678	4,4-dimethyloctane	C10H22	7.02474	1530.76	211.888	42	333.75
1679	4,5-dimethyloctane	C10H22	7.07898	1576.63	213.413	46	339.05
1680	dimethyloctatriacontylamine	C40H83N	8.94928	4837.48	273.15	380.663	574
1681	dimethyloctylamine	C10H23N	6.73915	1382.38	167.285	95.4244	377.45
1682	dimethylpentacosylamine	C27H57N	5.96301	1350	9	324.186	479
1683	2,2-dimethylpentadecane	C17H36	6.98123	1800.9	149.2	151.892	449.104
1684	2,3-dimethylpentadecane	C17H36	7.0381	1859.14	149.2	158.701	456.817
1685	2,4-dimethylpentadecane	C17H36	7.01201	1777.24	149.2	155.337	435.089
1686	dimethylpentadecylamine	C17H37N	6.90419	1772.89	123.647	200.203	477.35
1687	2,2-dimethylpentane	C7H16	7.03664	1321.9	38.893	-123.81	247.35
1688	2,3-dimethylpentane	C7H16	7.05945	1360.19	235.73	-113.15	264.2
1689	2,4-dimethylpentane	C7H16	7.02311	1303.23	234.125	-119.24	246.64
1690	3,3-dimethylpentane	C7H16	7.04247	1359.48	240.607	-134.45	263.25
1691	dimethylpentatriacontylamine	C37H77N	8.94756	4720.84	273.15	383.691	555
1692	dimethylpentylamine	C7H17N	6.62816	1131.33	179.901	39.7301	311.05

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1693	dimethyl phthalate	C10H10O4	7.70841	2379.23	209.14	-1	492.85
1694	2,2-dimethylpropanal	C5H10O	7.02634	1198.06	215	0.896527	252.59
1695	2,2-dimethylpropanenitrile	C5H9N	6.77837	1126.39	183.4	29.0771	292.632
1696	2,2-dimethylpropanoic acid	C5H10O2	7.06183	1327.97	153.82	71.8071	359.005
1697	1,2-dimethylpropyl acetate	C7H14O2	6.90195	1246.39	181.459	48.2972	302.85
1698	1,1-dimethylpropylamine	C5H13N	6.89943	1081.94	192.232	7.30299	246.15
1699	1,2-dimethylpropylamine	C5H13N	6.91414	1107.93	190.693	13.0817	254.25
1700	2,2-dimethylpropylamine	C5H13N	6.89078	1081.29	192.65	7.08331	243.95
1701	1,1-dimethylpropyl butanoate	C9H18O2	7.7438	1767.64	176.329	105.741	329.85
1702	1,2-dimethylpropyl butanoate	C9H18O2	7.674	1748.98	175.379	106.857	334.85
1703	2,2-dimethylpropyl butanoate	C9H18O2	7.57011	1700.94	175.569	103.595	333.85
1704	1,1-dimethylpropyl formate	C6H12O2	6.78399	1151.82	182.599	34.445	296.85
1705	1,2-dimethylpropyl formate	C6H12O2	6.89113	1211.91	182.029	41.8188	299.85
1706	2,2-dimethylpropyl formate	C6H12O2	6.75419	1159.95	181.649	38.1618	301.85
1707	1,1-dimethylpropyl propanoate	C8H16O2	7.48169	1579.34	178.989	84.0338	315.85
1708	1,2-dimethylpropyl propanoate	C8H16O2	7.45104	1576.08	178.229	85.5985	319.85
1709	2,2-dimethylpropyl propanoate	C8H16O2	7.32142	1520.95	178.229	82.0158	319.85
1710	2,3-dimethylpyridine	C7H9N	7.23968	1651.58	217.702	54.6767	382.25
1711	2,4-dimethylpyridine	C7H9N	7.21927	1628.65	216.999	52.5051	373.85
1712	2,5-dimethylpyridine	C7H9N	7.3137	1689.62	224.157	51.1351	371.05
1713	2,6-dimethylpyridine	C7H9N	7.16488	1526.96	212.378	-6.15	350.6
1714	3,4-dimethylpyridine	C7H9N	7.21549	1705.32	214.313	68.0542	410.65
1715	3,5-dimethylpyridine	C7H9N	7.22532	1685.34	216.024	62.5816	394.05

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1716	2,3-dimethylquinoline	C11H11N	6.927	1602.97	133.168	162.574	501.297
1717	2,4-dimethylquinoline	C11H11N	7.43865	2150.78	204.676	138.76	503.251
1718	2,6-dimethylquinoline	C11H11N	7.4351	2139.44	204.355	137.465	500.665
1719	2,7-dimethylquinoline	C11H11N	6.95173	1618.3	133.027	162.574	501.297
1720	2,8-dimethylquinoline	C11H11N	7.04778	1658.79	148.081	149.692	478.523
1721	3,4-dimethylquinoline	C11H11N	9.01091	3750.62	320.836	157.697	492.676
1722	3,6-dimethylquinoline	C11H11N	7.04343	1717.58	142.621	165.947	507.26
1723	3,7-dimethylquinoline	C11H11N	7.04323	1720.52	142.348	166.76	508.697
1724	3,8-dimethylquinoline	C11H11N	7.04535	1691.13	145.078	158.632	494.328
1725	4,5-dimethylquinoline	C11H11N	7.04452	1702.44	144.027	161.761	499.86
1726	4,6-dimethylquinoline	C11H11N	7.04302	1723.46	142.075	167.572	510.133
1727	4,8-dimethylquinoline	C11H11N	7.04284	1725.96	141.843	168.263	511.355
1728	5,6-dimethylquinoline	C11H11N	7.04284	1725.96	141.843	168.263	511.355
1729	5,7-dimethylquinoline	C11H11N	7.0426	1729.34	141.529	169.198	513.007
1730	6,7-dimethylquinoline	C11H11N	7.04263	1728.9	141.57	169.076	512.792
1731	dimethyl silane	C2H8Si	6.73312	853.361	241.12	-150.22	128.85
1732	2,3-dimethylstyrene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1733	3,4-dimethylstyrene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1734	2,6-dimethylstyrene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1735	2,4-dimethylstyrene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1736	3,5-dimethylstyrene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1737	2,5-dimethylstyrene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1738	dimethyl sulfate	C2H6O4S	6.79362	1496.99	193.786	-31.8	484.85

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1739	dimethyl sulfide	C2H6S	7.1438	1193.73	242.693	-98.27	229.89
1740	dimethyl sulfite	C2H6O3S	---	---	---	---	---
1741	dimethyl sulfoxide	C2H6OS	7.25197	1733.52	207.58	18.52	452.85
1742	dimethyl terephthalate	C10H10O4	8.04387	2819.15	258.023	130.65	498.85
1743	dimethyltetracosylamine	C26H55N	5.91347	1300	8.66667	319.03	470
1744	2,2-dimethyltetradecane	C16H34	6.97298	1753.29	154.45	139.087	435.526
1745	2,3-dimethyltetradecane	C16H34	7.03275	1812.11	154.45	145.929	443.11
1746	2,4-dimethyltetradecane	C16H34	7.00828	1735.39	154.45	143.106	422.467
1747	dimethyltetradecylamine	C16H35N	6.87237	1705.74	125.338	187.874	466.25
1748	2,2-dimethyltetrahydrofuran	C6H12O	6.9172	1219.8	210	14.2239	290.262
1749	2,3-dimethyltetrahydrofuran	C6H12O	6.90599	1235.13	210	17.5106	290.251
1750	2,4-dimethyltetrahydrofuran	C6H12O	6.90702	1238.46	210	18.0817	291.393
1751	2,5-dimethyltetrahydrofuran	C6H12O	7.10868	1387.32	235.638	-1.78851	283.627
1752	3,3-dimethyltetrahydrofuran	C6H12O	6.92651	1250.12	210	19.4055	00.748
1753	3,4-dimethyltetrahydrofuran	C6H12O	6.9215	1286.96	210	26.383	307.99
1754	dimethyltetratriacontylamine	C36H75N	8.51303	4343.29	273.15	383.278	548
1755	2,2-dimethylthiacyclohexane	C7H14S	6.91349	1466.94	209.735	88.82	383.869
1756	2,cis-3-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1757	2,trans-3-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1758	2,cis-4-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1759	2,trans-4-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1760	2,cis-5-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1761	2,trans-5-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206

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1762	2,cis-6-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1763	2,trans-6-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1764	3,3-dimethylthiacyclohexane	C7H14S	6.91349	1466.94	209.735	88.82	383.869
1765	3,cis-4-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1766	3,trans-4-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1767	3,cis-5-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1768	3,trans-5-dimethylthiacyclohexane	C7H14S	6.90019	1446.12	210.667	84.4478	368.206
1769	4,4-dimethylthiacyclohexane	C7H14S	6.91349	1466.94	209.735	88.82	383.869
1770	2,2-dimethylthiacyclopentane	C6H12S	6.93062	1384.11	214.893	65.8251	350.032
1771	2,cis-3-dimethylthiacyclopentane	C6H12S	6.91551	1362.9	215.826	61.4401	334.407
1772	2,trans-3-dimethylthiacyclopentane	C6H12S	6.91551	1362.9	215.826	61.4401	334.407
1773	2,cis-4-dimethylthiacyclopentane	C6H12S	6.91551	1362.9	215.826	61.4401	334.407
1774	2,trans-4-dimethylthiacyclopentane	C6H12S	6.91551	1362.9	215.826	61.4401	334.407
1775	2,cis-5-dimethylthiacyclopentane	C6H12S	6.89354	1413.37	209.691	30.1252	366.021
1776	2,trans-5-dimethylthiacyclopentane	C6H12S	6.92344	1439.4	214.056	28.9448	365.206
1777	3,3-dimethylthiacyclopentane	C6H12S	6.93062	1384.11	214.893	65.8251	350.032
1778	3,cis-4-dimethylthiacyclopentane	C6H12S	6.91551	1362.9	215.826	61.4401	334.407
1779	3,trans-4-dimethylthiacyclopentane	C6H12S	6.91551	1362.9	215.826	61.4401	334.407
1780	2,2-dimethylthiacyclopropane	C4H8S	6.96935	1261.97	222.66	31.2902	301.686
1781	2,cis-3-dimethylthiacyclopropane	C4H8S	6.95531	1197.14	226.143	15.4443	264.741
1782	2,trans-3-dimethylthiacyclopropane	C4H8S	6.95531	1197.14	226.143	15.4443	264.741
1783	2,3-dimethylthiophene	C6H8S	7.05405	1476.06	212.096	79.9582	362.15
1784	2,4-dimethylthiophene	C6H8S	7.05341	1472.79	212.267	79.1775	360.85

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1785	2,5-dimethylthiophene	C6H8S	7.05552	1460.01	213.027	75.7677	354.65
1786	3,4-dimethylthiophene	C6H8S	7.05425	1487.62	211.45	82.8807	367.25
1787	2,3-dimethylthiophenol	C8H10S	7.15604	1770.81	197.903	145.541	457.83
1788	2,4-dimethylthiophenol	C8H10S	7.15803	1742.88	199.48	138.416	445.434
1789	2,5-dimethylthiophenol	C8H10S	7.15877	1732.79	200.05	135.841	440.954
1790	2,6-dimethylthiophenol	C8H10S	7.15604	1770.81	197.903	145.541	457.83
1791	3,4-dimethylthiophenol	C8H10S	7.15604	1770.81	197.903	145.541	457.83
1792	3,5-dimethylthiophenol	C8H10S	7.15604	1770.81	197.903	145.541	457.83
1793	dimethyltriacontylamine	C32H67N	8.91994	4487.97	273.15	377.242	520
1794	dimethyltricosylamine	C25H53N	6.21713	1413.12	13.5588	312.616	563.275
1795	2,2-dimethyltridecane	C15H32	6.96928	1710.53	161.38	125.176	421.016
1796	2,3-dimethyltridecane	C15H32	7.0315	1769.77	161.38	132.041	428.491
1797	2,4-dimethyltridecane	C15H32	7.01049	1703	161.38	130.51	410.237
1798	dimethyltridecylamine	C15H33N	6.95521	1753.18	143.292	175.637	454.25
1799	dimethyltrtriacontylamine	C35H73N	8.93561	4632.83	273.15	383.281	542
1800	2,2-dimethylundecane	C13H28	6.93972	1604.16	174.22	95.8533	390.25
1801	2,3-dimethylundecane	C13H28	7.00409	1658.46	174.22	102.002	396.223
1802	2,4-dimethylundecane	C13H28	6.98655	1602.14	174.22	101.515	380.195
1803	dimethylundecylamine	C13H29N	6.87187	1600.97	148.14	147.422	427.35
1804	2,6-dimethyl-2-octanol	C10H22O	8.40589	2678.83	273	113.625	371.244
1805	m-dinitrobenzene	C6H4N2O4	7.67726	2265.85	172.552	90.85	531.85
1806	p-dinitrobenzene	C6H4N2O4	7.626	2196.41	164.021	173.45	529.85
1807	2,4-dinitrotoluene	C7H6N2O4	8.78892	3801.17	326.531	69.85	540.85

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1808	2,5-dinitrotoluene	C7H6N2O4	7.75934	2401.34	175.376	52.5	540.85
1809	2,6-dinitrotoluene	C7H6N2O4	7.8446	2316.41	181.812	65.85	496.85
1810	3,4-dinitrotoluene	C7H6N2O4	7.76013	2488.08	173.075	58.85	568.85
1811	3,5-dinitrotoluene	C7H6N2O4	8.23258	3032.95	251.868	92.5	540.85
1812	dinonadecylamine	C38H79N	8.94347	4772.22	273.15	381.457	564
1813	dinonylamine	C18H39N	7.79218	2571.72	189.626	221.665	488.35
1814	dinonyl disulfide	C18H38S2	7.45129	2406.77	157.581	215	529.15
1815	dinonyl ether	C18H38O	7.78823	2439.4	179.235	-0.15	462.85
1816	dinonylphenol	C24H42O	7.94799	3040.36	151.16	76.85	612.85
1817	dinonyl sulfide	C18H38S	7.13143	2069.41	135	301.85	401.85
1818	dioctadecylamine	C36H75N	8.93168	4684.28	273.15	382.481	551
1819	dioctylamine	C16H35N	7.64892	2327.91	186.226	194.36	459.25
1820	dioctyl disulfide	C16H34S2	7.57974	2466.8	178.96	196	511.31
1821	dioctyl ether	C16H34O	7.71618	2276.42	184.286	-7.6	433.85
1822	dioctyl phthalate	C24H38O4	7.77433	2614.83	150.346	24.85	532.85
1823	dioctyl sulfide	C16H34S	7.22342	2014.32	140	273.85	373.85
1824	1,4-dioxane	C4H8O2	7.29909	1485.85	234.976	11.8	313.85
1825	dipentadecylamine	C30H63N	8.90295	4397.06	273.15	335.677	507
1826	dipentylamine	C10H23N	7.14957	1585.69	168.463	111.079	371.25
1827	dipentyl disulfide	C10H22S2	7.51339	2180.25	206.724	128	453.79
1828	dipentyl sulfate	C10H22O4S	---	---	---	---	---
1829	dipentyl sulfide	C10H22S	7.16824	1809.06	195.094	176.85	276.85
1830	dipentyl sulfite	C10H22O3S	---	---	---	---	---

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1831	1,1-diphenyl-1-butene	C16H16	7.20804	2067.15	183.007	238.257	517.703
1832	1,1-diphenyl-1-decene	C22H28	7.41598	2487.18	166.421	319.836	570.631
1833	1,1-diphenyl-1-dodecene	C24H32	7.44141	2582.4	162.241	340.134	583.78
1834	1,1-diphenyl-1-heptene	C19H22	7.32733	2287.29	174.401	280.664	543.895
1835	1,1-diphenyl-1-hexadecene	C28H40	7.36385	2669.2	155.401	371.816	608.207
1836	1,1-diphenyl-1-hexene	C18H20	7.28999	2203.08	177.859	263.733	530.452
1837	1,1-diphenyl-1-nonene	C21H26	7.39183	2426.44	168.891	307.74	562.445
1838	1,1-diphenyl-1-octene	C20H24	7.36167	2363.02	171.361	295.582	554.866
1839	1,1-diphenyl-1-pentadecene	C27H38	7.40205	2662.65	156.921	365.063	602.285
1840	1,1-diphenyl-1-pentene	C17H18	7.24948	2136.7	180.336	251.455	524.484
1841	1,1-diphenyl-1-propene	C15H14	7.1649	2026.76	184.09	232.607	523.34
1842	1,1-diphenyl-1-tetradecene	C26H36	7.42714	2644.29	158.631	357.215	595.836
1843	1,1-diphenyl-1-tridecene	C25H34	7.43985	2618.44	160.341	349.2	590.09
1844	1,1-diphenyl-1-undecene	C23H30	7.43307	2537.11	164.331	330.037	576.876
1845	diphenylacetylene	C14H10	7.13222	2112.56	197.057	62.5	558.85
1846	diphenylamine	C12H11N	7.52551	2362.64	206.676	53.004	543.85
1847	1,1-diphenylbutane	C16H18	7.0577	1960.11	184.985	227.091	505.15
1848	1,1-diphenyldecane	C22H30	7.35095	2375.48	170.411	299.988	548.85
1849	1,1-diphenyldodecane	C24H34	7.56469	2583.91	165.661	325.235	559.65
1850	1,1-diphenylethane	C14H14	7.26963	2097.99	205.4	-17.95	501.85
1851	1,2-diphenylethane	C14H14	7.29419	2111.24	197.874	51.19	506.85
1852	1,1-diphenylethene	C14H12	7.13961	1973.74	186.351	221.567	518.491
1853	diphenyl ether	C12H10O	7.50605	2253.82	228.977	26.87	489.85

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1854	1,1-diphenylheptane	C19H24	7.36881	2286.82	175.541	275.706	529.55
1855	1,1-diphenylhexadecane	C28H42	7.734	2803.11	159.581	356.363	576.95
1856	1,1-diphenylhexane	C18H22	7.32681	2218.71	178.005	263.46	521.25
1857	diphenylmethane	C13H12	7.26088	2020.65	197.058	25.24	494.85
1858	diphenylmethane-4,4'-diisocyanate	C15H10N2O2	7.74262	2435.36	165.068	38.05	528.85
1859	1,1-diphenylnonane	C21H28	7.44432	2410.31	171.171	297.461	543.35
1860	1,1-diphenyloctane	C20H26	7.409	2351.31	173.261	287.061	536.85
1861	1,1-diphenylpentadecane	C27H40	7.68144	2745.53	160.911	349.372	573.55
1862	1,1-diphenylpentane	C17H20	7.28572	2151.32	180.501	251.084	513.25
1863	1,1-diphenylpropane	C15H16	7.20387	2024.96	185.189	227.829	501.15
1864	1,2-diphenylpropane	C15H16	7.19816	2023.82	185.105	228.162	508.009
1865	1,3-diphenylpropane	C15H16	7.25174	2102.19	182.247	242.376	523.903
1866	2,2-diphenylpropane	C15H16	7.08107	1960.53	185.574	224.575	515.119
1867	1,1-diphenyltetradecane	C26H38	7.64124	2691.69	162.431	341.612	569.05
1868	1,3-diphenyltriazene	C12H11N3	7.46274	2336.42	173.072	98.85	571.85
1869	1,1-diphenyltridecane	C25H36	7.60715	2641.79	163.951	333.925	564.85
1870	1,1-diphenylundecane	C23H32	7.52636	2528.9	167.371	316.599	554.75
1871	dipropyl disulfide	C6H14S2	6.86706	1478.81	179.478	73	399.85
1872	dipropylene glycol	C6H14O3	9.91532	3715.61	296.398	-40.15	380.85
1873	dipropyl ether	C6H14O	7.1768	1378.14	231.157	-123.2	257.45
1874	dipropyl sulfate	C6H14O4S	---	---	---	---	---
1875	dipropyl sulfide	C6H14S	7.23226	1610.82	227.33	83.925	336.58
1876	dipropyl sulfite	C6H14O3S	---	---	---	---	---

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1877	dipropyl sulfone	C6H14O2S	7.47607	2113.1	189.993	29.85	489.85
1878	ditetradecylamine	C28H59N	5.99654	1400	9.33333	329.124	490
1879	ditridecylamine	C26H55N	5.89939	1300	8.66667	319.883	472
1880	diundecylamine	C22H47N	6.76733	1784.19	77.0727	293.173	531.094
1881	m-divinylbenzene	C10H10	7.25031	1855.2	225.079	-66.9	418.85
1882	divinyl ether	C4H6O	7.18155	1146.68	238.323	-101.1	189.85
1883	DL-2,3 -dimethyl-1,4-butanediol	C6H14O2	9.53875	3307.6	273	137.289	379.562
1884	DL-2,3-butanediol	C4H10O2	9.26941	2777.13	254.001	81.8305	338.414
1885	DL-2,3-dibromobutane	C4H8Br2	7.0094	1348.9	166.223	77.6015	383.04
1886	DL-2,3-dichlorobutane	C4H8Cl2	6.67862	1126.98	177.244	39.4198	325.032
1887	DL-2,4-dimethyl-1,5-pentanediol	C7H16O2	9.56529	3396.12	273	146.887	386.957
1888	DL-2,4-pentanediol	C5H12O2	9.50761	3141.1	273	118.147	357.296
1889	DL-erythro-2,3-pentanediol	C5H12O2	9.50761	3146.74	273	118.848	358.426
1890	DL-erythro-4-methyl-2,3-pentanediol	C6H14O2	9.46086	3418.8	273	155.22	412.628
1891	DL-threo-2,3-pentanediol	C5H12O2	9.50761	3146.74	273	118.848	358.426
1892	DL-threo-4-methyl-2,3-pentanediol	C6H14O2	9.46086	3418.8	273	155.22	412.628
1893	docosane	C22H46	7.0838	2054	120.1	158.023	418.6
1894	1-docosene	C22H44	6.89383	1920.69	111.616	131.7	517.584
1895	docosylamine	C22H47N	7.01933	2108.85	102.568	313.98	561.822
1896	docosylbenzene	C28H50	6.49315	1771.43	52.3836	184.023	597.777
1897	docosylcyclohexane	C28H56	6.34928	1692.15	46.8678	183.38	601.263
1898	docosylcyclopentane	C27H54	6.68673	2017.04	99.9764	287.201	588.096
1899	1-docosyne	C22H42	8.22013	3616.74	311.379	223.873	519.973

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1900	dodecanal	C12H24O	7.70673	2201.53	206.189	12	411.85
1901	dodecane	C12H26	7.22883	1807.47	199.381	-9.58	385.05
1902	1,2-dodecanediol	C12H26O2	9.592	3899.21	273.001	221.005	450.009
1903	1,3-dodecanediol	C12H26O2	9.59203	3973.04	273.001	216.598	463.697
1904	1,4-dodecanediol	C12H26O2	9.59208	4114.01	273.001	248.215	489.828
1905	1,12-dodecanediol	C12H26O2	9.63162	4050.49	273.001	237.609	472.146
1906	dodecanenitrile	C12H23N	7.25091	1883.87	154.081	172.198	446.943
1907	1-dodecanethiol	C12H26S	7.62037	2309.1	212.597	-8	450.85
1908	2-dodecanethiol	C12H26S	7.08349	1804.21	164.1	157.714	446.85
1909	dodecanoic acid	C12H24O2	7.70218	2158.17	148.926	44	460.85
1910	1-dodecanol	C12H26O	6.88921	1589.5	134.693	23.8	447.85
1911	2-dodecanol	C12H26O	6.83609	1455.54	116	155.608	431.65
1912	2-dodecanone	C12H24O	7.3123	1852.68	171.372	122.131	414.308
1913	1-dodecene	C12H24	7.25069	1817.08	202.471	-35.22	383.85
1914	dodecyl acetate	C14H28O2	6.14197	1091.05	69.5593	150.15	447.15
1915	dodecylamine	C12H27N	7.90516	2434.67	225.374	28.32	422.85
1916	dodecylbenzene	C18H30	7.50144	2304.19	171.065	2.78	501.11
1917	dodecyl butanoate	C16H32O2	5.12874	800	5.33333	249.718	400.55
1918	dodecylcyclohexane	C18H36	7.15507	2073.96	157.512	179	499.68
1919	dodecylcyclopentane	C17H34	7.15194	2004.09	158.308	168	482.02
1920	1-dodecylcyclopentene	C17H32	7.31581	2130.48	182.38	182.511	466.773
1921	dodecyl formate	C13H26O2	7.37325	1961.4	155.391	177.268	440.05
1922	1-dodecyl naphthalene	C22H32	7.50542	2614.89	162.431	340.009	581.5

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1923	2-dodecyl-naphthalene	C22H32	7.50445	2636.82	161.291	345.456	589.084
1924	dodecyl propanoate	C15H30O2	8.00439	2455.63	151.61	224.601	459.95
1925	1-dodecyne	C12H22	7.16571	1769.54	197.96	113	395.01
1926	2-dodecyne	C12H22	7.18385	1848.7	203.627	104.094	413.113
1927	3-dodecyne	C12H22	7.19497	1835.75	206.118	98.8824	404.039
1928	n-dohexacontane	C62H126	7.21101	2620.2	-22.9	371.524	677.47
1929	dotriacontane	C32H66	7.1439	2296.1	71.6	236.973	517.494
1930	1-dotriacontene	C32H64	6.24451	1600	10.6667	205.618	515
1931	dotriacontylamine	C32H67N	8.72949	4539.45	273.15	402.819	553
1932	dotriacontylbenzene	C38H70	6.51602	1900	12.6667	242.522	560
1933	dotriacontylcyclohexane	C38H76	6.48157	1900	12.6667	242.196	565
1934	dotriacontylcyclopentane	C37H74	5.58191	1649.42	103.651	298.179	557
1935	1-dotriacontyne	C32H62	6.02721	1895.03	139.286	343.873	513
1936	eicosanal	C20H40O	7.28186	2184.32	135.318	212.4	511.056
1937	eicosane	C20H42	7.27683	2208.52	158.612	36.44	493.89
1938	1,2-eicosanediol	C20H42O2	8.60182	3964.66	273.001	301.351	576.839
1939	1,3-eicosanediol	C20H42O2	8.60183	4027.6	273.001	292.3	590.328
1940	1,4-eicosanediol	C20H42O2	8.60186	4147.77	273.001	327.873	616.079
1941	1,20-eicosanediol	C20H42O2	8.57105	4051.45	273.001	316.552	600.765
1942	eicosanenitrile	C20H39N	7.2474	2281.12	136.404	298.311	539.985
1943	1-eicosanethiol	C20H42S	7.14758	2154.87	122.026	229	541.42
1944	2-eicosanethiol	C20H42S	7.12936	2111.53	119.001	254.573	529.85
1945	eicosanoic acid	C20H40O2	7.39566	2344.88	122.37	176.85	549.73

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1946	1-eicosanol	C20H42O	7.04203	1914.84	104.163	65.4	518.85
1947	2-eicosanol	C20H42O	6.94626	1772.54	70.0004	254.098	518.05
1948	2-eicosanone	C20H40O	8.17892	3310.53	273.001	220.975	500.574
1949	1-eicosene	C20H40	7.45581	2299.83	160.304	28.61	497.85
1950	eicosyl acetate	C22H44O2	7.64398	2700	190	326.85	426.85
1951	eicosylamine	C20H43N	7.75427	2708.23	172.711	229.663	521.45
1952	eicosylbenzene	C26H46	6.78	1957.42	82.0069	169.589	578.5
1953	eicosyl butanoate	C24H48O2	5.09651	1200	8	339.632	583.59
1954	eicosylcyclohexane	C26H52	6.6272	1864.06	75.5616	168.835	580.226
1955	eicosylcyclopentane	C25H50	6.83951	2042.36	105.916	274.951	566.569
1956	eicosyl formate	C21H42O2	9.14753	4100	190	414.25	514.25
1957	eicosyl propanoate	C23H46O2	8.58931	4000	190	460.53	560.53
1958	1-eicosyne	C20H38	7.86389	2948.04	251.6	219	496.64
1959	2-eicosyne	C20H38	7.96194	3159.45	269.801	207.23	513.27
1960	3-eicosyne	C20H38	7.62458	2607.92	219.757	197.243	485.594
1961	alpha-epichlorohydrin	C3H5ClO	7.10839	1408.87	217.147	-57.2	336.85
1962	1,2-epoxybutane	C4H8O	7.19535	1337.15	246.496	-150	252.85
1963	epsilon-caprolactam	C6H11NO	7.49418	2131.64	192.056	69.21	532.85
1964	epsilon-caprolactone	C6H10O2	7.83109	2521.98	268.612	-1.3	497.85
1965	erythro-4,4-dimethyl-2,3-pentanediol	C7H16O2	9.33007	3480.41	273	170.197	437.153
1966	ethane	C2H6	6.95335	699.106	260.264	-182.8	32.27
1967	4-ethenyl-1,2-dimethylbenzene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1968	2-ethenyl-1,3-dimethylbenzene	C10H12	7.05759	1649.24	202.44	93.0981	406.189

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1969	2-ethenyl-1,4-dimethylbenzene	C10H12	7.05743	1651.24	202.325	93.581	407.08
1970	1-ethenyl-2,4-dimethylbenzene	C10H12	7.0551	1681.03	200.599	100.769	420.329
1971	1-ethenyl-3,5-dimethylbenzene	C10H12	7.05759	1649.24	202.44	93.0981	406.189
1972	2-ethoxyethanol	C4H10O2	8.17206	1925.93	228.985	-90.15	295.85
1973	2-(2-ethoxyethoxy)ethanol	C6H14O3	8.33772	2276.2	215.123	-78	358.85
1974	2-ethoxyethyl acetate	C6H12O3	7.3211	1640.21	213.092	-61.7	323.85
1975	1-ethyl,cis-decahydronaphthalene	C12H22	6.94771	1828.48	189.6	179.96	489.336
1976	2-ethyl-(1-thiaethyl)-benzene	C9H12S	7.17207	1818.12	195.68	155.846	457.72
1977	3-ethyl-(1-thiaethyl)-benzene	C9H12S	7.17101	1833.69	194.804	159.806	464.443
1978	4-ethyl-(1-thiaethyl)-benzene	C9H12S	7.17101	1833.69	194.804	159.806	464.443
1979	2-ethyl-1,2-butanediol	C6H14O2	9.45075	3107.58	273	116.732	351.138
1980	2-ethyl-1,3-butadiene	C6H10	6.91354	1208.81	224.75	-2.39601	258.408
1981	2-ethyl-1,3-butanediol	C6H14O2	9.53869	3194.79	273	123.298	357.312
1982	2-ethyl-1,3-pentanediol	C7H16O2	9.55208	3319.56	273	138.092	372.454
1983	2-ethyl-1,3-propanediol	C5H12O2	9.49492	3142.03	273	118.882	357.63
1984	2-ethyl-1,4-butanediol	C6H14O2	9.53869	3194.79	273	123.298	357.312
1985	2-ethyl-1,5-pentanediol	C7H16O2	9.6387	3279.47	273	128.818	354.832
1986	2-ethyl-1-butanol	C6H14O	7.49564	1498.18	178.145	-23.15	306.85
1987	2-ethyl-1-butene	C6H12	6.96578	1233.99	237.411	-131.54	238.85
1988	2-ethyl-1-heptanol	C9H20O	8.57327	2685.99	273	105.513	352.757
1989	3-ethyl-1-heptanol	C9H20O	8.5733	2732.39	273	112.051	363.564
1990	5-ethyl-1-heptanol	C9H20O	8.57327	2685.99	273	105.513	352.757
1991	2-ethyl-1-hexanol	C8H18O	7.05552	1461.65	165.52	-70	367.1

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1992	3-ethyl-1-hexanol	C8H18O	8.52318	2555.15	273	66.6363	335.489
1993	4-ethyl-1-hexanol	C8H18O	8.52318	2555.15	273	66.6363	335.489
1994	2-ethyl-1-hexene	C8H16	7.29597	1581.28	238.147	-100.15	300.85
1995	3-ethyl-1-hexene	C8H16	7.02826	1375.8	221.421	6.80308	283.093
1996	4-ethyl-1-hexene	C8H16	6.93567	1298.39	210.207	8.537	282.658
1997	2-ethyl-1-octanol	C10H22O	8.61878	2764.84	273	114.142	358.39
1998	3-ethyl-1-octanol	C10H22O	8.61878	2764.84	273	114.142	358.39
1999	2-ethyl-1-pentanol	C7H16O	8.34385	2324.35	259.469	57.0343	325.353
2000	3-ethyl-1-pentanol	C7H16O	8.47025	2453.76	273	55.4712	325.353
2001	2-ethyl-1-pentene	C7H14	7.01452	1325.43	226.639	-105.15	269.85
2002	3-ethyl-1-pentene	C7H14	7.08935	1346.26	235.778	-127.48	256.85
2003	3-ethyl-1-pentyne	C7H12	6.88599	1207.2	217.409	-5.98608	267.605
2004	3-ethyl-2,2,3-trimethylpentane	C10H22	6.99025	1608.63	221.938	47	372.85
2005	3-ethyl-2,2,4-trimethylpentane	C10H22	6.98282	1529.68	217.601	38	342.15
2006	3-ethyl-2,2-dimethylhexane	C10H22	6.99962	1527.84	214.832	40	338.55
2007	4-ethyl-2,2-dimethylhexane	C10H22	6.97668	1468.7	211.571	34	321.45
2008	3-ethyl-2,3,4-trimethylpentane	C10H22	7.02118	1619.09	221.599	47	369.15
2009	3-ethyl-2,3-dimethylhexane	C10H22	7.01446	1569.31	215.933	45	353.65
2010	4-ethyl-2,3-dimethylhexane	C10H22	7.04818	1569.99	215.824	44	344.15
2011	3-ethyl-2,3-pentanediol	C7H16O2	9.40578	3131.01	273	121.897	355.617
2012	3-ethyl-2,4-dimethylhexane	C10H22	7.05494	1572.89	216.708	43	342.95
2013	4-ethyl-2,4-dimethylhexane	C10H22	7.11162	1618.74	221.499	43	347.75
2014	3-ethyl-2,4-pentanediol	C7H16O2	9.49075	3176.08	273	123.334	353.778

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2015	3-ethyl-2,5-dimethylhexane	C10H22	7.03413	1529.46	214.141	39	330.35
2016	2-ethyl-2-heptanol	C9H20O	8.42444	2521.52	273	89.9483	336.251
2017	3-ethyl-2-heptanol	C9H20O	8.50271	2557.12	273	90.9722	333.196
2018	3-ethyl-2-hexanol	C8H18O	8.45078	2456.36	273	56.6776	322.758
2019	4-ethyl-2-hexanol	C8H18O	8.45078	2455.52	273	56.5654	322.555
2020	3-ethyl-cis-2-hexene	C8H16	7.05483	1441.41	224.33	13.7298	299.745
2021	3-ethyl-trans-2-hexene	C8H16	7.05483	1441.41	224.33	13.7298	299.745
2022	4-ethyl-cis-2-hexene	C8H16	7.01043	1378.58	220.827	8.537	288.881
2023	4-ethyl-trans-2-hexene	C8H16	7.01043	1378.58	220.827	8.537	288.881
2024	1-ethyl-2-isopropylbenzene	C11H16	7.0786	1649.31	202.9	103.684	389.616
2025	3-ethyl-2-methylheptane	C10H22	7.07029	1568.64	213.214	45	337.75
2026	4-ethyl-2-methylheptane	C10H22	7.0759	1550.6	213.414	42	328.65
2027	5-ethyl-2-methylheptane	C10H22	7.06932	1557.16	212.059	44	333.55
2028	3-ethyl-2-methylhexane	C9H20	7.05625	1490.43	218.943	26.85	314.95
2029	4-ethyl-2-methylhexane	C9H20	7.04242	1459.93	217	25	306.85
2030	3-ethyl-2-methylpentane	C8H18	7.03756	1416.51	225.113	9	293.85
2031	3-ethyl-2-pentanol	C7H16O	8.39655	2344.19	273	43.9299	309.658
2032	3-ethyl-2-pentanone	C7H14O	7.72556	1991.19	273	45.67	317.836
2033	3-ethyl-2-pentene	C7H14	7.00427	1331.43	226.883	-5.13508	274.505
2034	1-ethyl-2-propylbenzene	C11H16	7.13109	1714.69	200.43	115.227	403.415
2035	3-ethyl-2-thiapentane	C6H14S	6.99484	1388.02	205.518	78.435	325.235
2036	4-ethyl-3,3-dimethylhexane	C10H22	7.01947	1571.58	216.822	44	352.55
2037	3-ethyl-3,4-dimethylhexane	C10H22	7.02629	1574.73	217.757	44	351.35

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2038	ethyl-3-ethoxypropionate	C7H14O3	7.44459	1710.72	209.847	-50.15	335.85
2039	3-ethyl-3-heptanol	C9H20O	8.42444	2523.46	273	90.2276	336.72
2040	3-ethyl-3-hexanol	C8H18O	7.87807	1895.63	220.334	55.2709	313.8
2041	4-ethyl-3-hexanol	C8H18O	8.01738	2008.74	227.066	59.1857	317.355
2042	3-ethyl-3-hexene	C8H16	7.03608	1407.08	222.626	10.4858	292.477
2043	1-ethyl-3-isopropylbenzene	C11H16	7.07806	1655.9	202.52	105.32	392.478
2044	3-ethyl-3-methylheptane	C10H22	7.05165	1581.48	215.366	46	346.85
2045	4-ethyl-3-methylheptane	C10H22	7.09069	1591.99	215.945	45	341.15
2046	3-ethyl-3-methylhexane	C9H20	7.04317	1506.86	221.41	28	324.35
2047	3-ethyl-3-octanol	C10H22O	8.47466	2640.3	273	104.318	351.147
2048	6-ethyl-3-octanol	C10H22O	8.55069	2675.34	273	105.215	348.082
2049	3-ethyl-3-pentanol	C7H16O	7.72429	1710.58	210.673	43.7159	300.019
2050	1-ethyl-3-propylbenzene	C11H16	7.13162	1708.02	200.81	113.588	400.573
2051	4-ethyl-4-heptanol	C9H20O	8.42443	2505.72	273	87.6741	332.434
2052	1-ethyl-4-isopropylbenzene	C11H16	7.07683	1671.05	201.646	109.081	399.06
2053	3-ethyl-4-isopropylheptane	C12H26	6.92356	1523.45	181.835	75.3495	364.377
2054	4-ethyl-4-isopropylheptane	C12H26	6.87515	1525.18	181.835	77.763	374.881
2055	3-ethyl-4-methylheptane	C10H22	7.08435	1589.61	215.151	46	342.35
2056	4-ethyl-4-methylheptane	C10H22	7.05163	1570.23	215.67	44	342.55
2057	3-ethyl-4-methylhexane	C9H20	7.06079	1504.1	219.425	29	320.55
2058	3-ethyl-4-octanol	C10H22O	8.55068	2641.31	273	100.406	340.185
2059	4-ethyl-4-octanol	C10H22O	8.47464	2605.89	273	99.4011	343.016
2060	1-ethyl-4-propylbenzene	C11H16	7.13057	1721.36	200.05	116.866	406.257

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2061	3-ethyl-4-propylheptane	C12H26	6.97547	1547.11	181.835	77.0742	362.157
2062	4-ethyl-4-propylheptane	C12H26	6.92129	1530.67	181.835	76.6683	367.05
2063	3-ethyl-5-methylheptane	C10H22	7.04659	1535.39	210.362	44	333.45
2064	ethyl-sec-butylamine	C6H15N	6.94749	1165.73	188.656	24.4444	264.972
2065	ethyl-tert-butylamine	C6H15N	6.83428	1070.06	192.663	7.0805	243.882
2066	4a-ethyl-cis-decahydronaphthalene	C12H22	6.95338	1741.96	194.73	156.941	450.722
2067	4a-ethyl-trans-decahydronaphthalene	C12H22	6.95518	1716.33	196.25	150.12	439.281
2068	1-ethyl-trans-decahydronaphthalene	C12H22	6.94872	1812.46	190.55	175.697	482.185
2069	2-ethyl-trans-decahydronaphthalene	C12H22	6.9545	1725.94	195.68	152.678	443.571
2070	2-ethyl-cis-decahydronaphthalene	C12H22	6.95294	1748.37	194.35	158.646	453.582
2071	3-ethyl-o-xylene	C10H14	7.10646	1715.42	211.994	-49.51	406.85
2072	4-ethyl-o-xylene	C10H14	7.22714	1764.94	216.296	-66.93	393.85
2073	2-ethyl-m-xylene	C10H14	7.20901	1741.12	212.235	-16.26	397.85
2074	4-ethyl-m-xylene	C10H14	7.30983	1843.95	227.893	-62.88	391.85
2075	5-ethyl-m-xylene	C10H14	7.22685	1748.77	218.603	-84.33	381.85
2076	2-ethyl-p-xylene	C10H14	7.29636	1826.51	226.824	-53.63	389.85
2077	1-ethyl-[1,2,3,4-tetrahydronaphthalene]	C12H16	7.11255	1832.57	193.482	187.389	462.294
2078	2-ethyl-[1,2,3,4-tetrahydronaphthalene]	C12H16	7.11188	1842.66	192.906	190.115	466.638
2079	ethyl acetate	C4H8O2	7.25963	1338.46	228.608	-83.55	250.15
2080	ethylacetoacetate	C6H10O3	7.6595	1957.82	228.899	-39	369.85
2081	ethylacetylene	C4H6	7.1714	1070.62	241.457	-125.72	170.05
2082	ethyl acrylate	C5H8O2	7.26219	1428.92	226.634	-71.2	279.85
2083	ethyl alcohol	C2H6O	8.13484	1662.48	238.131	-114.1	243.1

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2084	ethyl aluminum sesquichloride	C6H15Al2Cl3	8.00942	1908.3	163.09	-20	226.85
2085	ethylamine	C2H7N	7.21885	1073.47	230.876	-81	183
2086	ethylbenzene	C8H10	7.1561	1559.55	228.582	-95	344.02
2087	ethyl benzoate	C9H10O2	7.50855	2047.03	228.94	-34.7	424.85
2088	2-ethylbiphenyl	C14H14	7.21197	1968.23	188.466	212.319	504.25
2089	3-ethylbiphenyl	C14H14	7.26929	2065.34	184.668	231.039	527.85
2090	4-ethylbiphenyl	C14H14	7.16265	2004.88	185.23	227.16	532.85
2091	2-ethylbutanal	C6H12O	7.18235	1397.14	208	36.8875	295.607
2092	2-ethylbutanenitrile	C6H11N	6.93608	1303.41	176.412	62.3535	329.41
2093	ethyl butanoate	C6H12O2	7.3746	1613.76	237.608	-98	297.85
2094	ethylbutylamine	C6H15N	7.00228	1214.51	186.679	33.1354	275.373
2095	ethyl butyl ether	C6H14O	7.2167	1400.33	230.763	-103	257.85
2096	ethyl sec-butyl ether	C6H14O	6.95756	1187.15	210	6.6155	247.572
2097	ethyl tert-butyl ether	C6H14O	6.83271	1117.6	210	-1.32152	243.517
2098	ethyl butyl sulfide	C6H14S	7.16605	1570.05	222.126	84.63	335.85
2099	2-ethyl butyric acid	C6H12O2	7.6032	1858.25	199.698	-15	381.85
2100	ethyl chloride	C2H5Cl	7.13047	1097.6	246.009	-136.4	187.2
2101	ethyl chloroformate	C3H5ClO2	8.05861	1577.17	211.753	-81.15	235
2102	ethyl cyanoacetate	C5H7NO2	7.34501	1731.5	181.865	-22.5	405.85
2103	ethylcyclobutane	C6H12	6.96049	1208.34	225.586	18.0074	254.954
2104	ethylcyclohexane	C8H16	6.96671	1473.49	228.828	-111.31	336
2105	1-ethylcyclohexene	C8H14	6.93892	1420.19	212.972	47.0507	344.531
2106	3-ethylcyclohexene	C8H14	6.94064	1403.09	213.994	42.8171	336.425

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2107	4-ethylcyclohexene	C8H14	6.94019	1407.51	213.73	43.9105	338.519
2108	ethylcyclopentane	C7H14	7.09118	1429.42	236.03	-138.44	296.37
2109	1-ethylcyclopentene	C7H12	6.95572	1324.87	218.797	23.0279	305.25
2110	3-ethylcyclopentene	C7H12	6.95891	1297.63	220.424	16.2926	292.205
2111	4-ethylcyclopentene	C7H12	6.95874	1299.03	220.34	16.638	292.874
2112	ethylcyclopropane	C5H10	6.98612	1100.65	232.173	-11.4313	207.783
2113	3-ethyldecane	C12H26	7.04446	1626.05	181.835	87.1797	375.81
2114	4-ethyldecane	C12H26	7.03774	1603.89	181.835	83.8087	369.48
2115	5-ethyldecane	C12H26	7.03484	1594.46	181.835	82.3743	366.787
2116	ethyldecylamine	C12H27N	6.77185	1337.69	102.786	142.585	404.55
2117	ethyl decyl sulfide	C12H26S	7.61843	2223.04	205.383	213.85	313.85
2118	2-ethyldiphenylmethane	C15H16	7.24487	2071.17	183.737	235.202	512.081
2119	3-ethyldiphenylmethane	C15H16	7.24473	2073.51	183.608	235.816	513.027
2120	4-ethyldiphenylmethane	C15H16	7.24366	2092.4	182.565	240.772	520.671
2121	ethyldocosylamine	C24H51N	6.3895	1538.64	33.5243	309.842	557.178
2122	ethyldodecylamine	C14H31N	7.20606	1802.96	140.846	172.164	434.25
2123	ethyl dodecyl sulfide	C14H30S	7.78265	2485.95	211.297	245.85	345.85
2124	ethyldotriacontylamine	C34H71N	8.89717	4597.4	273.15	384.379	541
2125	ethyleicosylamine	C22H47N	6.77558	1798.48	77.7688	294.905	533.549
2126	ethylene	C2H4	6.96636	649.806	262.73	-169.14	9.21
2127	ethylene carbonate	C3H4O3	7.47542	1944.57	185.23	36.4	516.85
2128	ethylenediamine	C2H8N2	7.64595	1600.32	218.58	11.14	319.85
2129	ethylene glycol	C2H6O2	9.69941	3147.1	264.246	-13	371.85

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2130	ethylene glycol diacetate	C6H10O4	7.03914	1418.58	150.643	-31	379.85
2131	ethylene glycol monopropyl ether	C5H12O2	8.48552	2290.88	257.391	-90	308.85
2132	ethyleneimine	C2H5N	7.13426	1171.65	219.609	-77.95	263.85
2133	ethylene oxide	C2H4O	7.26969	1114.78	243.301	-112.44	196
2134	ethylene sulfide	C2H4S	7.14085	1244.63	237.244	-35	281.85
2135	ethyl fluoride	C2H5F	7.24052	957.955	257.429	-143.2	102.16
2136	ethyl formate	C3H6O2	7.21764	1252.8	234.565	-79.6	235.25
2137	2-ethylfuran	C6H8O	7.0667	1266.23	210	16.5342	284.103
2138	3-ethylfuran	C6H8O	7.06575	1263.22	210	16.0345	283.112
2139	ethylheneicosylamine	C23H49N	6.60351	1688.72	58.6294	302.975	545.633
2140	ethylhentriacontylamine	C33H69N	8.89065	4544.34	273.15	382.108	533
2141	ethylheptacosylamine	C29H61N	6.02161	1450	9.66667	335.585	502
2142	ethylheptadecylamine	C19H41N	7.86353	2700.14	193.901	233.198	491.55
2143	ethyl heptadecyl sulfide	C19H40S	7.20937	2103.03	124	311.85	411.85
2144	3-ethylheptane	C9H20	7.21986	1628.26	232.057	-114.9	316.85
2145	4-ethylheptane	C9H20	7.12967	1538.44	220.874	30	311.8
2146	ethylheptatriacontylamine	C39H81N	8.91655	4811.39	273.15	383.211	574
2147	ethylheptylamine	C9H21N	7.08904	1487.11	172.681	92.31	349.05
2148	ethyl heptyl sulfide	C9H20S	7.15298	1737.33	199.813	156.85	256.85
2149	ethylhexacosylamine	C28H59N	5.97588	1400	9.33333	331.663	493
2150	ethylhexadecylamine	C18H39N	7.76234	2550.59	187.499	221.997	481.65
2151	ethyl hexadecyl sulfide	C18H38S	7.13143	2069.41	135	301.85	401.85
2152	2-ethylhexanal	C8H16O	7.35291	1689.29	217.09	-73.15	333.85

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2153	3-ethylhexane	C8H18	7.05503	1420.12	221.671	-1.11	292.25
2154	ethylhexatriacontylamine	C38H79N	8.93343	4788.53	273.15	384.793	568
2155	2-ethylhexyl acetate	C10H20O2	7.50916	1918.21	215.849	-93	365.85
2156	2-ethylhexyl acrylate	C11H20O2	7.77677	2222.15	237.874	-90	381.85
2157	ethylhexylamine	C8H19N	7.04831	1395.85	176.937	73.6108	326.65
2158	ethyl hexyl sulfide	C8H18S	7.09805	1717.84	220.489	136.85	236.85
2159	ethylidene diacetate	C6H10O4	6.9943	1371.33	164.375	18.85	361.85
2160	ethyl iodide	C2H5I	7.26806	1396.07	245.911	-111.1	287.85
2161	ethyl isobutanoate	C6H12O2	7.37463	1561.51	237.631	-88.15	280
2162	ethylisobutylamine	C6H15N	6.94749	1165.73	188.656	24.4444	264.972
2163	ethyl isobutyl ether	C6H14O	6.9574	1186.69	210	6.53895	247.425
2164	ethyl isocyanide	C3H5N	6.87239	1068.49	189.186	8.85578	262.179
2165	ethylisopropylamine	C5H13N	6.93178	1090.83	193.277	6.70487	240.65
2166	ethyl isopropyl ether	C5H12O	6.8725	1049.82	210	-15.4235	216.429
2167	ethyl isopropyl ketone	C6H12O	6.99939	1276.64	196.572	-73.15	293.85
2168	ethyl isovalerate	C7H14O2	7.23567	1578.65	228.203	-99.3	314.8
2169	ethyl lactate	C5H10O3	9.09091	2915.95	315.049	-26	314.85
2170	ethyl mercaptan	C2H6S	7.1629	1202.03	245.711	-147.89	226
2171	ethyl methacrylate	C6H10O2	7.18289	1492.18	229.851	-50	303.85
2172	ethyl methyl sulfate	C3H8O4S	---	---	---	---	---
2173	ethyl methyl sulfite	C3H8O3S	---	---	---	---	---
2174	1-ethylnaphthalene	C12H12	7.10905	1937.1	199.804	-13.81	502.85
2175	2-ethylnaphthalene	C12H12	7.2061	2000.9	204.264	118	501.75

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2176	ethyl nitrate	C2H5NO3	7.17012	1338.7	224.891	-10	100
2177	ethylnonacosylamine	C31H65N	8.88484	4449.89	273.15	377.14	518
2178	ethylnonadecylamine	C21H45N	6.95647	1924.23	99.1269	286.526	522.122
2179	3-ethylnonane	C11H24	7.01883	1554.65	187.7	70.5982	356.979
2180	4-ethylnonane	C11H24	7.01315	1535.99	187.7	67.7384	351.514
2181	5-ethylnonane	C11H24	7.00737	1517.34	187.7	64.8789	346.048
2182	ethylnonylamine	C11H25N	6.60191	1163.38	90.6435	126.711	387.65
2183	ethyl nonyl sulfide	C11H24S	7.09661	1759.04	170.4	196.85	296.85
2184	ethyloctacosylamine	C30H63N	8.89387	4408.47	273.15	338.185	510
2185	ethyloctadecylamine	C20H43N	7.98414	2870.99	201.573	244.589	500.75
2186	ethyl octadecyl sulfide	C20H42S	7.18259	2111.53	119.001	321.85	421.85
2187	3-ethyloctane	C10H22	7.11666	1601.8	211.642	50	340.45
2188	4-ethyloctane	C10H22	7.12109	1599.22	213.5	48	336.45
2189	ethyloctatriacontylamine	C40H83N	8.94057	4866.89	273.15	381.24	580
2190	ethyloctylamine	C10H23N	7.13621	1578.08	168.843	110.015	369.25
2191	ethyl octyl sulfide	C10H22S	7.16824	1809.06	195.094	176.85	276.85
2192	ethylpentacosylamine	C27H57N	5.92822	1350.9	327.276	484	
2193	ethylpentadecylamine	C17H37N	7.84024	2589.03	200.042	211.502	471.05
2194	ethyl pentadecyl sulfide	C17H36S	7.25728	2069.41	135	287.85	387.85
2195	3-ethylpentane	C7H16	7.10931	1402.17	238.129	-118.6	267.49
2196	ethylpentatriacontylamine	C37H77N	8.91205	4729.39	273.15	385.126	561
2197	ethylpentylamine	C7H17N	7.0104	1303.5	181.649	53.9257	301.85
2198	ethyl pentyl sulfide	C7H16S	7.05063	1575.03	210.873	116.85	216.85

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2199	m-ethylphenol	C8H10O	6.99776	1542.16	170.08	150.42	445.65
2200	p-ethylphenol	C8H10O	7.49026	1904.24	195.127	45.08	443.3
2201	ethyl propanoate	C5H10O2	7.19297	1375.07	219.783	-73.9	272.85
2202	1-ethylpropyl acetate	C7H14O2	6.95426	1276.08	181.269	51.7148	303.85
2203	1-ethylpropylamine	C5H13N	6.95953	1138.07	190.028	17.5589	257.75
2204	ethylpropylamine	C5H13N	6.90202	1095.37	192.099	9.8168	246.85
2205	1-ethylpropyl butanoate	C9H18O2	7.66369	1745.51	174.999	107.146	336.85
2206	ethyl propyl ether	C5H12O	7.11567	1232.15	227.094	-127.5	227.08
2207	1-ethylpropyl formate	C6H12O2	6.83139	1191.09	180.889	41.5681	305.85
2208	1-ethylpropyl propanoate	C8H16O2	7.39237	1554.41	177.469	85.3108	323.85
2209	ethyl propyl sulfate	C5H12O4S	---	---	---	---	---
2210	ethyl propyl sulfide	C5H12S	7.13461	1466.79	226.32	71.75	310.85
2211	2-ethylpyridine	C7H9N	7.25236	1627.2	222.825	44.9724	363.05
2212	3-ethylpyridine	C7H9N	7.45184	1856.94	239.241	56.6518	384.55
2213	4-ethylpyridine	C7H9N	7.27374	1741.83	227.308	58.3496	395.05
2214	3-ethylquinoline	C11H11N	7.05246	1708.38	143.521	162.896	502.522
2215	6-ethylquinoline	C11H11N	7.05314	1699.1	144.382	160.334	497.99
2216	8-ethylquinoline	C11H11N	7.05463	1678.94	146.255	154.764	488.135
2217	m-ethylstyrene	C10H12	7.06662	1644.77	202.891	91.3707	403.664
2218	p-ethylstyrene	C10H12	7.06603	1652.17	202.463	93.1525	406.952
2219	ethyltetracosylamine	C26H55N	5.87851	1300	8.66667	322.447	475
2220	ethyltetradecylamine	C16H35N	7.71755	2419.13	193.157	198.484	459.65
2221	ethyl tetradecyl sulfide	C16H34S	7.22342	2014.32	140	273.85	373.85

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2222	2-ethyltetrahydrofuran	C6H12O	6.99081	1311.09	210	27.7879	306.92
2223	3-ethyltetrahydrofuran	C6H12O	6.99984	1342.8	210	33.1415	317.545
2224	ethyltetratriacontylamine	C36H75N	8.92134	4700.44	273.15	385.876	555
2225	2-ethylthiacyclohexane	C7H14S	6.96647	1485.42	209.78	89.3101	373.273
2226	3-ethylthiacyclohexane	C7H14S	6.96647	1485.42	209.78	89.3101	373.273
2227	4-ethylthiacyclohexane	C7H14S	6.96647	1485.42	209.78	89.3101	373.273
2228	2-ethylthiacyclopentane	C6H12S	6.97349	1498.62	209.17	92.1507	386.127
2229	3-ethylthiacyclopentane	C6H12S	6.97127	1524.31	207.65	98.9735	398.388
2230	2-ethylthiacyclopropane	C4H8S	7.01195	1338.7	219.05	48.0506	321.574
2231	2-ethylthiophene	C6H8S	7.05715	1451.45	213.54	73.4683	350.45
2232	3-ethylthiophene	C6H8S	7.05608	1457.84	213.16	75.1732	353.55
2233	m-ethylthiophenol	C8H10S	7.167	1756.95	198.91	141.123	450.995
2234	p-ethylthiophenol	C8H10S	7.167	1756.95	198.91	141.123	450.995
2235	m-ethyltoluene	C9H12	7.07202	1610.69	222.972	-95.54	364
2236	p-ethyltoluene	C9H12	7.04821	1580.26	217.186	-62.32	367
2237	ethyltriacontylamine	C32H67N	8.90964	4516.5	273.15	380.272	526
2238	ethyltricosylamine	C25H53N	6.19192	1411.68	11.3466	316.343	569.44
2239	ethyltridecylamine	C15H33N	7.42041	2059.21	161.611	185.65	447.45
2240	ethyl tridecyl sulfide	C15H32S	7.22529	1980.43	146	259.85	359.85
2241	ethyltritriacontylamine	C35H73N	8.89	4633.98	273.15	385.347	548
2242	ethylundecylamine	C13H29N	6.988	1560.45	120.933	157.813	419.95
2243	ethyl undecyl sulfide	C13H28S	7.13871	1863.9	157.9	229.85	329.85
2244	ethyl vanillin	C9H10O3	8.18401	2413.87	161.324	77.5	474.85

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2245	ethyl vinyl ether	C4H8O	7.14878	1179.62	240.84	-115.8	202
2246	ethynylbenzene	C8H6	6.87809	1377.31	201.512	82	382.28
2247	fluoranthene	C16H10	7.85111	3122.76	245.485	110.18	631.85
2248	fluorene	C13H10	7.31877	2211.16	200.948	114.79	596.85
2249	cis-1-fluoro-1-butene	C4H7F	6.69721	860.982	204.401	-39.4646	182.1
2250	trans-1-fluoro-1-butene	C4H7F	6.69721	860.982	204.401	-39.4646	182.1
2251	2-fluoro-1-butene	C4H7F	6.6633	860.957	203.117	-37.1067	188.861
2252	3-fluoro-1-butene	C4H7F	6.66211	830.235	206.283	-46.1607	172.193
2253	4-fluoro-1-butene	C4H7F	6.71801	846.718	206.941	-45.3806	168.734
2254	cis-1-fluoro-1-decene	C10H19F	6.94912	1369.46	178.137	72.1299	320.331
2255	trans-1-fluoro-1-decene	C10H19F	6.94912	1369.46	178.137	72.1299	320.331
2256	cis-1-fluoro-1-dodecene	C12H23F	7.03576	1553.76	169.714	109.808	364.666
2257	trans-1-fluoro-1-dodecene	C12H23F	7.03576	1553.76	169.714	109.808	364.666
2258	cis-1-fluoro-1-eicosene	C20H39F	7.1506	2229.84	134.956	258.072	547.604
2259	trans-1-fluoro-1-eicosene	C20H39F	7.1506	2229.84	134.956	258.072	547.604
2260	cis-1-fluoro-1-heptadecene	C17H33F	7.17348	2004.76	148.38	203.557	476.948
2261	trans-1-fluoro-1-heptadecene	C17H33F	7.17348	2004.76	148.38	203.557	476.948
2262	cis-1-fluoro-1-heptene	C7H13F	6.81441	1104.58	190.965	15.989	252.815
2263	trans-1-fluoro-1-heptene	C7H13F	6.81441	1104.58	190.965	15.989	252.815
2264	cis-1-fluoro-1-hexadecene	C16H31F	7.16011	1919.19	152.723	184.985	454.092
2265	trans-1-fluoro-1-hexadecene	C16H31F	7.16011	1919.19	152.723	184.985	454.092
2266	cis-1-fluoro-1-hexene	C6H11F	6.77219	1020.76	195.352	-2.57751	229.725
2267	trans-1-fluoro-1-hexene	C6H11F	6.77219	1020.76	195.352	-2.57751	229.725

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2268	cis-1-fluoro-1-nonadecene	C19H37F	7.16988	2161.29	139.507	240.149	523.649
2269	trans-1-fluoro-1-nonadecene	C19H37F	7.16988	2161.29	139.507	240.149	523.649
2270	cis-1-fluoro-1-nonene	C9H17F	6.90382	1279.21	182.374	53.3516	298.034
2271	trans-1-fluoro-1-nonene	C9H17F	6.90382	1279.21	182.374	53.3516	298.034
2272	cis-1-fluoro-1-octadecene	C18H35F	7.17714	2085.86	143.979	221.961	500.115
2273	trans-1-fluoro-1-octadecene	C18H35F	7.17714	2085.86	143.979	221.961	500.115
2274	cis-1-fluoro-1-octene	C8H15F	6.85859	1190.81	186.645	34.6343	275.555
2275	trans-1-fluoro-1-octene	C8H15F	6.85859	1190.81	186.645	34.6343	275.555
2276	cis-1-fluoro-1-pentadecene	C15H29F	7.13833	1830.29	157.017	166.287	431.492
2277	trans-1-fluoro-1-pentadecene	C15H29F	7.13833	1830.29	157.017	166.287	431.492
2278	cis-1-fluoro-1-pentene	C5H9F	6.73282	939.521	199.824	-21.0619	206.189
2279	trans-1-fluoro-1-pentene	C5H9F	6.73282	939.521	199.824	-21.0619	206.189
2280	2-fluoro-1-pentene	C5H9F	6.70493	910.859	201.708	-27.4746	196.275
2281	3-fluoro-1-pentene	C5H9F	6.69709	907.589	201.66	-27.7918	196.525
2282	4-fluoro-1-pentene	C5H9F	6.69709	907.589	201.66	-27.7918	196.525
2283	5-fluoro-1-pentene	C5H9F	6.74026	992.044	195.043	-6.55395	231.354
2284	cis-1-fluoro-1-propene	C3H5F	6.66628	785.205	209.106	-57.7899	157.335
2285	trans-1-fluoro-1-propene	C3H5F	6.66628	785.205	209.106	-57.7899	157.335
2286	2-fluoro-1-propene	C3H5F	6.6505	722.052	215.542	-75.9709	123.466
2287	3-fluoro-1-propene	C3H5F	6.27804	722.052	215.542	-53	47
2288	cis-1-fluoro-1-tetradecene	C14H27F	7.10946	1739.13	161.273	147.503	409.093
2289	trans-1-fluoro-1-tetradecene	C14H27F	7.10946	1739.13	161.273	147.503	409.093
2290	cis-1-fluoro-1-tridecene	C13H25F	7.07484	1646.66	165.501	128.666	386.837

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2291	trans-1-fluoro-1-tridecene	C13H25F	7.07484	1646.66	165.501	128.666	386.837
2292	cis-1-fluoro-1-undecene	C11H21F	6.99347	1461.15	173.922	90.9548	342.519
2293	trans-1-fluoro-1-undecene	C11H21F	6.99347	1461.15	173.922	90.9548	342.519
2294	1-fluoro-2,2-dimethylbutane	C6H13F	7.01292	1234.88	222	1.07164	241.683
2295	1-fluoro-2,2-dimethylpropane	C5H11F	7.11983	1254.75	256	-33.6337	205.677
2296	1-fluoro-2,3-dimethylbutane	C6H13F	6.90281	1218.67	222	2.61014	256.31
2297	2-fluoro-2,3-dimethylbutane	C6H13F	6.88491	1156.58	222	-8.12643	235.155
2298	cis-1-fluoro-2-butene	C4H7F	6.69721	860.982	204.401	-39.4646	182.1
2299	trans-1-fluoro-2-butene	C4H7F	6.69721	860.982	204.401	-39.4646	182.1
2300	cis-2-fluoro-2-butene	C4H7F	6.64591	862.248	202.011	-35.1927	194.679
2301	trans-2-fluoro-2-butene	C4H7F	6.64591	862.248	202.011	-35.1927	194.679
2302	3-fluoro-2-ethyl-1-propene	C5H9F	6.70493	910.859	201.708	-27.4746	196.275
2303	1-fluoro-2-ethylbutane	C6H13F	6.8213	1107.79	222	-14.7111	227.86
2304	cis-1-fluoro-2-methyl-1-butene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2305	trans-1-fluoro-2-methyl-1-butene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2306	3-fluoro-2-methyl-1-butene	C5H9F	6.64921	893.407	201.039	-28.3025	199.797
2307	4-fluoro-2-methyl-1-butene	C5H9F	6.70493	910.859	201.708	-27.4746	196.275
2308	1-fluoro-2-methyl-1-propene	C4H7F	6.64323	874.479	200.575	-31.3025	202.239
2309	3-fluoro-2-methyl-1-propene	C4H7F	6.65918	879.599	200.949	-31.2096	200.269
2310	1-fluoro-2-methyl-cis-2-butene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2311	1-fluoro-2-methyl-trans-2-butene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2312	1-fluoro-2-methylbutane	C5H11F	7.00467	1173.73	228.72	-27.3436	221.301
2313	2-fluoro-2-methylbutane	C5H11F	7.01008	1190.88	243.601	-39.4711	213.017

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2314	1-fluoro-2-methylpentane	C6H13F	7.01953	1258.17	222	5.00771	249.258
2315	2-fluoro-2-methylpentane	C6H13F	6.89771	1200.45	222	-0.53894	250.106
2316	3-fluoro-2-methylpentane	C6H13F	6.95154	1196.79	222	-3.38444	238.657
2317	1-fluoro-2-methylpropane	C4H9F	7.1853	1170.82	256	-50.8873	171.406
2318	2-fluoro-2-methylpropane	C4H9F	6.90613	1016.15	240.339	-63.0011	173.681
2319	1-fluoro-cis-2-pentene	C5H9F	6.73282	939.521	199.824	-21.0619	206.189
2320	1-fluoro-trans-2-pentene	C5H9F	6.73282	939.521	199.824	-21.0619	206.189
2321	2-fluoro-cis-2-pentene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2322	2-fluoro-trans-2-pentene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2323	3-fluoro-cis-2-pentene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2324	3-fluoro-trans-2-pentene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48
2325	4-fluoro-cis-2-pentene	C5H9F	6.67678	921.607	199.146	-21.9022	209.758
2326	4-fluoro-trans-2-pentene	C5H9F	6.67678	921.607	199.146	-21.9022	209.758
2327	5-fluoro-cis-2-pentene	C5H9F	6.73282	939.521	199.824	-21.0619	206.189
2328	5-fluoro-trans-2-pentene	C5H9F	6.73282	939.521	199.824	-21.0619	206.189
2329	1-fluoro-3,3-dimethylbutane	C6H13F	6.95633	1213.28	222	-0.566364	244.143
2330	2-fluoro-3,3-dimethylbutane	C6H13F	6.8355	1154.77	222	-6.49303	244.249
2331	cis-1-fluoro-3-methyl-1-butene	C5H9F	6.67678	921.607	199.146	-21.9022	209.758
2332	trans-1-fluoro-3-methyl-1-butene	C5H9F	6.67678	921.607	199.146	-21.9022	209.758
2333	2-fluoro-3-methyl-1-butene	C5H9F	6.64921	893.407	201.039	-28.3025	199.797
2334	3-fluoro-3-methyl-1-butene	C5H9F	6.58229	866.995	200.859	-31.0325	200.741
2335	4-fluoro-3-methyl-1-butene	C5H9F	6.69709	907.589	201.66	-27.7918	196.525
2336	1-fluoro-3-methyl-2-butene	C5H9F	6.68457	924.918	199.199	-21.5846	209.48

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2337	2-fluoro-3-methyl-2-butene	C5H9F	6.63686	910.446	198.555	-22.1027	212.872
2338	1-fluoro-3-methylbutane	C5H11F	7.2535	1353.35	256	-21.7103	217.695
2339	2-fluoro-3-methylbutane	C5H11F	7.1899	1309.96	256	-26.6961	213.623
2340	1-fluoro-3-methylpentane	C6H13F	7.02577	1280.79	222	8.82935	256.613
2341	2-fluoro-3-methylpentane	C6H13F	6.9578	1218.41	222	0.309549	245.849
2342	3-fluoro-3-methylpentane	C6H13F	6.88491	1156.58	222	-8.12643	235.155
2343	1-fluoro-4-methylpentane	C6H13F	7.02204	1267.22	222	6.53634	252.2
2344	2-fluoro-4-methylpentane	C6H13F	6.9578	1218.41	222	0.309549	245.849
2345	fluorobenzene	C6H5F	7.13144	1351.52	233.227	-42.21	286.94
2346	1-fluorobutane	C4H9F	7.1435	1166.07	241.052	-51.2472	187.55
2347	2-fluorobutane	C4H9F	7.01419	1087.22	237.935	-51.7051	185.397
2348	1-fluorodecane	C10H21F	7.22115	1682.91	201.538	68.9768	349.95
2349	1-fluorodocosane	C22H45F	7.23258	2319.49	169.001	301.337	510.4
2350	1-fluorododecane	C12H25F	7.21559	1781.81	186.05	100.618	385.45
2351	1-fluorodotriacontane	C32H65F	6.41051	2152.1	155.714	359.62	504
2352	1-fluoroeicosane	C20H41F	6.96318	1886.95	121.221	195.213	483.65
2353	fluoroform	CHF3	7.18249	725.191	250.743	-155.18	25.74
2354	1-fluoroheneicosane	C21H43F	7.29345	2314.43	171.501	292.088	499.381
2355	1-fluorohentriacontane	C31H63F	6.4717	2168.65	157.932	356.353	496
2356	1-fluoroheptacosane	C27H55F	6.72239	2187.78	156.501	338.32	568.088
2357	1-fluoroheptadecane	C17H35F	7.10635	1905.49	147.948	164.104	453.05
2358	1-fluoroheptane	C7H15F	7.19226	1467.98	222.585	14.4824	282.65
2359	1-fluoroheptatriacontane	C37H75F	6.16488	2089.01	147.105	364.739	539

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2360	1-fluorohexacosane	C26H53F	6.84942	2234.33	159.001	332.234	556.106
2361	1-fluorohexadecane	C16H33F	7.12174	1882.45	154.876	152.626	441.45
2362	1-fluorohexane	C6H13F	7.1708	1374.62	228.926	-6.16347	254.95
2363	2-fluorohexane	C6H13F	7.02478	1277.17	222	8.21787	255.436
2364	3-fluorohexane	C6H13F	7.02066	1262.24	222	5.69559	250.582
2365	1-fluorohexatriacontane	C36H73F	6.21142	2100.63	148.706	364.681	532
2366	1-fluorononacosane	C29H59F	6.28875	1873.62	119.782	348.551	593.186
2367	1-fluorononadecane	C19H39F	7.0266	1907.35	131.071	185.419	474.15
2368	1-fluorononane	C9H19F	7.21771	1621.13	208.799	51.9285	329.75
2369	1-fluorononatriacontane	C39H79F	6.08238	2069.72	144.471	362.536	552
2370	1-fluorooctacosane	C28H57F	6.58577	2134.06	154.001	344.059	580.846
2371	1-fluorooctadecane	C18H37F	7.06312	1909.3	140.517	174.386	463.95
2372	1-fluorooctane	C8H17F	7.21056	1551.57	216.05	33.7768	307.35
2373	1-fluorooctatriacontane	C38H77F	6.12661	2080.31	145.926	363.482	545
2374	1-fluoropentacosane	C25H51F	6.96541	2273.08	161.501	325.827	544.867
2375	1-fluoropentadecane	C15H31F	7.15848	1872.96	163.845	140.281	428.95
2376	1-fluoropentane	C5H11F	7.13705	1265.03	234.417	-28.2878	223.55
2377	2-fluoropentane	C5H11F	6.92088	1110.92	219.675	-26.2955	220.4
2378	3-fluoropentane	C5H11F	6.93892	1115.98	222	-17.6756	216.944
2379	1-fluoropentatriacontane	C35H71F	6.25923	2112.77	150.371	364.127	525
2380	1-fluoropropane	C3H7F	7.00443	975.851	239.849	-70	148.85
2381	2-fluoropropane	C3H7F	6.82343	860.678	227.642	-49	142.53
2382	1-fluorotetracontane	C40H81F	6.04614	2062.04	143.445	360.287	558

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2383	1-fluorotetracosane	C24H49F	7.06817	2298.86	164.001	318.23	533.114
2384	1-fluorotetradecane	C14H29F	7.13255	1807.54	167.131	127.615	415.55
2385	1-fluorotetratriacontane	C34H69F	6.30833	2125.4	152.098	363.09	518
2386	p-fluorotoluene	C7H7F	7.1726	1484.79	229.351	68	317.33
2387	1-fluorotriacontane	C30H61F	6.53464	2185.66	160.185	352.656	488
2388	1-fluorotricosane	C23H47F	7.15775	2315.97	166.501	310.357	522.044
2389	1-fluorotridecane	C13H27F	7.17668	1800.39	177.098	114.384	401.05
2390	1-fluorotritriacontane	C33H67F	6.35875	2138.52	153.881	361.582	511
2391	1-fluoroundecane	C11H23F	7.21326	1731.73	193.713	85.0032	368.45
2392	formaldehyde	CH2O	7.46432	1078.39	254.377	-92	134.85
2393	formamide	CH3NO	7.63804	2012.7	203.234	2.55	497.85
2394	formanilide	C7H7NO	7.53199	2137.43	188.545	50	513.85
2395	formic acid	CH2O2	8.41278	2247.58	305.729	8.4	306.85
2396	fumaric acid	C4H4O4	7.50353	1665.01	70.1806	287	497.85
2397	furan	C4H4O	7.13277	1145.36	238.023	-85.6	217
2398	furfural	C5H4O2	7.71516	1917.45	234.93	-36.5	383.85
2399	furfuryl alcohol	C5H6O2	8.2317	2128.37	227.76	-14.63	358.85
2400	glutaric acid	C5H8O4	8.04576	2432.01	148.479	97.5	533.85
2401	glutaric anhydride	C5H6O3	7.88053	2538.84	218.256	54.85	564.85
2402	glutaronitrile	C5H6N2	7.85683	2587.97	234.088	-28.94	508.85
2403	glycerol	C3H8O3	9.90788	3821.36	253.806	18.18	449.85
2404	glyceryl triacetate	C9H14O6	7.74878	2162.45	185.221	4.1	430.85
2405	guaiacol	C7H8O2	7.89985	2204.47	234.222	31.5	423.85

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2406	halothane	C2HBrClF3	6.55116	951.73	209.103	-50	247.85
2407	heneicosane	C21H44	7.07687	2022.5	125.5	148.625	406.5
2408	heneicosanenitrile	C21H41N	7.19134	2290.31	134.33	306.849	550.897
2409	1-heneicosene	C21H42	6.98584	1963.02	123.199	122.614	506.202
2410	heneicosylamine	C21H45N	7.19297	2231.36	122.458	304.788	549.252
2411	heneicosylbenzene	C27H48	6.64024	1865.35	67.1797	176.968	587.777
412	heneicosylcyclohexane	C27H54	6.49605	1785.33	61.8343	176.335	590.993
2413	heneicosylcyclopentane	C26H52	6.76888	2033	102.882	281.3	576.979
2414	1-heneicosyne	C21H40	8.04371	3273.97	280.135	211.873	509.268
2415	hentriacontane	C31H64	7.14547	2276.9	75.9	230.274	509.238
2416	1-hentriacontene	C31H62	6.01819	1461.55	8.8505	199.401	507
2417	hentriacontylamine	C31H65N	8.7196	4485.06	273.15	399.974	545
2418	hentriacontylbenzene	C37H68	6.46377	1850	12.3333	237.621	554
2419	hentriacontylcyclohexane	C37H74	6.43623	1850	12.3333	237.163	558
2420	hentriacontylcyclopentane	C36H72	5.72218	1718.57	103.839	301.001	551
2421	1-hentriacontyne	C31H60	6.09198	1921.05	143.242	331.873	505
2422	n-heptacontane	C70H142	7.22067	2662.5	-39.5	393.296	702.459
2423	heptacosane	C27H56	7.11471	2188.5	94.8	200.296	472.04
2424	1-heptacosene	C27H54	6.2286	1551.84	42.5433	172.138	576.776
2425	heptacosylamine	C27H57N	5.76543	1350	9	347.451	509
2426	heptacosylbenzene	C33H60	6.1121	1546.49	1.60011	215.845	527
2427	heptacosylcyclohexane	C33H66	6.23447	1650	11	215.4	531
2428	heptacosylcyclopentane	C32H64	6.27543	1965.46	106.993	302.622	522

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2429	1-heptacosyne	C27H52	8.3422	4496.67	404.357	283.873	574.342
2430	heptadecanal	C17H34O	7.59576	2366.09	176.828	181.901	479.053
2431	heptadecane	C17H36	7.25896	2028.11	161.086	21.98	460.22
2432	1,2-heptadecanediol	C17H36O2	9.11678	4059.62	273.001	274.279	524.443
2433	1,3-heptadecanediol	C17H36O2	9.11679	4128.22	273.001	267.366	537.917
2434	1,4-heptadecanediol	C17H36O2	9.11683	4259.2	273.001	301.182	563.639
2435	1,17-heptadecanediol	C17H36O2	9.11084	4174.12	273.001	290.166	547.471
2436	heptadecanenitrile	C17H33N	7.33198	2189.36	142.861	267.747	505.998
2437	1-heptadecanethiol	C17H36S	7.39235	2295	160.685	198	512.86
2438	2-heptadecanethiol	C17H36S	7.22832	2069.41	135	224.823	503.85
2439	heptadecanoic acid	C17H34O2	7.35248	2072.1	100.784	176.85	516.001
2440	1-heptadecanol	C17H36O	6.96026	1797.05	116.512	53.9	496.85
2441	2-heptadecanol	C17H36O	6.89532	1657.99	85.0003	221.004	491.25
2442	2-heptadecanone	C17H34O	7.4683	2226.6	166.364	177.869	472.825
2443	1-heptadecene	C17H34	7.36258	2126.37	174.12	11.25	462.85
2444	heptadecyl acetate	C19H38O2	7.6754	2550	190	291.85	391.85
2445	heptadecylamine	C17H37N	7.56304	2397.6	169.063	198.793	494.65
2446	heptadecylbenzene	C23H40	7.08791	2133.92	118.218	145.622	549.855
2447	heptadecyl butanoate	C21H42O2	5.10563	1050	7	336.632	514.95
2448	heptadecylcyclohexane	C23H46	6.9428	2046.35	112.781	144.855	550.825
2449	heptadecylcyclopentane	C22H44	6.9848	2027.13	116.941	251.114	535.639
2450	heptadecyl formate	C18H36O2	9.11363	3650	190	345.61	445.61
2451	heptadecyl propanoate	C20H40O2	8.25996	3400	190	392.07	492.07

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2452	1-heptadecyne	C17H32	7.13747	1929.84	154.361	184	463.06
2453	2-heptadecyne	C17H32	7.37031	2251.56	190.518	172.978	480.645
2454	3-heptadecyne	C17H32	7.36546	2203.59	191.363	164.667	466.451
2455	n-heptahexacontane	C67H136	7.21879	2647.9	-33.6	385.615	693.675
2456	1-heptanal	C7H14O	7.32102	1635.48	215.534	-43	329.85
2457	heptane	C7H16	7.04605	1341.89	223.733	-90.59	267.11
2458	1,2-heptanediol	C7H16O2	9.63878	3453.33	273	150.115	388.105
2459	1,3-heptanediol	C7H16O2	9.63881	3527.68	273	159.224	402.335
2460	1,4-heptanediol	C7H16O2	7.16002	1435.29	93.4098	176.612	429.502
2461	1,6-heptanediol	C7H16O2	9.6387	3279.47	273	128.818	354.832
2462	1,7-heptanediol	C7H16O2	10.5427	4544.41	331.118	166.649	410.031
2463	2,3-heptanediol	C7H16O2	9.56529	3396.12	273	146.887	386.957
2464	2,4-heptanediol	C7H16O2	9.56529	3396.12	273	146.887	386.957
2465	2,6-heptanediol	C7H16O2	9.56529	3396.12	273	146.887	386.957
2466	heptanenitrile	C7H13N	7.03431	1467.06	168.71	95.2825	369.946
2467	2-heptanethiol	C7H16S	7.08682	1575.03	210.873	47.8887	358.85
2468	heptanoic acid	C7H14O2	7.32832	1656.28	149.408	-7.32	406.85
2469	1-heptanol	C7H16O	7.18822	1482.06	167.773	-34	358.75
2470	2-heptanol	C7H16O	7.92389	1897.51	217.061	-30.15	314.85
2471	3-heptanol	C7H16O	7.71058	1690.91	193.402	58.5748	312.679
2472	4-heptanol	C7H16O	7.8339	1789.72	206.635	55.254	309.953
2473	2-heptanone	C7H14O	7.16218	1551.82	211.559	-35	338.4
2474	3-heptanone	C7H14O	7.22074	1520.57	202.967	41.4679	327.01

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2475	4-heptanone	C7H14O	7.60043	1857.3	249.527	31.8632	322.158
2476	heptatriacontane	C37H76	7.16756	2380	51.2	267.821	555.071
2477	1-heptatriacontene	C37H74	6.47072	1850	12.3333	233.636	553
2478	heptatriacontylamine	C37H77N	8.74357	4767.3	273.15	407.052	590
2479	1-heptatriacontyne	C37H72	5.74292	1772.73	119.38	403.873	550
2480	1-heptene	C7H14	7.0899	1371.22	232.136	-118.88	264.14
2481	cis-2-heptene	C7H14	7.06158	1400.63	236.608	-109.15	275.85
2482	trans-2-heptene	C7H14	7.1336	1414.38	234.628	-109.48	269.85
2483	cis-3-heptene	C7H14	7.02687	1361.01	232.516	-136.64	271.85
2484	trans-3-heptene	C7H14	7.17463	1442.86	240.362	-136.63	266.85
2485	1-heptyl-[1,2,3,4-tetrahydronaphthalene]	C17H26	7.31141	2210.91	178.011	263.256	515.261
2486	2-heptyl-[1,2,3,4-tetrahydronaphthalene]	C17H26	7.31065	2224.89	177.251	266.873	520.569
2487	heptyl acetate	C9H18O2	7.00947	1541.36	180.932	75.5563	370.75
2488	heptylamine	C7H17N	7.38735	1682.44	216.434	-19	333.85
2489	heptylbenzene	C13H20	7.25666	1945.86	198.582	-48	440.85
2490	heptyl butanoate	C11H22O2	6.82421	1528.67	162.554	123.335	402.35
2491	heptylcyclohexane	C13H26	7.10051	1835.18	189.998	111	435.48
2492	heptylcyclopentane	C12H24	7.11422	1770.7	194.118	95	405.85
2493	1-heptylcyclopentene	C12H22	7.1397	1773.36	197.39	115.781	407.626
2494	heptyl formate	C8H16O2	6.94976	1418.49	170.515	88.6828	360.45
2495	heptyl mercaptan	C7H16S	7.21232	1700.98	215.759	-43.23	371.85
2496	1-heptylnaphthalene	C17H22	7.39867	2313.01	174.971	278.771	538.291
2497	2-heptylnaphthalene	C17H22	7.3983	2320.14	174.591	280.582	540.951

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2498	heptyl propanoate	C10H20O2	6.8848	1503.8	165.575	112.511	386.45
2499	1-heptyne	C7H12	7.2638	1554.66	254.993	14	286.54
2500	2-heptyne	C7H12	6.91852	1318.37	214.515	15.0709	308.748
2501	3-heptyne	C7H12	6.92415	1306.53	215.972	11.3291	301.436
2502	hexachloro-1,3-butadiene	C4Cl6	6.60811	1484.18	183.191	-21	467.85
2503	hexachlorobenzene	C6Cl6	6.63176	1444.53	75.7115	228.55	551.85
2504	hexachlorocyclopentadiene	C5Cl6	7.09079	1829.59	195.584	11.34	472.85
2505	hexachloroethane	C2Cl6	6.69959	1377.5	173.867	33	424.85
2506	hexacosane	C26H54	7.10961	2164.3	99.6	192.453	462.202
2507	1-hexacosene	C26H52	6.38418	1641.95	57.6761	164.684	564.534
2508	hexacosylamine	C26H55N	6.1621	1485.48	3.7122	341.956	611.838
2509	hexacosylbenzene	C32H58	6.24846	1635.45	15.6376	209.99	520
2510	hexacosylcyclohexane	C32H64	6.1268	1576.82	11.777	209.476	524
2511	hexacosylcyclopentane	C31H62	6.40455	2016.72	108.323	300.961	514
2512	1-hexacosyne	C26H50	8.45447	4513.25	400.747	271.873	562.854
2513	hexadecanal	C16H32O	7.60512	2321.81	180.46	171.056	466.952
2514	hexadecane	C16H34	7.36235	2094.08	180.407	18.17	447.45
2515	1,2-hexadecanediol	C16H34O2	9.25172	4058.27	273.001	264.323	508.371
2516	1,3-hexadecanediol	C16H34O2	9.25174	4128.37	273.001	258.005	521.863
2517	1,4-hexadecanediol	C16H34O2	9.25178	4262.18	273.001	291.317	547.621
2518	1,16-hexadecanediol	C16H34O2	9.30068	4181.48	273.001	280.395	531.164
2519	hexadecanenitrile	C16H31N	7.33475	2142.14	144.954	256.59	494.981
2520	1-hexadecanethiol	C16H34S	7.38074	2235.41	162.757	188	501.53

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2521	2-hexadecanethiol	C16H34S	7.19413	2014.32	140	212.338	494.85
2522	hexadecanoic acid	C16H32O2	8.58266	3341.95	235.116	62.51	502.85
2523	1-hexadecanol	C16H34O	6.93175	1747.21	119.31	49.2	487.85
2524	2-hexadecanol	C16H34O	6.87873	1619.16	91.0003	208.754	481.05
2525	2-hexadecanone	C16H32O	7.5392	2262.56	178.696	167.304	463.36
2526	1-hexadecene	C16H32	7.45309	2193.98	194.974	4.36	448.85
2527	hexadecyl acetate	C18H36O2	7.71781	2500	190	276.85	376.85
2528	hexadecylamine	C16H35N	7.48138	2275.78	166.673	187.658	484.35
2529	hexadecylbenzene	C22H38	6.59124	1709.22	83.6545	231.985	537.35
2530	hexadecyl butanoate	C20H40O2	5.10929	1000	6.66667	335.632	492.07
2531	hexadecylcyclohexane	C22H44	6.95175	2003.81	113.214	224	540.27
2532	hexadecylcyclopentane	C21H42	6.91514	1897.48	106.324	215	524.1
2533	1-hexadecylcyclopentene	C21H40	7.34912	2320.21	173.261	221.872	502.505
2534	hexadecyl formate	C17H34O2	9.10049	3500	190	322.73	422.73
2535	hexadecyl propanoate	C19H38O2	8.13369	3200	190	369.19	469.19
2536	1-hexadecyne	C16H30	7.10989	1864.84	156.948	172	451.11
2537	2-hexadecyne	C16H30	7.34772	2187.32	193.671	160.746	469.038
2538	3-hexadecyne	C16H30	7.34926	2150.63	195.292	153.093	455.998
2539	1,2-hexadiene	C6H10	6.96077	1226.27	224.56	-0.936721	260.921
2540	1,cis-3-hexadiene	C6H10	6.94618	1212.01	225.13	-3.51824	253.549
2541	1,trans-3-hexadiene	C6H10	6.94618	1212.01	225.13	-3.51824	253.549
2542	1,cis-4-hexadiene	C6H10	6.94975	1186.71	226.65	-9.8063	241.377
2543	1,trans-4-hexadiene	C6H10	6.94975	1186.71	226.65	-9.8063	241.377

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2544	1,5-hexadiene	C6H10	7.05328	1270.64	245.07	-140.68	233.85
2545	2,3-hexadiene	C6H10	6.94918	1196.43	226.08	-7.43736	250.763
2546	cis-2,trans-4-hexadiene	C6H10	7.06647	1332.12	234.758	-96.1	264.85
2547	cis-2,cis-4-hexadiene	C6H10	6.92807	1229.56	223.8	1.76744	266.308
2548	trans-2,trans-4-hexadiene	C6H10	6.97629	1249.62	223.221	-44.9	261.85
2549	hexaethylbenzene	C18H30	7.6139	2455.63	220.811	134	461.63
2550	hexafluoroacetone	C3F6O	7.04955	872.277	236.513	-125.45	83.99
2551	hexafluorobenzene	C6F6	7.22141	1329.93	226.134	5.1	243.58
2552	hexafluoroethane	C2F6	6.99088	723.544	254.242	-100.7	19.65
2553	1,1,1,2,2,3-hexafluoropropane	C3H2F6	6.89584	841.265	208.329	-23.15	128.064
2554	1,1,1,2,3,3-hexafluoropropane	C3H2F6	6.70224	814.052	206.923	-23.15	134.179
2555	1,1,1,3,3,3-hexafluoropropane	C3H2F6	6.79355	833.01	213.597	-56.9111	133.7
2556	1,1,2,2,3,3-hexafluoropropane	C3H2F6	6.78562	844.924	206.38	-23.15	143.941
2557	hexafluoropropylene	C3F6	6.93705	900.849	251.69	-156.5	94.85
2558	n-hexahexacontane	C66H134	7.21737	2642.7	-31.6	382.979	690.645
2559	hexamethylbenzene	C12H18	7.39576	2358.05	258.827	178	484.85
2560	hexamethylcyclotrisiloxane	C6H18O3Si3	6.89602	1350.23	201.168	64	281.05
2561	hexamethyldisilazane	C6H19NSi2	7.30838	1581.26	231.139	20	270.85
2562	hexamethyldisiloxane	C6H18OSi2	7.12803	1433.96	237.103	-68.22	245.55
2563	hexamethylenediamine	C6H16N2	7.54526	1828.87	190.197	40.8	389.85
2564	hexamethyleneimine	C6H13N	7.1137	1427.99	205.657	-37	341.85
2565	2,2,3,3,4,4-hexamethylhexane	C12H26	6.63649	1494.14	181.835	83.2481	418.283
2566	2,2,3,3,4,5-hexamethylhexane	C12H26	6.66965	1442.92	181.835	72.6642	389.839

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2567	2,2,3,3,5,5-hexamethylhexane	C12H26	6.61085	1405.61	181.835	68.681	388.599
2568	2,2,3,4,4,5-hexamethylhexane	C12H26	6.67849	1472.87	181.835	77.5424	399.668
2569	2,2,3,4,5,5-hexamethylhexane	C12H26	6.65789	1404.45	181.835	66.3934	377.201
2570	2,3,3,4,4,5-hexamethylhexane	C12H26	6.67849	1472.87	181.835	77.5424	399.668
2571	2,2,3,3,4,4-hexamethylpentane	C11H24	6.6044	1421.29	187.7	65.903	399.409
2572	hexamethyl phosphoramidate	C6H18N3OP	8.0642	2397.83	229.599	7	233
2573	hexanal	C6H12O	7.34663	1588.31	227.359	-56	305.85
2574	hexane	C6H14	6.9895	1216.92	227.451	-95.31	234.28
2575	1,2-hexanediol	C6H14O2	9.61605	3347.42	273	138.284	376.948
2576	1,3-hexanediol	C6H14O2	9.61609	3421.52	273	147.387	391.332
2577	1,4-hexanediol	C6H14O2	9.61615	3562.99	273	164.766	418.793
2578	1,5-hexanediol	C6H14O2	10.4322	4270.05	328.464	144.781	387.213
2579	1,6-hexanediol	C6H14O2	8.862	2626.62	196.146	42	396.85
2580	2,3-hexanediol	C6H14O2	9.53869	3182.47	273	121.77	354.882
2581	2,5-hexanediol	C6H14O2	9.53874	3287.68	273	134.819	375.635
2582	3,4-hexanediol	C6H14O2	9.53875	3307.6	273	137.289	379.562
2583	hexanenitrile	C6H11N	7.57546	1927.95	247.07	-80.3	348.9
2584	2-hexanethiol	C6H14S	6.9792	1426.46	209.155	29.416	333.85
2585	hexanoic acid	C6H12O2	7.47273	1747.23	174.802	-3	393.85
2586	1-hexanol	C6H14O	7.34748	1538.76	187.498	-44.6	338.2
2587	2-hexanol	C6H14O	7.3119	1461.05	189.837	-50.15	313.05
2588	3-hexanol	C6H14O	7.38185	1516.14	201.443	36.128	306.15
2589	2-hexanone	C6H12O	7.24056	1522.85	221.597	-55.8	313.9

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2590	3-hexanone	C6H12O	7.19422	1482.66	220.234	-55.65	309.67
2591	hexatriacontane	C36H74	7.16373	2364.6	55.1	262.005	548.025
2592	1-hexatriacontene	C36H72	6.42412	1800	12	228.433	546
2593	hexatriacontylamine	C36H75N	8.73437	4718.85	273.15	407.575	583
2594	hexatriacontylbenzene	C42H78	6.71994	2100	14	260.902	583
2595	hexatriacontylcyclohexane	C42H84	6.68516	2100	14	260.587	588
2596	hexatriacontylcyclopentane	C41H82	5.04958	1379.63	104.138	282.048	582
2597	1-hexatriacontyne	C36H70	5.79493	1796.17	123.369	391.873	543
2598	1-hexene	C6H12	7.07214	1270.42	239.628	-139.76	230.88
2599	cis-2-hexene	C6H12	7.09973	1315.64	242.963	-141.15	239.85
2600	trans-2-hexene	C6H12	7.0103	1252.84	235.52	-132.98	239.85
2601	cis-3-hexene	C6H12	7.07141	1279.52	238.882	-137.82	235.85
2602	trans-3-hexene	C6H12	7.05706	1263.56	235.469	-113.42	235.85
2603	1-hexyl-[1,2,3,4-tetrahydronaphthalene]	C16H24	7.27463	2135.62	181.051	248.34	504.201
2604	2-hexyl-[1,2,3,4-tetrahydronaphthalene]	C16H24	7.27366	2152.93	180.101	252.857	510.923
2605	hexyl acetate	C8H16O2	7.47682	1820.45	224.594	-80.9	344.85
2606	hexylamine	C6H15N	7.34589	1579.36	222.214	-21.3	309.85
2607	hexylbenzene	C12H18	7.29541	1948.01	215.155	-61.15	424.85
2608	hexyl butanoate	C10H20O2	6.81383	1463.2	166.031	108.146	384.05
2609	hexylcyclohexane	C12H24	7.07462	1764.46	196.02	94	418.66
2610	hexylcyclopentane	C11H22	7.08212	1694.02	200.103	78	394.52
2611	1-hexylcyclopentene	C11H20	7.0991	1691.53	201	99.8785	392.334
2612	hexylene glycol	C6H14O2	8.61143	2229.3	191.516	-50	347.85

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2613	hexyl formate	C7H14O2	6.92151	1333.68	174.562	70.4022	339.15
2614	hexyl mercaptan	C6H14S	7.19912	1628.29	224.406	-80.53	349.85
2615	1-hexylnaphthalene	C16H20	7.40324	2323.85	191.851	-18	539.85
2616	2-hexylnaphthalene	C16H20	7.36137	2243.1	177.631	265.641	530.342
2617	hexyl propanoate	C9H18O2	6.88448	1438.51	169.299	96.7299	366.85
2618	1-hexyne	C6H10	7.21967	1336.56	236.713	-131.9	243.05
2619	2-hexyne	C6H10	6.89243	1229.19	221.889	-89.5	275.85
2620	3-hexyne	C6H10	7.01524	1318.15	237.623	-103.1	270.85
2621	hydracrylonitrile	C3H5NO	8.73052	2834.99	263.638	-46	416.85
2622	hydrazobenzene	C12H12N2	7.54296	2186.08	169.05	131	518.85
2623	hydrogen cyanide	CHN	8.02579	1608.28	286.893	-13.24	183.5
2624	p-hydroquinone	C6H6O2	8.09136	2463.24	187.741	171.5	548.85
2625	p-hydroxybenzaldehyde	C7H6O2	7.96259	2654.79	212.413	117	570.85
2626	hydroxycaproic acid	C6H12O3	8.39777	2557.41	160.705	60.85	484.85
2627	2-hydroxyethyl acrylate	C5H8O3	8.38431	2402.31	225.655	-60.15	388.85
2628	8-hydroxyquinoline	C9H7NO	7.50383	2097.73	186.907	72.85	514.85
2629	indane	C9H10	7.19185	1723.24	221.757	-51.41	411.75
2630	indene	C9H8	7.11961	1655.45	207.927	-1.45	413.85
2631	indole	C8H7N	7.18748	1870.12	181.239	0.53	516.85
2632	cis-1-iodo-1-butene	C4H7I	6.63024	1231.85	160.543	78.5059	412.93
2633	trans-1-iodo-1-butene	C4H7I	6.64197	1128.39	172.511	45.9637	349.944
2634	2-iodo-1-butene	C4H7I	6.61076	1115.7	172.271	45.0614	351.208
2635	3-iodo-1-butene	C4H7I	6.60308	1112.65	172.068	44.9944	352.275

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2636	4-iodo-1-butene	C4H7I	6.65789	1133.27	173.189	45.5565	346.372
2637	cis-1-iodo-1-decene	C10H19I	6.91334	1628.09	153.739	145.75	448.741
2638	trans-1-iodo-1-decene	C10H19I	6.91334	1628.09	153.739	145.75	448.741
2639	cis-1-iodo-1-dodecene	C12H23I	7.00642	1789.62	148.783	208.682	474.83
2640	trans-1-iodo-1-dodecene	C12H23I	7.00642	1789.62	148.783	208.682	474.83
2641	cis-1-iodo-1-eicosene	C20H39I	7.15514	2259.86	132.707	305.664	559.441
2642	trans-1-iodo-1-eicosene	C20H39I	7.15514	2259.86	132.707	305.664	559.441
2643	cis-1-iodo-1-heptadecene	C17H33I	7.16381	2130.27	138.38	274.16	529.583
2644	trans-1-iodo-1-heptadecene	C17H33I	7.16381	2130.27	138.38	274.16	529.583
2645	cis-1-iodo-1-heptene	C7H13I	6.76948	1377.62	162.266	98.0379	403.863
2646	trans-1-iodo-1-heptene	C7H13I	6.76948	1377.62	162.266	98.0379	403.863
2647	cis-1-iodo-1-hexadecene	C16H31I	7.14616	2070.62	140.453	261.91	518.672
2648	trans-1-iodo-1-hexadecene	C16H31I	7.14616	2070.62	140.453	261.91	518.672
2649	cis-1-iodo-1-hexene	C6H11I	6.72413	1293.37	165.524	80.9724	386.718
2650	trans-1-iodo-1-hexene	C6H11I	6.72413	1293.37	165.524	80.9724	386.718
2651	cis-1-iodo-1-nonadecene	C19H37I	7.16957	2224.29	134.633	295.633	549.305
2652	trans-1-iodo-1-nonadecene	C19H37I	7.16957	2224.29	134.633	295.633	549.305
2653	cis-1-iodo-1-nonene	C9H17I	6.86484	1546.84	156.261	130.844	435.47
2654	trans-1-iodo-1-nonene	C9H17I	6.86484	1546.84	156.261	130.844	435.47
2655	cis-1-iodo-1-octadecene	C18H35I	7.17203	2181.84	136.442	285.411	539.78
2656	trans-1-iodo-1-octadecene	C18H35I	7.17203	2181.84	136.442	285.411	539.78
2657	cis-1-iodo-1-octene	C8H15I	6.81674	1461.31	159.275	114.398	419.604
2658	trans-1-iodo-1-octene	C8H15I	6.81674	1461.31	159.275	114.398	419.604

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2659	cis-1-iodo-1-pentadecene	C15H29I	7.1202	2007.04	142.426	249.558	508.289
2660	trans-1-iodo-1-pentadecene	C15H29I	7.1202	2007.04	142.426	249.558	508.289
2661	cis-1-iodo-1-pentene	C5H9I	6.68153	1208.91	169.076	63.2111	368.023
2662	trans-1-iodo-1-pentene	C5H9I	6.68153	1208.91	169.076	63.2111	368.023
2663	2-iodo-1-pentene	C5H9I	6.65578	1149.14	174.061	47.8385	341.786
2664	3-iodo-1-pentene	C5H9I	6.64805	1145.23	173.967	47.5073	342.278
2665	4-iodo-1-pentene	C5H9I	6.64805	1145.23	173.967	47.5073	342.278
2666	5-iodo-1-pentene	C5H9I	6.69732	1218.44	169.256	64.1533	367.075
2667	cis-1-iodo-1-propene	C3H5I	6.61126	1016.02	180.169	17.726	309.637
2668	trans-1-iodo-1-propene	C3H5I	6.61126	1016.02	180.169	17.726	309.637
2669	2-iodo-1-propene	C3H5I	6.57705	1025.18	177.359	23.6604	324.429
2670	3-iodo-1-propene	C3H5I	6.91697	1287.53	216.99	20	322.66
2671	cis-1-iodo-1-tetradecene	C14H27I	7.08726	1940.44	144.3	237.13	498.421
2672	trans-1-iodo-1-tetradecene	C14H27I	7.08726	1940.44	144.3	237.13	498.421
2673	cis-1-iodo-1-tridecene	C13H25I	7.04904	1865.63	146.582	222.919	486.412
2674	trans-1-iodo-1-tridecene	C13H25I	7.04904	1865.63	146.582	222.919	486.412
2675	cis-1-iodo-1-undecene	C11H21I	6.96081	1710.19	151.164	193.576	462.299
2676	trans-1-iodo-1-undecene	C11H21I	6.96081	1710.19	151.164	193.576	462.299
2677	1-iodo-2,2-dimethylbutane	C6H13I	7.58102	1570.86	177.982	79.3726	321.151
2678	1-iodo-2,2-dimethylpropane	C5H11I	7.40715	1423.64	180.523	59.5495	307.774
2679	1-iodo-2,3-dimethylbutane	C6H13I	7.44317	1547.56	174.203	85.1924	341.039
2680	2-iodo-2,3-dimethylbutane	C6H13I	7.44743	1510.28	177.282	75.6833	324.835
2681	1-iodo-cis-2-butene	C4H7I	6.64055	1139.88	171.181	49.5794	356.943

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2682	1-iodo-trans-2-butene	C4H7I	6.64055	1139.88	171.181	49.5794	356.943
2683	2-iodo-cis-2-butene	C4H7I	6.59909	1079.28	175.313	35.4024	335.194
2684	2-iodo-trans-2-butene	C4H7I	6.59909	1079.28	175.313	35.4024	335.194
2685	3-iodo-2-ethyl-1-propene	C5H9I	6.65578	1149.14	174.061	47.8385	341.786
2686	1-iodo-2-ethylbutane	C6H13I	7.37958	1525.77	173.153	85.3445	346.566
2687	cis-1-iodo-2-methyl-1-butene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2688	trans-1-iodo-2-methyl-1-butene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2689	3-iodo-2-methyl-1-butene	C5H9I	6.59887	1144.98	171.101	52.4515	357.366
2690	4-iodo-2-methyl-1-butene	C5H9I	6.65372	1165.94	172.179	53.0535	351.692
2691	1-iodo-2-methyl-1-propene	C4H7I	6.59909	1079.28	175.313	35.4024	335.194
2692	3-iodo-2-methyl-1-propene	C4H7I	6.6172	1066.69	178.018	29.5067	320.958
2693	1-iodo-2-methyl-cis-2-butene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2694	1-iodo-2-methyl-trans-2-butene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2695	1-iodo-2-methylbutane	C5H11I	7.53791	1512.7	178.815	70.7719	316.762
2696	2-iodo-2-methylbutane	C5H11I	7.40919	1407.78	181.879	55.4375	300.64
2697	1-iodo-2-methylpentane	C6H13I	7.57656	1610.11	174.886	89.09	337.442
2698	2-iodo-2-methylpentane	C6H13I	7.44743	1510.28	177.282	75.6833	324.835
2699	3-iodo-2-methylpentane	C6H13I	7.51703	1544.67	177.384	78.3593	324.294
2700	1-iodo-2-methylpropane	C4H9I	7.50285	1405.79	183.749	49.5486	290.796
2701	2-iodo-2-methylpropane	C4H9I	6.76368	1210.96	211.863	42	314.75
2702	1-iodo-cis-2-pentene	C5H9I	6.6849	1180.08	172.264	54.3356	351.24
2703	1-iodo-trans-2-pentene	C5H9I	6.6849	1180.08	172.264	54.3356	351.24
2704	2-iodo-cis-2-pentene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654

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2705	2-iodo-trans-2-pentene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2706	3-iodo-cis-2-pentene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2707	3-iodo-trans-2-pentene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2708	4-iodo-cis-2-pentene	C5H9I	6.62978	1157.82	171.326	53.3765	356.177
2709	4-iodo-trans-2-pentene	C5H9I	6.62978	1157.82	171.326	53.3765	356.177
2710	5-iodo-cis-2-pentene	C5H9I	6.6849	1180.08	172.264	54.3356	351.24
2711	5-iodo-trans-2-pentene	C5H9I	6.6849	1180.08	172.264	54.3356	351.24
2712	1-iodo-3,3-dimethylbutane	C6H13I	7.51432	1568.33	175.476	84.3018	334.336
2713	2-iodo-3,3-dimethylbutane	C6H13I	7.38243	1500.38	175.298	78.7751	335.277
2714	cis-1-iodo-3-methyl-1-butene	C5H9I	6.62978	1157.82	171.326	53.3765	356.177
2715	trans-1-iodo-3-methyl-1-butene	C5H9I	6.62978	1157.82	171.326	53.3765	356.177
2716	2-iodo-3-methyl-1-butene	C5H9I	6.60102	1127.37	173.128	46.8926	346.694
7217	3-iodo-3-methyl-1-butene	C5H9I	6.53477	1095.72	172.634	44.0135	349.298
2718	4-iodo-3-methyl-1-butene	C5H9I	6.64805	1145.23	173.967	47.5073	342.278
2719	1-iodo-3-methyl-2-butene	C5H9I	6.63748	1161.77	171.426	53.7078	355.654
2720	2-iodo-3-methyl-2-butene	C5H9I	6.59059	1143.62	170.562	53.0867	360.203
2721	1-iodo-3-methylbutane	C5H11I	7.53703	1519.92	178.227	72.5878	319.858
2722	2-iodo-3-methylbutane	C5H11I	7.4757	1468.83	179.666	65.1967	312.283
2723	1-iodo-3-methylpentane	C6H13I	7.57438	1630.12	173.308	94.0437	345.746
2724	2-iodo-3-methylpentane	C6H13I	7.51703	1544.67	177.384	78.3593	324.294
2725	3-iodo-3-methylpentane	C6H13I	7.44743	1510.28	177.282	75.6833	324.835
2726	1-iodo-4-methylpentane	C6H13I	7.5747	1627.11	173.545	93.3007	344.501
2727	2-iodo-4-methylpentane	C6H13I	7.51657	1548.64	177.064	79.3566	325.979

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2728	iodobenzene	C6H5I	7.1286	1736.98	220.463	-31.32	448
2729	1-iodobutane	C4H9I	9.30096	3155.24	360.93	19.176	301.212
2730	2-iodobutane	C4H9I	7.50303	1404.5	183.858	49.2185	290.223
2731	1-iodododecane	C10H21I	9.52782	4189.76	366.622	124.682	427.204
2732	1-iododocosane	C22H45I	7.52371	2720.74	158.001	334.556	585.261
2733	1-iodododecane	C12H25I	9.47246	4307.24	355.238	153.142	457.419
2734	1-iododotriacontane	C32H65I	6.60042	2454.72	143.942	409.303	566
2735	1-iodoeicosane	C20H41I	8.08037	3214.07	211.144	242.798	560.809
2736	iodoform	CHI3	7.42936	2270.36	281.13	137	521.4
2737	1-iodoheneicosane	C21H43I	7.64434	2753.32	160.001	327.802	573.287
2738	1-iodohentriacontane	C31H63I	6.65151	2468.61	145.683	408.146	559
2739	1-iodoheptacosane	C27H55I	6.52165	2083.58	102.28	355.25	647.299
2740	1-iodoheptadecane	C17H35I	8.83561	3911.58	285.879	213.327	523.71
2741	1-iodoheptane	C7H15I	9.48545	3807.89	372.599	76.157	373.413
2742	1-iodoheptatriacontane	C37H75I	6.36369	2393.43	136.199	407.742	601
2743	1-iodohexacosane	C26H53I	6.92099	2492.79	150.001	356.562	639.837
2744	1-iodohexadecane	C16H33I	9.01052	4044.82	302.872	202.067	510.103
2745	1-iodohexane	C6H13I	9.44303	3626.39	371.287	58.2261	352.058
2746	2-iodohexane	C6H13I	7.5762	1613.44	174.623	89.9156	338.826
2747	3-iodohexane	C6H13I	7.57656	1610.11	174.886	89.09	337.442
2748	1-iodohexatriacontane	C36H73I	6.40862	2404.57	137.605	409.065	594
2749	1-iodononacosane	C29H59I	5.9734	1664.05	45.0763	365.242	686.206
2750	1-iodononadecane	C19H39I	8.35035	3459.86	237.569	233.138	547.795

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2751	1-iodononane	C9H19I	9.53154	4093.33	370.47	109.317	410.688
2752	1-iodononatriacontane	C39H79I	6.291	2378.05	134.336	401.969	613
2753	1-iodooctacosane	C28H57I	6.27013	1912.49	79.2691	363.429	670.585
2754	1-iodooctadecane	C18H37I	8.60077	3690.42	262.183	223.349	535.437
2755	1-iodooctane	C8H17I	9.51257	3959.7	371.972	93.1873	392.829
2756	1-iodooctatriacontane	C38H77I	6.32689	2385.47	135.226	405.103	607
2757	1-iodopentacosane	C25H51I	7.08693	2565.73	152.001	352.377	625.853
2758	1-iodopentadecane	C15H31I	9.23707	4272.69	328.202	190.513	498.303
2759	1-iodopentane	C5H11I	9.38224	3410.1	367.516	39.3087	328.259
2760	2-iodopentane	C5H11I	7.53911	1502.85	179.618	68.2958	312.539
2761	3-iodopentane	C5H11I	7.5383	1509.41	179.083	69.9466	315.354
2762	1-iodopentatriacontane	C35H71I	6.44741	2413.64	138.735	410.705	588
2763	1-iodopropane	C3H7I	7.32543	1566.19	249.929	-101.3	319.85
2764	2-iodopropane	C3H7I	7.20587	1433.28	241.89	-90	304.85
2765	1-iodotetracontane	C40H81I	6.256	2371.18	133.532	398.344	619
2766	1-iodotetracosane	C24H49I	7.24442	2631.26	154.001	347.724	612.734
2767	1-iodotetradecane	C14H29I	9.33822	4317.84	338.665	179.172	485.792
2768	1-iodotetratriacontane	C34H67I	6.49333	2424.13	140.036	412.758	581
2769	1-iodotriacontane	C30H61I	6.74173	2526.01	153.252	366.511	551
2770	1-iodotricosane	C23H47I	7.39061	2683.33	156.001	341.778	599.215
2771	1-iodotridecane	C13H27I	9.37559	4263.77	342.491	166.579	471.256
2772	1-iodotritriacontane	C33H67I	6.54301	2438.7	141.91	410.832	574
2773	1-iodoundecane	C11H23I	9.51548	4271.88	362.373	139.288	442.843

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2774	isobutane	C4H10	6.93388	953.92	247.077	-159.61	134.99
2775	isobutanol	C4H10O	7.45936	1386.1	195.079	-108	274.58
2776	isobutene	C4H8	6.99506	984.226	246.124	-140.34	144.75
2777	isobutyl acetate	C6H12O2	7.42094	1584.82	232.421	-98.85	287.85
2778	isobutyl acrylate	C7H12O2	7.28452	1545.97	219.06	-61.15	306.85
2779	isobutylamine	C4H11N	7.31147	1329.9	232.428	-84.6	240.58
2780	isobutylbenzene	C10H14	7.22936	1726.18	224.166	-51.45	377
2781	isobutyl butanoate	C8H16O2	7.12551	1576.62	214.532	50.4729	337.85
2782	isobutylcyclopentane	C9H18	6.95436	1461.75	210.89	34.6027	344.06
2783	isobutyl formate	C5H10O2	7.48932	1586.24	246.128	-95.8	278.2
2784	isobutyl isobutyrate	C8H16O2	7.13476	1554.49	217.922	-80.7	328.85
2785	isobutyl isocyanide	C5H9N	6.89754	1180.5	183.897	33.8913	290.016
2786	isobutyl mercaptan	C4H10S	7.13583	1389.59	238.087	-144.84	285.85
2787	1-isobutyl naphthalene	C14H16	7.38845	2212.41	211.314	135	499.531
2788	2-isobutyl naphthalene	C14H16	8.51736	3993.45	396.231	135	545.337
2789	2-isobutylphenol	C10H14O	7.18027	1727.74	165	150.206	459.849
2790	3-isobutylphenol	C10H14O	7.18027	1727.74	165	150.206	459.849
2791	4-isobutylphenol	C10H14O	7.18049	1728.47	165	150.327	460.064
2792	isobutyl propanoate	C7H14O2	6.73991	1194.11	172.829	35.2085	318.85
2793	isobutyraldehyde	C4H8O	7.27632	1294.63	230.435	-65	233.85
2794	isobutyric acid	C4H8O2	7.83371	1878.15	224.503	-46	336
2795	isobutyronitrile	C4H7N	7.22199	1443.15	228.824	-71.45	291.85
2796	isodecanol	C10H22O	8.0139	2167.2	202.353	-60	370.85

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2797	isopentane	C5H12	7.03015	1140.45	247.012	-159.9	187.28
2798	isopentyl acetate	C7H14O2	7.19136	1566.48	221.306	-78.5	325.85
2799	isopentyl formate	C6H12O2	7.20108	1483.57	219.297	19.9463	304.85
2800	isopentyl isovalerate	C10H20O2	7.75828	2194.42	255.911	-58.15	363.85
2751	1-iodononane	C9H19I	9.53154	4093.33	370.47	109.317	410.688
2752	1-iodononatriacontane	C39H79I	6.291	2378.05	134.336	401.969	613
2753	1-iodooctacosane	C28H57I	6.27013	1912.49	79.2691	363.429	670.585
2754	1-iodooctadecane	C18H37I	8.60077	3690.42	262.183	223.349	535.437
2755	1-iodooctane	C8H17I	9.51257	3959.7	371.972	93.1873	392.829
2756	1-iodooctatriacontane	C38H77I	6.32689	2385.47	135.226	405.103	607
2757	1-iodopentacosane	C25H51I	7.08693	2565.73	152.001	352.377	625.853
2758	1-iodopentadecane	C15H31I	9.23707	4272.69	328.202	190.513	498.303
2759	1-iodopentane	C5H11I	9.38224	3410.1	367.516	39.3087	328.259
2760	2-iodopentane	C5H11I	7.53911	1502.85	179.618	68.2958	312.539
2761	3-iodopentane	C5H11I	7.5383	1509.41	179.083	69.9466	315.354
2762	1-iodopentatriacontane	C35H71I	6.44741	2413.64	138.735	410.705	588
2763	1-iodopropane	C3H7I	7.32543	1566.19	249.929	-101.3	319.85
2764	2-iodopropane	C3H7I	7.20587	1433.28	241.89	-90	304.85
2765	1-iodotetracontane	C40H81I	6.256	2371.18	133.532	398.344	619
2766	1-iodotetracosane	C24H49I	7.24442	2631.26	154.001	347.724	612.734
2767	1-iodotetradecane	C14H29I	9.33822	4317.84	338.665	179.172	485.792
2768	1-iodotetraatriacontane	C34H67I	6.49333	2424.13	140.036	412.758	581
2769	1-iodotriacontane	C30H61I	6.74173	2526.01	153.252	366.511	551

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2770	1-iodotricosane	C23H47I	7.39061	2683.33	156.001	341.778	599.215
2771	1-iodotridecane	C13H27I	9.37559	4263.77	342.491	166.579	471.256
2772	1-iodotritriacontane	C33H67I	6.54301	2438.7	141.91	410.832	574
2773	1-iodoundecane	C11H23I	9.51548	4271.88	362.373	139.288	442.843
2774	isobutane	C4H10	6.93388	953.92	247.077	-159.61	134.99
2775	isobutanol	C4H10O	7.45936	1386.1	195.079	-108	274.58
2776	isobutene	C4H8	6.99506	984.226	246.124	-140.34	144.75
2777	isobutyl acetate	C6H12O2	7.42094	1584.82	232.421	-98.85	287.85
2778	isobutyl acrylate	C7H12O2	7.28452	1545.97	219.06	-61.15	306.85
2779	isobutylamine	C4H11N	7.31147	1329.9	232.428	-84.6	240.58
2780	isobutylbenzene	C10H14	7.22936	1726.18	224.166	-51.45	377
2781	isobutyl butanoate	C8H16O2	7.12551	1576.62	214.532	50.4729	337.85
2782	isobutylcyclopentane	C9H18	6.95436	1461.75	210.89	34.6027	344.06
2783	isobutyl formate	C5H10O2	7.48932	1586.24	246.128	-95.8	278.2
2784	isobutyl isobutyrate	C8H16O2	7.13476	1554.49	217.922	-80.7	328.85
2785	isobutyl isocyanide	C5H9N	6.89754	1180.5	183.897	33.8913	290.016
2786	isobutyl mercaptan	C4H10S	7.13583	1389.59	238.087	-144.84	285.85
2787	1-isobutyl naphthalene	C14H16	7.38845	2212.41	211.314	135	499.531
2788	2-isobutyl naphthalene	C14H16	8.51736	3993.45	396.231	135	545.337
2789	2-isobutylphenol	C10H14O	7.18027	1727.74	165	150.206	459.849
2790	3-isobutylphenol	C10H14O	7.18027	1727.74	165	150.206	459.849
2791	4-isobutylphenol	C10H14O	7.18049	1728.47	165	150.327	460.064
2792	isobutyl propanoate	C7H14O2	6.73991	1194.11	172.829	35.2085	318.85

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2793	isobutyraldehyde	C4H8O	7.27632	1294.63	230.435	-65	233.85
2794	isobutyric acid	C4H8O2	7.83371	1878.15	224.503	-46	336
2795	isobutyronitrile	C4H7N	7.22199	1443.15	228.824	-71.45	291.85
2796	isodecanol	C10H22O	8.0139	2167.2	202.353	-60	370.85
2797	isopentane	C5H12	7.03015	1140.45	247.012	-159.9	187.28
2798	isopentyl acetate	C7H14O2	7.19136	1566.48	221.306	-78.5	325.85
2799	isopentyl formate	C6H12O2	7.20108	1483.57	219.297	19.9463	304.85
2800	isopentyl isovalerate	C10H20O2	7.75828	2194.42	255.911	-58.15	363.85
2851	malononitrile	C3H2N2	7.81263	2293.92	246.777	31.84	441.85
2852	3-mercaptopropionic acid	C3H6O2S	7.89705	2241.03	218.905	17.5	455.85
2853	mesitylene	C9H12	7.26105	1695.83	222.415	-44.69	364.21
2854	mesityl oxide	C6H10O	7.11665	1480.62	219.745	-53	326.85
2855	meso-2,3-butanediol	C4H10O2	9.47429	2979.26	273	99.5396	335.921
2856	meso-2,3-dibromobutane	C4H8Br2	7.01039	1339.81	167.143	74.9947	378.198
2857	meso-2,3-dichlorobutane	C4H8Cl2	6.67983	1117.89	178.257	36.6093	319.7
2858	meso-2,3-dimethyl-1,4-butanediol	C6H14O2	9.53875	3307.6	273	137.289	379.562
2859	meso-2,4-dimethyl-1,5-pentanediol	C7H16O2	9.56529	3396.12	273	146.887	386.957
2860	meso-2,4-pentanediol	C5H12O2	9.50761	3141.1	273	118.147	357.296
2861	methacrolein	C4H6O	7.12901	1298.1	237.564	-81	256.85
2862	2-methacrylamide	C4H7NO	7.40149	1843.79	193.007	110.5	467.85
2863	methacrylic acid	C4H6O2	7.31085	1534.44	185.373	15	369.85
2864	methacrylonitrile	C4H5N	7.31473	1521.42	252.833	-35.8	280.85
2865	methane	CH4	6.84566	435.621	271.361	-182.48	-82.57

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2866	methanesulfonic acid	CH4O3S	9.21833	3354.46	241.453	19.66	287.85
2867	methoxyacetic acid	C3H6O3	7.65398	1849.97	182.467	7.85	417.85
2868	2-methoxyethanol	C3H8O2	8.09715	1805.18	221.663	-85.1	290.85
2869	2-(2-methoxyethoxy)ethanol	C5H12O3	8.28868	2210.73	215.198	-23.15	356.85
2870	p-methoxyphenol	C7H8O2	7.5936	2038.72	189.743	55.85	484.85
2871	3-methoxypropionitrile	C4H7NO	7.543	1855.32	232.101	-63.03	364.85
2872	2-methyl-(1-thiaethyl)-benzene	C8H10S	7.1366	1740.11	199.152	139.616	445.801
2873	3-methyl-(1-thiaethyl)-benzene	C8H10S	7.1366	1740.11	199.152	139.616	445.801
2874	4-methyl-(1-thiaethyl)-benzene	C8H10S	7.13486	1764.45	197.77	145.852	456.625
2875	3-methyl-(1-thiapropyl)-benzene	C9H12S	7.1742	1787.73	197.39	148.117	444.594
2876	4-methyl-(1-thiapropyl)-benzene	C9H12S	7.17396	1791.1	197.2	148.976	446.053
2877	methyl-1,1-dimethylpropylamine	C6H15N	6.82068	1158.51	183.579	33.2266	291.69
2878	2-methyl-1,1-diphenylethane	C15H16	7.18886	2038.09	184.09	232.883	514.576
2879	3-methyl-1,1-diphenylethane	C15H16	7.18905	2034.7	184.28	231.981	513.174
2880	4-methyl-1,1-diphenylethane	C15H16	7.18866	2041.49	183.9	233.785	515.977
2881	3-methyl-1,2-butadiene	C5H8	6.9337	1119.33	235.331	-113.62	216.85
2882	2-methyl-1,2-butanediol	C5H12O2	9.41665	3019.56	273	107.319	344.391
2883	3-methyl-1,2-butanediol	C5H12O2	9.50761	3134.47	273	117.322	355.966
2884	methyl-1,2-dimethylpropylamine	C6H15N	6.9412	1208.83	184.452	36.7795	287.097
2885	2-methyl-1,2-diphenylethane	C15H16	7.24367	2092.3	182.57	240.745	520.629
2886	3-methyl-1,2-diphenylethane	C15H16	7.24386	2088.85	182.76	239.842	519.237
2887	4-methyl-1,2-diphenylethane	C15H16	7.24543	2061.32	184.28	232.62	508.099
2888	2-methyl-1,2-hexanediol	C7H16O2	9.48101	3261.16	273	134.447	371.479

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2889	3-methyl-1,2-pentadiene	C6H10	6.9164	1193.32	225.7	-6.31012	255.692
2890	4-methyl-1,2-pentadiene	C6H10	6.90404	1189.67	225.7	-6.48388	254.893
2891	2-methyl-1,2-pentanediol	C6H14O2	9.4508	3218.31	273	130.616	373.371
2892	2-methyl-1,2-propanediol	C4H10O2	9.381	2931.59	273	97.9045	338.06
2893	2-methyl-1,3-butanediol	C5H12O2	11.3636	5013.74	391.049	108.657	342.005
2894	3-methyl-1,3-butanediol	C5H12O2	9.42897	3090.73	273	115.681	358.863
2895	2-methyl-1,cis-3-pentadiene	C6H10	6.89808	1207.43	224.56	-1.82649	262.047
2896	2-methyl-1,trans-3-pentadiene	C6H10	6.89808	1207.43	224.56	-1.82649	262.047
2897	3-methyl-1,cis-3-pentadiene	C6H10	6.89766	1210.56	224.37	-1.04225	263.58
2898	3-methyl-1,trans-3-pentadiene	C6H10	6.89766	1210.56	224.37	-1.04225	263.58
2899	4-methyl-1,3-pentadiene	C6H10	6.89795	1208.37	224.503	-1.59122	262.507
2900	2-methyl-1,3-pentanediol	C6H14O2	9.53873	3284.36	273	134.406	374.978
2901	3-methyl-1,3-pentanediol	C6H14O2	9.45078	3172.18	273	124.832	364.108
2902	1-methyl-1,3-propanediol	C4H10O2	9.55716	3251.38	273	129.397	379.822
2903	2-methyl-1,4-butanediol	C5H12O2	9.50757	3068.19	273	109.069	342.67
2904	2-methyl-1,4-pentadiene	C6H10	6.925	1130.35	229.5	-22.0156	220.238
2905	3-methyl-1,4-pentadiene	C6H10	6.91499	1143.89	228.55	-18.1936	228.675
2906	4-methyl-1,4-pentanediol	C6H14O2	9.45081	3246.9	273	134.201	379.11
2907	4-methyl-1,5-hexanediol	C7H16O2	9.56529	3396.12	273	146.887	386.957
2908	5-methyl-1,5-hexanediol	C7H16O2	9.48101	3261.16	273	134.447	371.479
2909	2-methyl-1,5-pentanediol	C6H14O2	9.53875	3307.6	273	137.289	379.562
2910	3-methyl-1,5-pentanediol	C6H14O2	9.61613	3511.8	273	158.477	408.855
2911	3-methyl-1,6-hexanediol	C7H16O2	9.6387	3279.47	273	128.818	354.832

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2912	2-methyl-1-butanethiol	C5H12S	7.07323	1438.31	224.075	12.752	317.85
2913	3-methyl-1-butanethiol	C5H12S	6.76876	1261.91	206.224	12.5243	330.85
2914	2-methyl-1-butanol	C5H12O	7.43675	1395.79	177.668	-70.15	291.85
2915	3-methyl-1-butanol	C5H12O	7.50977	1559.43	205.685	-112.15	306.3
2916	2-methyl-1-butene	C5H10	6.9903	1118.31	240.98	-137.57	191.85
2917	3-methyl-1-butene	C5H10	7.0492	1117.71	248.08	-168.49	177.22
2918	2-methyl-1-butene-3-yne	C5H6	6.92374	1110.19	242.35	-113	218.85
2919	3-methyl-1-butyne	C5H8	7.23284	1184.88	243.26	-89.7	190.05
2920	2-methyl-1-decene	C11H22	7.11965	1667.84	202.767	69.7718	364.528
2921	2-methyl-1-dodecene	C13H26	7.19556	1839.61	195.053	101.87	400.725
2922	1-methyl-1-ethylcyclohexane	C9H18	7.04666	1592.23	230.051	41.1735	360.23
2923	1-methyl-1-ethylcyclopentane	C8H16	7.21303	1573.21	241.621	-138.15	308.85
2924	1-methyl-1-ethylcyclopropane	C6H12	6.95009	1159.68	228.214	6.06031	234.79
2925	2-methyl-1-ethylnaphthalene	C13H14	7.279	2055.64	194.383	133	497.633
2926	methyl-1-ethylpropylamine	C6H15N	6.94496	1182.68	187.003	29.2943	273.671
2927	2-methyl-1-heptadecene	C18H36	7.31191	2189.63	179.15	167.754	472.271
2928	2-methyl-1-heptanol	C8H18O	8.3426	2344.8	253.71	65.6318	329.779
2929	3-methyl-1-heptanol	C8H18O	8.25743	2311.67	243.95	74.5755	343.752
2930	4-methyl-1-heptanol	C8H18O	8.25322	2293.32	243.671	72.5093	339.99
2931	5-methyl-1-heptanol	C8H18O	7.95729	2018.72	211.061	79.0974	344.558
2932	6-methyl-1-heptanol	C8H18O	7.67593	1763.38	180.045	84.0951	346.036
2933	2-methyl-1-heptene	C8H16	7.07956	1448.12	225.593	12.6015	295.384
2934	3-methyl-1-heptene	C8H16	7.03175	1381.24	221.753	7.2414	284.108

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2935	4-methyl-1-heptene	C8H16	7.03707	1392.19	222.163	8.4443	286.719
2936	5-methyl-1-heptene	C8H16	7.0398	1396.3	222.431	8.75209	287.445
2937	6-methyl-1-heptene	C8H16	7.03956	1395.74	222.416	8.68399	287.3
2938	2-methyl-1-hexadecene	C17H34	7.30228	2131.15	182	156.155	459.442
2939	2-methyl-1-hexanol	C7H16O	7.62555	1642.6	183.193	64.7251	321.265
2940	3-methyl-1-hexanol	C7H16O	7.42439	1506.24	159.509	74.9471	333.53
2941	4-methyl-1-hexanol	C7H16O	7.46454	1542.97	163.619	75.0629	334.893
2942	5-methyl-1-hexanol	C7H16O	7.704	1748.87	190.596	20	331.85
2943	2-methyl-1-hexene	C7H14	7.06007	1357.85	233.064	-102.87	264.85
2944	3-methyl-1-hexene	C7H14	7.05288	1319.14	232.284	-128.15	254.85
2945	4-methyl-1-hexene	C7H14	7.14435	1400.33	241.714	-141.45	260.85
2946	5-methyl-1-hexene	C7H14	6.97852	1268.49	224.251	-12.0765	257.504
2947	3-methyl-1-hexyne	C7H12	6.88617	1210.72	217.275	-5.24181	269.119
2948	4-methyl-1-hexyne	C7H12	6.88592	1230.8	216.308	-0.748416	278.204
2949	5-methyl-1-hexyne	C7H12	6.8861	1233.82	216.197	-0.116222	279.491
2950	1-methyl-1-isopropylcyclopentane	C9H18	6.89912	1442.09	210.88	55.09	352.9
2951	2-methyl-1-isopropyl-naphthalene	C14H16	7.89318	3035.91	293.423	147	544.392
2952	methyl-1-methylbutylamine	C6H15N	6.9412	1208.83	184.452	36.7795	287.097
2953	2-methyl-1-nonadecene	C20H40	7.30164	2281.24	174.02	187.986	495.604
2954	2-methyl-1-nonanol	C10H22O	8.61882	2840.31	273	124.708	375.62
2955	4-methyl-1-nonanol	C10H22O	8.88007	3050.97	292.558	118.16	364.941
2956	5-methyl-1-nonanol	C10H22O	8.61879	2793.54	273	118.16	364.941
2957	7-methyl-1-nonanol	C10H22O	8.61879	2793.54	273	118.16	364.941

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2958	3-methyl-1-nonanol	C10H22O	8.61879	2793.54	273	118.16	364.941
2959	2-methyl-1-nonene	C10H20	7.0804	1576.54	207.004	52.2784	343.759
2960	2-methyl-1-octadecene	C19H38	7.3121	2239.97	176.49	178.379	484.308
2961	2-methyl-1-octanol	C9H20O	8.57328	2691.68	273	106.315	354.083
2962	3-methyl-1-octanol	C9H20O	8.57328	2691.68	273	106.315	354.083
2963	4-methyl-1-octanol	C9H20O	8.57328	2691.68	273	106.315	354.083
2964	5-methyl-1-octanol	C9H20O	8.57328	2691.68	273	106.315	354.083
2965	6-methyl-1-octanol	C9H20O	8.57329	2726.7	273	111.249	362.238
2966	7-methyl-1-octanol	C9H20O	8.57329	2726.7	273	111.249	362.238
2967	2-methyl-1-octene	C9H18	7.04178	1482	211.517	33.7749	320.846
2968	2-methyl-1-pentadecene	C16H32	7.28454	2065.52	185.04	143.627	445.766
2969	2-methyl-1-pentanol	C6H14O	7.89558	1844.53	219.821	-50.15	308.85
2970	3-methyl-1-pentanol	C6H14O	7.22812	1389.6	167.247	55.8706	330.05
2971	4-methyl-1-pentanol	C6H14O	7.12665	1312.92	157.425	56.8714	330.35
2972	2-methyl-1-pentene	C6H12	6.96749	1218.09	235.963	-135.73	233.85
2973	3-methyl-1-pentene	C6H12	7.07154	1245.54	243.032	-152.95	221.85
2974	4-methyl-1-pentene	C6H12	7.00315	1215.15	240.912	-153.64	222.85
2975	3-methyl-1-pentyne	C6H10	6.85717	1114.1	222.482	-26.373	239.667
2976	4-methyl-1-pentyne	C6H10	6.85559	1124.6	221.764	-23.7527	245.046
2977	cis-(1-methyl-1-propenyl)benzene	C10H12	7.01598	1571.12	205.94	77.7132	387.698
2978	trans-(1-methyl-1-propenyl)benzene	C10H12	7.01051	1638.28	202.007	94.0646	418.29
2979	(2-methyl-1-propenyl)benzene	C10H12	7.01225	1616.25	203.297	88.701	408.255
2980	1-methyl-1-propylcyclopentane	C9H18	6.95411	1455.23	211.26	54.438	344.884

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2981	2-methyl-1-propylnaphthalene	C14H16	8.69093	4211.46	412.589	135	539.195
2982	2-methyl-1-tetradecene	C15H30	7.26001	1993.72	188.27	130.214	431.18
2983	2-methyl-1-tridecene	C14H28	7.39515	1993.08	191.5	120.155	416.933
2984	2-methyl-1-undecene	C12H24	7.15844	1755.52	198.796	86.2632	383.381
2985	methyl-2,2-dimethylpropylamine	C6H15N	6.82068	1158.51	183.579	33.2266	291.69
2986	2-methyl-2,3-butanediol	C5H12O2	9.33578	2885.37	273	94.158	327.455
2987	1-methyl-2,3-diethylbenzene	C11H16	7.12204	1723.41	199.746	118.045	407.686
2988	2-methyl-2,3-pentadiene	C6H10	6.90066	1195.18	225.32	-4.95083	260.942
2989	2-methyl-2,3-pentanediol	C6H14O2	9.37249	3282.26	273	142.719	397.347
2990	3-methyl-2,3-pentanediol	C6H14O2	9.37249	3282.26	273	142.719	397.347
2991	1-methyl-2,4-diethylbenzene	C11H16	7.12246	1718.08	200.05	116.735	405.416
2992	2-methyl-2,4-hexanediol	C7H16O2	9.4059	3372.69	273	152.373	404.124
2993	3-methyl-2,4-hexanediol	C7H16O2	9.4909	3508.9	273	164.858	419.438
2994	4-methyl-2,4-hexanediol	C7H16O2	9.4059	3372.69	273	152.373	404.124
2995	5-methyl-2,4-hexanediol	C7H16O2	9.4909	3508.9	273	164.858	419.438
2996	2-methyl-2,4-pentanediol	C6H14O2	9.37239	3054.29	273	113.85	350.801
2997	3-methyl-2,4-pentanediol	C6H14O2	6.80996	1158.1	83.2459	155.22	412.628
2998	1-methyl-2,5-diethylbenzene	C11H16	7.12191	1725.07	199.651	118.455	408.396
2999	2-methyl-2,5-hexanediol	C7H16O2	9.4059	3372.69	273	152.373	404.124
3000	1-methyl-2,6-diethyl benzene	C11H16	7.12148	1730.74	199.328	119.848	410.808
3001	1-methyl-2-(1-methylethenyl)benzene	C10H12	7.08891	1592.69	206.282	77.5292	373.961
3002	cis-1-methyl-2-(1-propenyl)benzene	C10H12	7.05035	1646.38	202.44	92.969	409.46
3003	2-methyl-2-butanethiol	C5H12S	6.89364	1290.08	222.36	-3	292.85

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3004	3-methyl-2-butanethiol	C5H12S	7.01231	1383.58	225.124	4.99971	305.85
3005	3-methyl-2-butanol	C5H12O	6.89288	1154.86	176.346	-85.15	300.85
3006	2-methyl-2-butene	C5H10	7.098	1184.97	242.425	-133.76	197.85
3007	trans-2-methyl-2-butenoic acid	C5H8O2	6.65803	1199.04	118.94	92.9783	433.113
3008	cis-2-methyl-2-butenoic acid	C5H8O2	6.70775	1207.06	130.413	81.0655	412.898
3009	3-methyl-2-butenoic acid	C5H8O2	6.727	1250.36	130.09	88.2367	427.872
3010	1-methyl-2-butylbenzene	C11H16	7.12979	1731.38	199.48	119.325	410.519
3011	1-methyl-2-sec-butylbenzene	C11H16	7.07699	1669.07	201.76	108.59	398.202
3012	1-methyl-2-tert-butyl benzene	C11H16	6.95995	1637.22	200.915	110.286	414.58
3013	2-methyl-2-ethyl-1,3-propanediol	C6H14O2	9.45083	3277.13	273	137.991	385.18
3014	2-methyl-2-ethyl-1-butanol	C7H16O	7.25486	1374.63	157.27	62.5	320.014
3015	3-methyl-2-ethyl-1-butanol	C7H16O	7.77355	1798.76	205.638	59.9179	323.366
3016	3-methyl-2-ethyl-1-butene	C7H14	6.90882	1239.76	221.419	-11.6047	262.673
3017	1-methyl-2-ethyl-1-hexanol	C9H20O	8.50273	2596.48	273	96.5739	342.524
3018	3-methyl-2-ethyl-1-hexanol	C9H20O	8.5301	2646.23	275.418	99.7749	347.855
3019	4-methyl-2-ethyl-1-hexanol	C9H20O	8.50275	2631.07	273	101.495	350.72
3020	5-methyl-2-ethyl-1-hexanol	C9H20O	8.50274	2618.98	273	99.7749	347.855
3021	2-methyl-2-ethyl-1-pentanol	C8H18O	7.60887	1726.89	188.143	73.1558	338.384
3022	3-methyl-2-ethyl-1-pentanol	C8H18O	8.45081	2505.66	273	63.294	334.713
3023	4-methyl-2-ethyl-1-pentanol	C8H18O	7.81361	1874.62	203.533	71.5966	334.24
3024	3-methyl-2-ethyl-1-pentene	C8H16	6.91701	1311.24	213.37	8.23484	288.352
3025	4-methyl-2-ethyl-1-pentene	C8H16	6.94182	1327.67	216.631	6.81365	286.601
3026	1-methyl-cis-2-ethylcyclohexane	C9H18	6.86386	1438.48	205.051	47.8583	358.876

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3027	1-methyl-trans-2-ethylcyclohexane	C9H18	6.8615	1421.58	205.419	44.6224	352.397
3028	1-methyl-cis-2-ethylcyclopentane	C8H16	6.93565	1405.78	218.642	18.1947	324.189
3029	1-methyl-trans-2-ethylcyclopentane	C8H16	6.94761	1392.25	221.146	12.9398	313.99
3030	1-methyl-cis-2-ethylcyclopropane	C6H12	6.93943	1190.3	226.268	14.7118	245.382
3031	1-methyl-trans-2-ethylcyclopropane	C6H12	6.94328	1163.96	227.855	7.6076	232.654
3032	1-methyl-2-ethylnaphthalene	C13H14	7.28826	2077.74	195.416	135	501.867
3033	4-methyl-2-ethylphenol	C9H12O	7.17063	1661.88	165	138.724	446.604
3034	3-methyl-2-ethylthiophene	C7H10S	7.09708	1557.53	208.41	97.1631	378.85
3035	2-methyl-2-heptanol	C8H18O	7.47686	1538.11	177.959	59.5184	310.676
3036	3-methyl-2-heptanol	C8H18O	8.4637	2459.13	274.376	55.1022	320.192
3037	4-methyl-2-heptanol	C8H18O	7.91215	1944.7	214.918	66.4276	327.621
3038	5-methyl-2-heptanol	C8H18O	8.14773	2171.02	240.298	63.4364	328.026
3039	6-methyl-2-heptanol	C8H18O	7.75764	1804.95	198.206	68.8906	328.026
3040	2-methyl-2-heptene	C8H16	7.05896	1450.88	224.654	14.806	302.07
3041	3-methyl-cis-2-heptene	C8H16	7.05859	1448.35	224.68	14.3774	301.198
3042	3-methyl-trans-2-heptene	C8H16	7.05859	1448.35	224.68	14.3774	301.198
3043	4-methyl-cis-2-heptene	C8H16	7.01426	1385.39	221.166	9.18486	290.336
3044	4-methyl-trans-2-heptene	C8H16	7.01426	1385.39	221.166	9.18486	290.336
3045	5-methyl-cis-2-heptene	C8H16	7.02922	1412.53	222.499	11.7813	296.158
3046	5-methyl-trans-2-heptene	C8H16	7.02922	1412.53	222.499	11.7813	296.158
3047	6-methyl-cis-2-heptene	C8H16	7.02543	1405.67	222.156	11.1337	294.703
3048	6-methyl-trans-2-heptene	C8H16	7.02543	1405.67	222.156	11.1337	294.703
3049	2-methyl-2-hexanol	C7H16O	7.56106	1573.52	193.405	46.4225	300.433

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3050	3-methyl-2-hexanol	C7H16O	8.03712	1995.65	235.031	48.558	309.658
3051	4-methyl-2-hexanol	C7H16O	7.2193	1301.26	148.933	60.2954	308.287
3052	5-methyl-2-hexanol	C7H16O	7.81367	1788.52	211.573	50.9171	308.287
3053	3-methyl-2-hexanone	C7H14O	7.72556	2000.88	273	47.2208	320.71
3054	4-methyl-2-hexanone	C7H14O	7.21533	1515.46	210.625	33.2005	319.273
3055	5-methyl-2-hexanone	C7H14O	7.25964	1590.91	218.518	-73.9	327.85
3056	2-methyl-2-hexene	C7H14	7.00221	1327.58	226.709	-5.52712	273.615
3057	3-methyl-cis-2-hexene	C7H14	7.00901	1339.87	227.305	-4.32858	276.36
3058	3-methyl-trans-2-hexene	C7H14	7.00139	1326.08	226.639	-5.67673	273.274
3059	4-methyl-cis-2-hexene	C7H14	6.95452	1260.55	223.124	-11.4288	260.895
3060	4-methyl-trans-2-hexene	C7H14	6.95918	1268.64	223.505	-10.6165	262.754
3061	5-methyl-cis-2-hexene	C7H14	6.96645	1281.3	224.11	-9.35981	265.634
3062	5-methyl-trans-2-hexene	C7H14	6.9614	1272.35	223.695	-10.264	263.569
3063	4-methyl-2-hexyne	C7H12	6.8449	1242.3	213.849	5.29906	294.901
3064	5-methyl-2-hexyne	C7H12	6.84669	1253.52	213.616	7.44112	299.352
3065	4-methyl-2-isobutyl-1-pentanol	C10H22O	8.47589	2668.85	273	108.331	356.78
3066	1-methyl-2-isobutylbenzene	C11H16	7.07699	1669.07	201.76	108.59	398.202
3067	3-methyl-2-isopropyl-1-butanol	C8H18O	8.37846	2451.95	273	59.3119	332.862
3068	3-methyl-2-isopropyl-1-butene	C8H16	6.82481	1237.38	209.737	2.69523	281.74
3069	4-methyl-2-isopropyl-1-hexanol	C10H22O	8.47588	2652.06	273	105.933	352.819
3070	5-methyl-2-isopropyl-1-hexanol	C10H22O	8.4822	2722.28	273	115.614	369.701
3071	4-methyl-2-isopropyl-1-pentanol	C9H20O	8.42617	2550.87	273	94.081	342.106
3072	1-methyl-cis-2-isopropylcyclopentane	C9H18	6.88901	1438.46	210.88	54.9166	345.87

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3073	1-methyl-trans-2-isopropylcyclopentane	C9H18	6.89117	1416.5	212.21	49.4238	335.581
3074	3-methyl-2-isopropyl-naphthalene	C14H16	7.89318	3035.91	293.423	147	544.392
3075	3-methyl-2-isopropylphenol	C10H14O	7.1575	1680.74	165	142.91	446.196
3076	4-methyl-2-isopropylphenol	C10H14O	7.1575	1680.74	165	142.91	446.196
3077	5-methyl-2-isopropylphenol	C10H14O	7.16423	1702.66	165	146.542	452.655
3078	methyl-2-methylbutylamine	C6H15N	6.9412	1208.83	184.452	36.7795	287.097
3079	2-methyl-2-nonanol	C10H22O	8.4747	2723.39	273	116.189	370.783
3080	3-methyl-2-nonanol	C10H22O	8.55074	2760.4	273	117.239	367.824
3081	5-methyl-2-nonanol	C10H22O	8.55074	2760.4	273	117.239	367.824
3082	6-methyl-2-nonanol	C10H22O	8.55074	2760.4	273	117.239	367.824
3083	7-methyl-2-nonanol	C10H22O	8.55074	2760.4	273	117.239	367.824
3084	8-methyl-2-nonanol	C10H22O	8.55074	2760.4	273	117.239	367.824
3085	2-methyl-2-octanol	C9H20O	8.42443	2500.17	273	86.8761	331.095
3086	3-methyl-2-octanol	C9H20O	8.50271	2551.5	273	90.172	331.863
3087	5-methyl-2-octanol	C9H20O	8.50271	2551.5	273	90.172	331.863
3088	7-methyl-2-octanol	C9H20O	8.50271	2551.5	273	90.172	331.863
3089	4-methyl-2-pentanol	C6H14O	7.55995	1625.62	215.719	-90.15	301.25
3090	2-methyl-2-pentanol	C6H14O	7.18816	1283.65	176.604	30.8326	286.35
3091	3-methyl-2-pentanol	C6H14O	7.17326	1316.3	172.445	40.7812	304.85
3092	3-methyl-2-pentanone	C6H12O	7.09264	1420.94	219.968	13.2536	306.75
3093	4-methyl-2-pentanone	C6H12O	7.15329	1421.73	216.266	-84	298.25
3094	3-methyl-trans-2-pentene	C6H12	6.89621	1180.05	223.43	-23	247.85
3095	2-methyl-2-pentene	C6H12	6.9866	1245.72	236.107	-135.08	240.85

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3096	3-methyl-cis-2-pentene	C6H12	7.05827	1283.19	239.469	-134.84	241.85
3097	4-methyl-cis-2-pentene	C6H12	6.98469	1204.59	237.146	-134.85	225.85
3098	4-methyl-trans-2-pentene	C6H12	7.01711	1227.64	238.197	-140.8	227.85
3099	4-methyl-2-pentyne	C6H10	6.81352	1147.44	218.638	-15.0974	267.427
3100	2-methyl-2-propyl-1,3-propanediol	C7H16O2	9.48106	3364.15	273	147.311	391.826
3101	4-methyl-2-propyl-1-hexanol	C10H22O	8.55072	2727.23	273	112.55	360.125
3102	4-methyl-2-propyl-1-pentanol	C9H20O	8.50898	2617.1	273	99.1771	347.793
3103	1-methyl-2-propylbenzene	C10H14	7.43034	1969.2	247.906	66.9533	387.55
3104	1-methyl-cis-2-propylcyclopentane	C9H18	6.94184	1472.49	210.01	59.4434	347.728
3105	1-methyl-trans-2-propylcyclopentane	C9H18	6.94375	1452.74	211.19	54.5576	338.672
3106	1-methyl-2-propylnaphthalene	C14H16	8.14486	3344.76	323.135	145	539.195
3107	3-methyl-2-propylnaphthalene	C14H16	8.04483	3196.57	306.748	147	539.195
3108	3-methyl-2-propylphenol	C10H14O	7.26114	1869.74	165	171.153	489.304
3109	4-methyl-2-propylphenol	C10H14O	7.27815	1933.6	165	181.574	507.646
3110	5-methyl-2-propylphenol	C10H14O	7.27815	1933.6	165	181.574	507.646
3111	N-methyl-2-pyrrolidone	C5H9NO	7.36115	1869.62	215.294	-24	450.85
3112	3-methyl-2-thiahexane	C6H14S	7.00711	1423.32	205.939	82	335.769
3113	4-methyl-2-thiahexane	C6H14S	7.00923	1428.66	206.055	82.5	337.246
3114	5-methyl-2-thiahexane	C6H14S	7.00466	1417.7	205.782	81.5	334.291
3115	3-methyl-2-thiapentane	C5H12S	6.83558	1258.24	206.159	68.5	311.85
3116	4-methyl-2-thiapentane	C5H12S	6.86134	1276.67	208.229	68.75	311.85
3117	2-methyl-3,3-diethylheptane	C12H26	6.87928	1538.75	181.835	79.8891	378.99
3118	4-methyl-3,3-diethylheptane	C12H26	6.882	1547.8	181.835	81.3065	381.729

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3119	2-methyl-3,3-diethylhexane	C11H24	6.85594	1485.5	187.7	65.9747	365.757
3120	1-methyl-3,4-diethylbenzene	C11H16	7.12282	1713.42	200.316	115.588	403.429
3121	2-methyl-3,4-diethylheptane	C12H26	6.92356	1523.45	181.835	75.3495	364.377
3122	3-methyl-3,4-diethylheptane	C12H26	6.87653	1529.7	181.835	78.4716	376.251
3123	4-methyl-3,4-diethylheptane	C12H26	6.87653	1529.7	181.835	78.4716	376.251
3124	2-methyl-3,4-diethylhexane	C11H24	6.90276	1474.85	187.7	62.1573	352.136
3125	3-methyl-3,4-diethylhexane	C11H24	6.85594	1485.5	187.7	65.9747	365.757
3126	3-methyl-3,4-hexanediol	C7H16O2	9.4059	3372.69	273	152.373	404.124
3127	1-methyl-3,5-diethylbenzene	C11H16	7.12359	1703.76	200.867	113.212	399.313
3128	2-methyl-3,5-diethylheptane	C12H26	6.92356	1523.45	181.835	75.3495	364.377
3129	3-methyl-3,5-diethylheptane	C12H26	6.87097	1511.61	181.835	75.637	370.772
3130	4-methyl-3,5-diethylheptane	C12H26	6.9307	1546.39	181.835	78.9079	371.186
3131	1-methyl-3-(1-methylethenyl)benzene	C10H12	7.08531	1634.92	203.85	87.6734	392.56
3132	cis-1-methyl-3-(1-propenyl)benzene	C10H12	7.05035	1646.38	202.44	92.969	409.46
3133	2-methyl-3-butenic acid	C5H8O2	6.93065	1376.94	163.148	89.3373	399.221
3134	3-methyl-3-butenic acid	C5H8O2	6.93888	1380.51	163.338	89.4204	398.221
3135	1-methyl-3-butylbenzene	C11H16	7.13057	1721.36	200.05	116.866	406.257
3136	1-methyl-3-sec-butylbenzene	C11H16	7.07752	1662.49	202.14	106.955	395.34
3137	1-methyl-3-tert-butylbenzene	C11H16	6.9628	1601.36	203.041	101.18	398.331
3138	2-methyl-3-ethyl-1,4-butanediol	C7H16O2	9.56529	3396.12	273	146.887	386.957
3139	1-methyl-3-ethyl-1-hexanol	C9H20O	8.50274	2614.2	273	99.0947	346.722
3140	2-methyl-3-ethyl-1-pentanol	C8H18O	8.4508	2494.52	273	61.7987	332.011
3141	3-methyl-3-ethyl-1-pentanol	C8H18O	8.37086	2458.72	273	60.5726	335.328

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3142	4-methyl-3-ethyl-1-pentanol	C8H18O	8.4508	2494.52	273	61.7987	332.011
3143	2-methyl-3-ethyl-1-pentene	C8H16	7.04278	1411.64	229.177	4.43136	286.163
3144	3-methyl-3-ethyl-1-pentene	C8H16	6.83038	1274.67	210.736	7.88918	294.253
3145	4-methyl-3-ethyl-1-pentene	C8H16	6.91771	1301.96	215.016	4.99527	283.281
3146	2-methyl-3-ethyl-2-hexanol	C9H20O	8.35368	2468.27	273	85.9386	334.285
3147	2-methyl-3-ethyl-2-pentanol	C8H18O	7.44388	1542.07	180.146	59.1617	315.526
3148	3-methyl-3-ethyl-2-pentanol	C8H18O	8.29869	2345.13	273	48.3079	318.326
3149	4-methyl-3-ethyl-2-pentanol	C8H18O	8.37844	2402.46	273	52.6056	320.637
3150	2-methyl-3-ethyl-2-pentene	C8H16	6.88139	1304.15	208.99	12.7515	297.533
3151	4-methyl-3-ethyl-cis-2-pentene	C8H16	6.93583	1350.33	217.002	10.4858	296.863
3152	4-methyl-3-ethyl-trans-2-pentene	C8H16	6.92848	1338.24	216.32	9.41065	294.373
3153	2-methyl-3-ethyl-3-heptanol	C10H22O	8.40584	2574.66	273	98.5927	346.199
3154	5-methyl-3-ethyl-3-heptanol	C10H22O	8.40584	2573.83	273	98.4731	346
3155	2-methyl-3-ethyl-3-hexanol	C9H20O	8.3537	2501.66	273	90.7937	342.498
3156	4-methyl-3-ethyl-3-hexanol	C9H20O	8.35368	2472.92	273	86.6151	335.429
3157	5-methyl-3-ethyl-3-hexanol	C9H20O	8.35366	2435.42	273	81.1631	326.206
3158	2-methyl-3-ethyl-3-isopropylhexane	C12H26	6.87515	1525.18	181.835	77.763	374.881
3159	2-methyl-3-ethyl-3-pentanol	C8H18O	8.29869	2345.94	273	48.4193	318.531
3160	1-methyl-cis-3-ethylcyclohexane	C9H18	6.90042	1444.71	211.416	40.9666	346.949
3161	1-methyl-trans-3-ethylcyclohexane	C9H18	6.84202	1401.49	202.805	44.5514	351.367
3162	1-methyl-cis-3-ethylcyclopentane	C8H16	6.93371	1379.73	219.331	13.1933	313.841
3163	1-methyl-trans-3-ethylcyclopentane	C8H16	6.964	1406.31	223.315	12.4848	313.841
3164	1-methyl-3-ethylnaphthalene	C13H14	7.19948	1964.44	181.872	135	497.633

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3165	2-methyl-3-ethylnaphthalene	C13H14	7.40725	2222.98	214.1	196	503.29
3166	2-methyl-3-ethylnonane	C12H26	6.98272	1570.35	181.835	80.6464	368.928
3167	3-methyl-3-ethylnonane	C12H26	6.93115	1562.76	181.835	81.6486	376.582
3168	4-methyl-3-ethylnonane	C12H26	6.98128	1565.7	181.835	79.9319	367.573
3169	5-methyl-3-ethylnonane	C12H26	6.97984	1561.05	181.835	79.2174	366.219
3170	2-methyl-3-ethyloctane	C11H24	6.95851	1507.53	187.7	65.3036	352.464
3171	3-methyl-3-ethyloctane	C11H24	6.90687	1503.33	187.7	66.8052	361.348
3172	4-methyl-3-ethyloctane	C11H24	6.95993	1512.13	187.7	66.0157	353.839
3173	3-methyl-3-ethylpentane	C8H18	7.04885	1456.81	231.249	-90.87	303.35
3174	2-methyl-3-ethylphenol	C9H12O	7.17761	1684.34	165	142.438	453.285
3175	4-methyl-3-ethylphenol	C9H12O	7.19089	1728.34	165	149.706	466.357
3176	2-methyl-3-ethylthiophene	C7H10S	7.09826	1544.3	209.17	93.7377	372.843
3177	2-methyl-3-heptanol	C8H18O	7.85222	1872.41	209.037	64.2199	322.218
3178	3-methyl-3-heptanol	C8H18O	7.71862	1760.81	202.968	59.1108	316.516
3179	4-methyl-3-heptanol	C8H18O	8.74829	2695.03	303.916	43.9059	305.738
3180	5-methyl-3-heptanol	C8H18O	8.5737	2501.01	285.723	44.5008	303.307
3181	6-methyl-3-heptanol	C8H18O	8.45076	2410.95	273	50.5845	311.749
3182	2-methyl-cis-3-heptene	C8H16	7.00658	1371.77	220.489	7.88918	287.425
3183	2-methyl-trans-3-heptene	C8H16	6.98758	1355.85	218.15	8.29348	287.425
3184	3-methyl-cis-3-heptene	C8H16	7.05483	1441.41	224.33	13.7298	299.745
3185	3-methyl-trans-3-heptene	C8H16	7.05483	1441.41	224.33	13.7298	299.745
3186	4-methyl-cis-3-heptene	C8H16	7.05859	1448.35	224.68	14.3774	301.198
3187	4-methyl-trans-3-heptene	C8H16	7.05859	1448.35	224.68	14.3774	301.198

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3188	5-methyl-cis-3-heptene	C8H16	7.00658	1371.77	220.489	7.88918	287.425
3189	5-methyl-trans-3-heptene	C8H16	7.00658	1371.77	220.489	7.88918	287.425
3190	6-methyl-cis-3-heptene	C8H16	7.01782	1391.99	221.474	9.83828	291.792
3191	6-methyl-trans-3-heptene	C8H16	7.04781	1417.59	225.194	9.20272	291.792
3192	2-methyl-3-hexanol	C7H16O	7.57243	1559.4	187.38	49.8838	300.062
3193	3-methyl-3-hexanol	C7H16O	7.61898	1621.96	199.517	45.5292	300.433
3194	4-methyl-3-hexanol	C7H16O	8.39654	2327.64	273	41.6926	305.545
3195	5-methyl-3-hexanol	C7H16O	8.06327	2001.09	238.127	45.1818	304.174
3196	2-methyl-3-hexanone	C7H14O	7.30388	1571.09	222.203	27.0224	310.649
3197	4-methyl-3-hexanone	C7H14O	7.72555	1981.5	273	44.1192	314.961
3198	5-methyl-3-hexanone	C7H14O	7.72555	1981.5	273	44.1192	314.961
3199	2-methyl-cis-3-hexene	C7H14	6.95346	1258.61	223.041	-11.632	260.434
3200	2-methyl-trans-3-hexene	C7H14	6.95297	1257.88	222.997	-11.6946	260.286
3201	3-methyl-cis-3-hexene	C7H14	6.92412	1264.07	217.231	-3.85456	273.602
3202	3-methyl-trans-3-hexene	C7H14	6.9519	1279.99	220.868	-5.81227	270.844
3203	2-methyl-3-hexyne	C7H12	6.84592	1228.67	214.669	2.03431	288.286
3204	1-methyl-3-isobutylbenzene	C11H16	7.07752	1662.49	202.14	106.955	395.34
3205	2-methyl-3-isopropyl-3-hexanol	C10H22O	8.33135	2534.5	273	96.7715	346.892
3206	2-methyl-3-isopropyl-3-pentanol	C9H20O	8.27782	2434.05	273	84.9116	336.449
3207	1-methyl-cis-3-isopropylcyclopentane	C9H18	6.89086	1419.64	212.02	50.2084	337.051
3208	1-methyl-trans-3-isopropylcyclopentane	C9H18	6.89086	1419.64	212.02	50.2084	337.051
3209	2-methyl-3-isopropylheptane	C11H24	6.90178	1471.67	187.7	61.6608	351.168
3210	1-methyl-3-isopropyl-naphthalene	C14H16	7.80195	2905.61	278.174	149	544.392

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3211	2-methyl-3-isopropyloctane	C12H26	6.925	1528.04	181.835	76.0611	365.738
3212	2-methyl-3-isopropylphenol	C10H14O	7.22148	1906.77	165	180.272	512.626
3213	4-methyl-3-isopropylphenol	C10H14O	7.16327	1699.49	165	146.017	451.722
3214	methyl-3-methylbutylamine	C6H15N	6.94331	1193.97	185.901	32.5276	279.47
3215	2-methyl-3-nonanol	C10H22O	8.55072	2729.5	273	112.87	360.651
3216	3-methyl-3-nonanol	C10H22O	8.47469	2695.41	273	112.192	364.171
3217	5-methyl-3-nonanol	C10H22O	8.55072	2732.05	273	113.231	361.243
3218	2-methyl-3-octanol	C9H20O	8.50272	2569.21	273	92.6927	336.061
3219	3-methyl-3-octanol	C9H20O	8.42446	2561.17	273	95.654	345.828
3220	4-methyl-3-octanol	C9H20O	8.50272	2579.61	273	94.1732	338.526
3221	6-methyl-3-octanol	C9H20O	8.50272	2579.61	273	94.1732	338.526
3222	7-methyl-3-octanol	C9H20O	8.50272	2579.61	273	94.1732	338.526
3223	2-methyl-3-pentanol	C6H14O	7.17751	1306.1	177.468	33.9605	291.25
3224	3-methyl-3-pentanol	C6H14O	7.40879	1473.55	203.023	26.904	289.25
3225	1-methyl-3-propylbenzene	C10H14	7.4265	1952.01	247.44	64.8626	383.25
3226	1-methyl-cis-3-propylcyclopentane	C9H18	6.94324	1457.93	210.88	55.8401	341.049
3227	1-methyl-trans-3-propylcyclopentane	C9H18	6.94324	1457.93	210.88	55.8401	341.049
3228	2-methyl-3-propylphenol	C10H14O	7.23302	1770.7	165	154.964	460.801
3229	4-methyl-3-propylphenol	C10H14O	7.27815	1933.6	165	181.574	507.646
3230	2-methyl-3-thiahexane	C6H14S	7.06541	1450.58	214.597	78.525	325.501
3231	4-methyl-3-thiahexane	C6H14S	7.08037	1469.65	216.304	79.325	327.865
3232	5-methyl-3-thiahexane	C6H14S	7.06796	1460.62	214.614	79.61	328.707
3233	2-methyl-3-thiapentane	C5H12S	6.67507	1153.47	196.624	66.19	311.85

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3234	2-methyl-4,4-diethylheptane	C12H26	6.86673	1498.05	181.835	73.5112	366.663
3235	3-methyl-4,4-diethylheptane	C12H26	6.88064	1543.27	181.835	80.5978	380.359
3236	2-methyl-4,4-diethylhexane	C11H24	6.84644	1454.19	187.7	61.0316	356.016
3237	3-methyl-4,4-diethylhexane	C11H24	6.86124	1503.41	187.7	68.7997	371.323
3238	2-methyl-4,5-diethylheptane	C12H26	6.92066	1514.28	181.835	73.9262	361.653
3239	3-methyl-4,5-diethylheptane	C12H26	6.92786	1537.21	181.835	77.4845	368.462
3240	1-methyl-4-(1-methylethenyl)benzene	C10H12	7.08504	1638.22	203.66	88.466	394.013
3241	cis-1-methyl-4-(1-propenyl)benzene	C10H12	7.04942	1658.11	201.76	95.8021	414.709
3242	trans-1-methyl-4-(1-propenyl)benzene	C10H12	7.04816	1674.48	200.81	99.7589	422.04
3243	1-methyl-4-butylbenzene	C11H16	7.13005	1728.04	199.67	118.506	409.099
3244	1-methyl-4-sec-butylbenzene	C11H16	7.07673	1672.37	201.57	109.408	399.633
3245	1-methyl-4-tert-butylbenzene	C11H16	6.96189	1612.58	202.376	104.028	403.413
3246	2-methyl-4-tert-butylheptane	C12H26	6.80389	1439.12	181.835	66.123	358.099
3247	3-methyl-4-tert-butylheptane	C12H26	6.81105	1461.4	181.835	69.6513	364.988
3248	4-methyl-4-tert-butylheptane	C12H26	6.7673	1476.22	181.835	74.1293	379.967
3249	2-methyl-4-ethyl-3-hexanol	C9H20O	8.43197	2508.29	273	87.6534	332.276
3250	3-methyl-4-ethyl-3-hexanol	C9H20O	8.35368	2472.92	273	86.6151	335.429
3251	2-methyl-4-ethyl-3-isopropylhexane	C12H26	6.91626	1500.52	181.835	71.7914	357.568
3252	1-methyl-cis-4-ethylcyclohexane	C9H18	6.76719	1334.33	192.336	46.3186	351.367
3253	1-methyl-trans-4-ethylcyclohexane	C9H18	7.05785	1592.63	233.283	37.4935	346.949
3254	1-methyl-4-ethylnaphthalene	C13H14	7.1896	1956.82	180.146	136	499.044
3255	2-methyl-4-ethylnaphthalene	C13H14	7.30903	2094.43	198.973	133	499.044
3256	2-methyl-4-ethylnonane	C12H26	6.97839	1556.4	181.835	78.503	364.865

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3257	3-methyl-4-ethylnonane	C12H26	6.98272	1570.35	181.835	80.6464	368.928
3258	4-methyl-4-ethylnonane	C12H26	6.92413	1539.84	181.835	78.0911	369.773
3259	5-methyl-4-ethylnonane	C12H26	6.97984	1561.05	181.835	79.2174	366.219
3260	2-methyl-4-ethyloctane	C11H24	6.9499	1479.93	187.7	61.0312	344.217
3261	3-methyl-4-ethyloctane	C11H24	6.95851	1507.53	187.7	65.3036	352.464
3262	4-methyl-4-ethyloctane	C11H24	6.89899	1477.48	187.7	62.7637	353.466
3263	2-methyl-4-ethylphenol	C9H12O	7.17851	1687.28	165	142.923	454.157
3264	3-methyl-4-ethylphenol	C9H12O	7.18209	1699	165	144.861	457.643
3265	2-methyl-4-ethyl thiophene	C7H10S	7.09649	1564.14	208.03	98.8758	381.854
3266	3-methyl-4-ethyl thiophene	C7H10S	6.97206	1535.05	209.702	91.3399	368.638
3267	2-methyl-4-heptanol	C8H18O	7.74252	1768.07	197.572	64.6543	320.192
3268	3-methyl-4-heptanol	C8H18O	8.43894	2425.81	271.744	54.3523	318.3
3269	4-methyl-4-heptanol	C8H18O	7.72914	1770.52	204.081	59.0308	316.652
3270	1-methyl-4-isobutylbenzene	C11H16	7.07699	1669.07	201.76	108.59	398.202
3271	2-methyl-4-isopropylheptane	C11H24	6.89275	1443.1	187.7	57.193	342.456
3272	3-methyl-4-isopropylheptane	C11H24	6.89993	1465.77	187.7	60.7389	349.37
3273	4-methyl-4-isopropylheptane	C11H24	6.84781	1458.67	187.7	61.7377	357.408
3274	1-methyl-4-isopropyl-naphthalene	C14H16	8.03471	3243.56	317.079	144	544.392
3275	2-methyl-4-isopropyloctane	C12H26	6.91626	1500.52	181.835	71.7914	357.568
3276	3-methyl-4-isopropyloctane	C12H26	6.92356	1523.45	181.835	75.3495	364.377
3277	4-methyl-4-isopropyloctane	C12H26	6.87237	1516.13	181.835	76.3456	372.142
3278	2-methyl-4-isopropylphenol	C10H14O	5.8197	768.23	31.4019	180.272	512.626
3279	3-methyl-4-isopropylphenol	C10H14O	7.17063	1723.86	165	150.053	458.899

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3280	2-methyl-4-nonanol	C10H22O	8.55072	2732.05	273	113.231	361.243
3281	4-methyl-4-nonanol	C10H22O	8.47469	2695.41	273	112.192	364.171
3282	5-methyl-4-nonanol	C10H22O	8.55072	2732.05	273	113.231	361.243
3283	7-methyl-4-nonanol	C10H22O	8.55072	2732.05	273	113.231	361.243
3284	2-methyl-4-octanol	C9H20O	8.50272	2569.21	273	92.6927	336.061
3285	3-methyl-4-octanol	C9H20O	8.5027	2546.72	273	89.4918	330.73
3286	4-methyl-4-octanol	C9H20O	8.42444	2516.81	273	89.2701	335.113
3287	5-methyl-4-octanol	C9H20O	8.50271	2557.12	273	90.9722	333.196
3288	6-methyl-4-octanol	C9H20O	8.50271	2557.12	273	90.9722	333.196
3289	7-methyl-4-octanol	C9H20O	8.50271	2557.12	273	90.9722	333.196
3290	1-methyl-4-propylbenzene	C10H14	7.19301	1743.52	223.943	65.8282	385.35
3291	2-methyl-4-propylheptane	C11H24	6.94697	1470.73	187.7	59.6072	341.468
3292	3-methyl-4-propylheptane	C11H24	6.95423	1493.72	187.7	63.1673	348.341
3293	4-methyl-4-propylheptane	C11H24	6.89618	1468.42	187.7	61.3458	350.7
3294	2-methyl-4-propyloctane	C12H26	6.96806	1523.87	181.835	73.5024	355.386
3295	3-methyl-4-propyloctane	C12H26	6.97693	1551.75	181.835	77.7886	363.511
3296	4-methyl-4-propyloctane	C12H26	6.91841	1521.51	181.835	75.2455	364.327
3297	2-methyl-4-propylphenol	C10H14O	7.23324	1771.44	165	155.085	461.015
3298	3-methyl-4-propylphenol	C10H14O	7.26114	1869.74	165	171.153	489.304
3299	"2-methyl-5,5-diethylheptane"	C12H26	6.87237	1516.13	181.835	76.3456	372.142
3300	"3-methyl-5,5-diethylheptane"	C12H26	6.87376	1520.66	181.835	77.0543	373.511
3301	4-methyl-5-ethyl-3-heptanol	C10H22O	8.48214	2609.38	273	99.5012	343.056
3302	1-methyl-5-ethylnaphthalene	C13H14	7.15085	1899.15	174.762	134	493.399

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3303	2-methyl-5-ethylnaphthalene	C13H14	7.18995	1942.91	180.881	133	493.399
3304	2-methyl-5-ethylnonane	C12H26	6.97547	1547.11	181.835	77.0742	362.157
3305	3-methyl-5-ethylnonane	C12H26	6.974	1542.46	181.835	76.3598	360.803
3306	4-methyl-5-ethylnonane	C12H26	6.97839	1556.4	181.835	78.503	364.865
3307	5-methyl-5-ethylnonane	C12H26	6.92271	1535.26	181.835	77.3797	368.412
3308	2-methyl-5-ethyloctane	C11H24	6.95279	1489.12	187.7	62.4553	346.966
3309	3-methyl-5-ethyloctane	C11H24	6.9499	1479.93	187.7	61.0312	344.217
3310	4-methyl-5-ethyloctane	C11H24	6.95567	1498.32	187.7	63.8794	349.715
3311	2-methyl-5-ethylphenol	C9H12O	7.17866	1687.76	165	143.004	454.302
3312	3-methyl-5-ethylphenol	C9H12O	7.19089	1728.34	165	149.706	466.357
3313	3-methyl-5-ethylthiophene	C7H10S	7.0991	1535.05	209.702	91.3399	368.638
3314	2-methyl-5-ethyl thiophene	C7H10S	7.09734	1554.55	208.581	96.3924	377.499
3315	2-methyl-5-isopropyloctane	C12H26	6.91773	1505.11	181.835	72.503	358.929
3316	3-methyl-5-isopropyloctane	C12H26	6.9192	1509.69	181.835	73.2146	360.291
3317	4-methyl-5-isopropyloctane	C12H26	6.92211	1518.86	181.835	74.6378	363.015
3318	2-methyl-5-isopropylphenol	C10H14O	7.17085	1724.6	165	150.174	459.114
3319	3-methyl-5-isopropylphenol	C10H14O	7.17663	1744.1	165	153.403	464.856
3320	2-methyl-5-nonanol	C10H22O	8.55072	2732.05	273	113.231	361.243
3321	3-methyl-5-nonanol	C10H22O	8.55072	2732.05	273	113.231	361.243
3322	5-methyl-5-nonanol	C10H22O	7.81933	2099.66	223.16	112.192	364.171
3323	2-methyl-5-propyloctane	C12H26	6.96806	1523.87	181.835	73.5024	355.386
3324	3-methyl-5-propyloctane	C12H26	6.97253	1537.81	181.835	75.6454	359.448
3325	4-methyl-5-propyloctane	C12H26	6.97547	1547.11	181.835	77.0742	362.157

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3326	2-methyl-5-propylphenol	C10H14O	7.23302	1770.7	165	154.964	460.801
3327	3-methyl-5-propylphenol	C10H14O	7.25589	1850.66	165	168.037	483.817
3328	1-methyl-6-ethylnaphthalene	C13H14	7.08391	1835.44	163.688	138	497.633
3329	2-methyl-6-ethylnaphthalene	C13H14	7.2996	2068.06	198.005	192	493.41
3330	2-methyl-6-ethylnonane	C12H26	6.97839	1556.4	181.835	78.503	364.865
3331	3-methyl-6-ethylnonane	C12H26	6.97984	1561.05	181.835	79.2174	366.219
3332	4-methyl-6-ethylnonane	C12H26	6.97547	1547.11	181.835	77.0742	362.157
3333	2-methyl-6-ethyloctane	C11H24	6.95851	1507.53	187.7	65.3036	352.464
3334	3-methyl-6-ethyloctane	C11H24	6.95851	1507.53	187.7	65.3036	352.464
3335	4-methyl-6-ethyloctane	C11H24	6.95567	1498.32	187.7	63.8794	349.715
3336	2-methyl-6-ethylphenol	C9H12O	7.15755	1620.88	165	131.942	434.404
3337	3-methyl-6-ethylphenol	C9H12O	7.17338	1670.67	165	140.177	449.219
3338	1-methyl-6-isopropylnaphthalene	C14H16	8.03471	3243.56	317.079	144	544.392
3339	2-methyl-6-isopropylphenol	C10H14O	6.3495	1093.05	89.6205	158.125	473.253
3340	2-methyl-6-propylphenol	C10H14O	7.23302	1770.7	165	154.964	460.801
3341	1-methyl-7-ethylnaphthalene	C13H14	7.34074	2120.02	204.35	130	494.81
3342	2-methyl-7-ethylnaphthalene	C13H14	7.2996	2068.06	198.005	192	493.41
3343	2-methyl-7-ethylnonane	C12H26	6.98415	1575	181.835	81.3609	370.282
3344	3-methyl-7-ethylnonane	C12H26	6.98128	1565.7	181.835	79.9319	367.573
3345	4-methyl-7-ethylnonane	C12H26	6.98128	1565.7	181.835	79.9319	367.573
3346	1-methyl-7-isopropylnaphthalene	C14H16	7.05887	1843.91	160.333	144	500.734
3347	1-methyl-8-ethylnaphthalene	C13H14	7.33925	2133.84	203.608	133	500.456
3348	2-methyl-8-ethylnaphthalene	C13H14	7.18995	1942.91	180.881	133	493.399

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3349	2-methyl-8-isopropyl-naphthalene	C14H16	7.08735	1878.83	164.644	144	502.13
3350	methyl-butylamine	C5H13N	7.00538	1158.82	189.857	19.7616	258.65
3351	methyl-sec-butylamine	C5H13N	6.93168	1096.24	192.118	8.85841	246.75
3352	methyl-tert-butylamine	C5H13N	6.89149	1068.41	193.391	3.93738	240.05
3353	1-methyl-cis-decahydronaphthalene	C11H20	6.90657	1754.55	192.83	164.761	479.357
3354	1-methyl-trans-decahydronaphthalene	C11H20	6.90824	1729.18	194.35	157.95	467.694
3355	2-methyl-cis-decahydronaphthalene	C11H20	6.91243	1668.93	197.96	141.776	439.993
3356	2-methyl-trans-decahydronaphthalene	C11H20	6.9143	1643.57	199.48	134.965	428.33
3357	4a-methyl-cis-decahydronaphthalene	C11H20	6.91266	1665.76	198.15	140.924	438.535
3358	4a-methyl-trans-decahydronaphthalene	C11H20	6.91501	1634.05	200.05	132.411	423.956
3359	methyl-propylamine	C4H11N	6.98544	1062.68	195.899	-2.97554	226.85
3360	1-methyl-[1,2,3,4-tetrahydronaphthalene]	C11H14	7.07391	1751.37	197.088	169.855	448.983
3361	2-methyl-[1,2,3,4-tetrahydronaphthalene]	C11H14	7.07405	1749.42	197.2	169.322	448.117
3362	methyl 1,1-dimethylpropyl ether	C6H14O	6.85338	1177.07	210	8.93868	263.679
3363	methyl 1,2-dimethylpropyl ether	C6H14O	6.90692	1179.65	210	7.25468	254.437
3364	methyl 1-ethylpropyl ether	C6H14O	6.96815	1218.03	210	11.8211	257.565
3365	methyl 1-methylbutyl ether	C6H14O	6.9727	1231.66	210	14.1179	261.973
3366	methyl 2,2-dimethylpropyl ether	C6H14O	6.84847	1162.52	210	6.43039	258.75
3367	methyl 2-methylbutyl ether	C6H14O	6.97119	1227.11	210	13.3523	260.504
3368	methyl 3-methylbutyl ether	C6H14O	6.97119	1227.11	210	13.3523	260.504
3369	N-methylacetamide	C3H7NO	7.41637	1829.08	198.275	28	444.85
3370	methyl acetate	C3H6O2	7.28036	1276.29	233.155	-98	233.65
3371	methyl acetoacetate	C5H8O3	7.53543	1813.98	218.017	-80	368.85

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3372	methylacetylene	C3H4	7.11874	923.311	241.079	-102.7	129.24
3373	methyl acrylate	C4H6O2	7.29607	1387.88	234.137	-76.83	262.85
3374	methylal	C3H8O2	7.16103	1197.95	238.031	-104.8	207.45
3375	methyl alcohol	CH4O	8.09126	1582.91	239.096	-97.68	239.43
3376	methylamine	CH5N	7.36379	1025.4	235.062	-93.46	156.9
3377	N-methylaniline	C7H9N	7.74401	2085.01	232.863	-57	428.4
3378	methyl benzoate	C8H8O2	7.3207	1825.16	211.583	-12.4	419.85
3379	2-methylbenzofuran	C9H8O	7.22082	1766.5	209.527	16.85	424.85
3380	1-methylbiphenyl	C13H12	7.19863	1924.86	190.493	202.527	502.65
3381	3-methylbiphenyl	C13H12	7.19885	1985.81	187.187	218.26	527.85
3382	4-methylbiphenyl	C13H12	7.23977	1995.09	187.7	216.268	520.25
3383	methyl bromide	CH3Br	7.34062	1146.12	253.43	-93.68	193.85
3384	2-methylbutanal	C5H10O	7.17	1316.78	215	16.303	270.577
3385	3-methylbutanal	C5H10O	7.17084	1319.61	215	16.7663	271.47
3386	2-methylbutanenitrile	C5H9N	6.89173	1223.31	179.596	46.3322	312.652
3387	3-methylbutanenitrile	C5H9N	6.8899	1237.49	178.172	50.4523	320.148
3388	methyl butanoate	C5H10O2	7.20355	1402.13	221.612	-85.8	281.35
3389	3-methylbutanoic acid	C5H10O2	7.69432	1822.54	203.53	-29.3	360.85
3390	1-methylbutyl acetate	C7H14O2	6.94421	1275.46	180.889	52.4081	305.85
3391	2-methylbutyl acetate	C7H14O2	6.94136	1295.27	178.989	58.0559	315.85
3392	1-methylbutylamine	C5H13N	6.95763	1145.45	189.268	19.7373	261.75
3393	2-methylbutylamine	C5H13N	6.96309	1156.53	187.805	23.011	269.45
3394	3-methylbutylamine	C5H13N	6.96096	1160.26	187.368	24.2107	271.75

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3395	1-methylbutyl butanoate	C9H18O2	7.38164	1606.79	174.999	97.13	336.85
3396	2-methylbutyl butanoate	C9H18O2	7.09876	1485.13	173.099	91.0829	346.85
3397	3-methylbutyl butanoate	C9H18O2	7.67441	2015.89	241.539	68.6805	345.85
3398	methyl butyl ether	C5H12O	7.10128	1182.58	210	0.266964	228.85
3399	methyl sec-butyl ether	C5H12O	7.15243	1273.31	239.086	-123.15	224.85
3400	methyl tert-butyl ether	C5H12O	7.07597	1233.7	238.879	-108.6	223.95
3401	1-methylbutyl formate	C6H12O2	6.87062	1206.71	181.839	41.8958	300.85
3402	2-methylbutyl formate	C6H12O2	6.82506	1190.68	181.269	41.3748	303.85
3403	1-methylbutyl propanoate	C8H16O2	7.36008	1543.28	177.469	84.8619	323.85
3404	2-methylbutyl propanoate	C8H16O2	7.12228	1451.68	175.189	81.966	335.85
3405	methyl butyl sulfide	C5H12S	7.14399	1490.96	226.299	74.215	317.85
3406	2-methylbutyricacid	C5H10O2	7.68526	1883.34	215	-80.15	369.85
3407	methyl chloride	CH3Cl	7.15229	963.608	249.811	-97.72	143.1
3408	methyl chloroacetate	C3H5ClO2	7.40326	1554.93	214.006	-32.12	326.85
3409	methyl chloroformate	C2H3ClO2	7.44868	1364.54	227.876	-81.15	251.85
3410	methyl chlorosilane	CH5ClSi	7.04725	1054.78	244.46	-134.1	168.85
3411	methyl cyanoacetate	C4H5NO2	7.53151	1895.57	202.5	-13.07	413.85
3412	methylcyclobutane	C5H10	6.94406	1070.84	233.243	-16.6517	204.604
3413	methylcyclohexane	C7H14	7.00107	1375.13	232.819	-126.57	299.04
3414	1-methylcyclohexanol	C7H14O	7.66323	1686.73	195.694	26	329.85
3415	cis-2-methylcyclohexanol	C7H14O	8.10339	2130.94	243.025	7	340.85
3416	trans-2-methylcyclohexanol	C7H14O	8.03432	2068.83	234.941	-4	342.85
3417	cis-3-methylcyclohexanol	C7H14O	7.70311	1761.78	197.34	-5.5	344.85

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3418	trans-3-methylcyclohexanol	C7H14O	7.74609	1790.81	200.079	-0.5	343.85
3419	cis-4-methylcyclohexanol	C7H14O	7.51059	1600.23	174.638	52	348.85
3420	trans-4-methylcyclohexanol	C7H14O	7.56987	1652.14	181.341	54	348.85
3421	1-methylcyclohexene	C7H12	6.90891	1322.59	218.044	25.4459	317.794
3422	3-methylcyclohexene	C7H12	6.91169	1297.95	219.531	19.3013	305.735
3423	4-methylcyclohexene	C7H12	6.91159	1298.8	219.48	19.5126	306.149
3424	N-methylcyclohexylamine	C7H15N	7.21504	1577.43	215.096	-8.5	348.85
3425	methylcyclopentadiene	C6H8	7.16296	1344.84	241.277	-123.15	267.85
3426	methylcyclopentane	C6H12	7.06372	1304.45	240.043	-142.42	259.64
3427	1-methylcyclopentene	C6H10	6.93473	1234.35	228.685	-5	268.84
3428	3-methylcyclopentene	C6H10	7.24211	1452.03	262.926	-10	262.56
3429	4-methylcyclopentene	C6H10	6.98436	1257.37	231.251	-2	270.6
3430	methylcyclopropane	C4H8	6.97325	980.512	238.861	-41.7041	163.984
3431	2-methyldecane	C11H24	7.0205	1560.21	187.7	71.449	358.605
3432	3-methyldecane	C11H24	7.02164	1563.99	187.7	72.0281	359.712
3433	4-methyldecane	C11H24	7.01869	1554.19	187.7	70.5267	356.843
3434	5-methyldecane	C11H24	7.01601	1545.32	187.7	69.1683	354.246
3435	methyldecylamine	C11H25N	6.65525	1211.31	94.7237	130.312	393.45
3436	methyl decyl sulfide	C11H24S	7.09661	1759.04	170.4	196.85	296.85
3437	methyl dichlorosilane	CH4Cl2Si	7.23413	1272.21	250.69	-90.6	209.85
3438	methyl diethanolamine	C5H13NO2	8.74332	2501.48	179.692	-21	404.85
3439	methyldiethylamine	C5H13N	6.83838	1030.8	194.462	-2.19451	234.411
3440	methyldiisopropylamine	C7H17N	6.80578	1162.39	184.154	33.9863	288.666

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3441	2-methyldiphenylmethane	C14H14	7.20293	2015	185.705	225.359	511.001
3442	3-methyldiphenylmethane	C14H14	7.20318	2010.7	185.945	224.222	509.216
3443	4-methyldiphenylmethane	C14H14	7.20264	2019.97	185.428	226.675	513.069
3444	methyldipropylamine	C7H17N	6.92018	1208.86	185.17	36.9221	283.315
3445	methyldocosylamine	C23H49N	6.56977	1645.8	54.1411	300.383	541.957
3446	2-methyldodecane	C13H28	7.05546	1685.39	174.22	104.105	394.874
3447	3-methyldodecane	C13H28	7.05661	1689.2	174.22	104.681	395.938
3448	methyl dodecanoate	C13H26O2	7.33074	1992.81	180.98	5	438.85
3449	methyldodecylamine	C13H29N	6.95296	1544.49	118.283	159.088	423.65
3450	methyl dodecyl sulfide	C13H28S	7.13871	1863.9	157.9	229.85	329.85
3451	methyldotriacontylamine	C33H69N	8.9459	4555.79	273.15	377.768	528
3452	methyleicosylamine	C21H45N	6.91462	1870.01	93.5845	283.922	518.429
3453	2-methylenebutanoic acid	C5H8O2	6.82278	1270.53	142.308	75.8913	400.773
3454	(1-methylenepropyl)benzene	C10H12	7.02158	1600.08	204.42	84.1699	398.113
455	methylethanolamine	C3H9NO	7.69194	1731.91	201.98	-4.5	356.85
3456	methylethyl-sec-butylamine	C7H17N	6.86671	1157.66	187.438	27.3568	271.378
3457	methylethyl-tert-butylamine	C7H17N	6.74447	1135.47	183.885	31.6827	290.077
3458	methylethylamine	C3H9N	6.86968	943.96	200.649	-25.6	201.85
3459	methylethylbutylamine	C7H17N	6.91904	1217.03	184.379	39.2622	287.482
3460	methyl ethyl ether	C3H8O	6.62951	760.22	195.446	-113.15	164.65
3461	methylethylisobutylamine	C7H17N	6.86509	1168.74	186.338	30.5785	277.169
3462	methylethylisopropylamine	C6H15N	6.81952	1103.08	188.56	17.9154	265.472
3463	methyl ethyl ketone	C4H8O	7.29427	1400.37	237.655	-86.67	262.35

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3464	methylethylpropylamine	C6H15N	6.87728	1122.49	189.371	18.4917	261.206
3465	methyl ethyl sulfide	C3H8S	6.98835	1211.78	228.013	-26	259.65
3466	methyl fluoride	CH3F	7.17217	755.926	254.481	-141.8	44.55
3467	N-methylformamide	C2H5NO	7.49425	1885	209.081	-3.8	447.85
3468	methyl formate	C2H4O2	7.26545	1178.19	236.959	-99	214.05
3469	2-methylfuran	C5H6O	7.17114	1275.53	232.604	-19.8387	253.85
3470	3-methylfuran	C5H6O	6.99595	1133.72	210	-4.57238	255.447
3471	methylglutaronitrile	C6H8N2	7.62007	2204.98	202.259	-45	468.85
3472	methylheneicosylamine	C22H47N	6.75141	1764.54	74.8838	292.307	529.866
3473	methylhentriacontylamine	C32H67N	8.94899	4509.57	273.15	375.03	520
3474	methylheptacosylamine	C28H59N	6.01047	1400	9.33333	327.431	488
3475	2-methylheptadecane	C18H38	7.06388	1904.55	143.3	170.781	466.178
3476	3-methylheptadecane	C18H38	7.0654	1909.43	143.3	171.506	467.442
3477	methylheptadecylamine	C18H39N	7.53255	2335.59	168.091	219.608	481.95
3478	methyl heptadecyl sulfide	C18H38S	7.13143	2069.41	135	301.85	401.85
3479	2-methylheptane	C8H18	7.12709	1473.84	229.44	-108.99	286.49
3480	3-methylheptane	C8H18	7.12293	1477.48	229.359	-120.55	290.52
3481	4-methylheptane	C8H18	7.12417	1473.51	229.542	-120.95	288.59
3482	methylheptatriacontylamine	C38H79N	8.97849	4781.49	273.15	378.956	561
3483	methylheptylamine	C8H19N	7.08179	1428.49	175.037	79.8376	336.65
3484	methyl heptyl sulfide	C8H18S	7.08052	1717.84	220.489	138.55	238.55
3485	methylhexacosylamine	C27H57N	5.95598	1350	9	323.873	480
3486	2-methylhexadecane	C17H36	7.07554	1871.69	149.2	158.869	453.076

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3487	3-methylhexadecane	C17H36	7.07706	1876.56	149.2	159.594	454.349
3488	methylhexadecylamine	C17H37N	7.54861	2317.61	175.511	208.771	471.85
3489	methyl hexadecyl sulfide	C17H36S	7.25728	2069.41	135	287.85	387.85
3490	2-methylhexane	C7H16	7.0583	1340.21	230.768	-118.25	257.22
3491	3-methylhexane	C7H16	7.08748	1370.78	234.008	-119.4	262.1
3492	methylhexatriacontylamine	C37H77N	8.96561	4740.97	273.15	380.918	556
3493	methylhexylamine	C7H17N	7.04774	1339.28	179.407	61.0114	313.65
3494	methyl hexyl sulfide	C7H16S	7.05063	1575.03	210.873	116.85	216.85
3495	2-methylindene	C10H10	7.08766	1657.67	209.192	80	410.85
3496	1-methylindene	C10H10	7.10152	1711.34	206.962	76.85	429.85
3497	methyl iodide	CH3I	7.33367	1316.43	253.207	-66.45	254.85
3498	methylisobutylamine	C5H13N	6.93253	1094.01	193.011	7.52545	242.05
3499	methyl isobutyl ether	C5H12O	7.1429	1261.86	237.516	-113.15	223.85
3500	methyl isocyanate	C2H3NO	7.05663	1162.78	239.607	-17	231.85
3501	methyl isocyanide	C2H3N	6.83764	995.205	192.506	-6.85129	244.707
3502	methyl isopropenyl ketone	C5H8O	7.12747	1390.61	229.46	-53.6	292.85
3503	methylisopropylamine	C4H11N	6.36271	676.394	143.86	4.06748	214.45
3504	methyl isopropyl ether	C4H10O	7.17957	1184.12	244.686	-145.22	191.35
3505	methyl isopropyl ketone	C5H10O	7.04182	1260.87	208.621	-92	279.85
3506	methyl isopropyl sulfide	C4H10S	7.06781	1326.81	232.139	33	277.85
3507	methyl mercaptan	CH4S	7.07246	1008.88	234.729	-122.97	196.8
3508	methyl methacrylate	C5H8O2	6.95921	1254.41	207.274	-48.2	290.85
3509	1-methylnaphthalene	C11H10	7.26987	2027.9	217.356	-30.48	498.89

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3510	2-methylnaphthalene	C11H10	7.03802	1805.88	193.348	34.58	487.85
3511	methyl nitrate	CH3NO3	---	---	---	---	---
3512	methyl nitrite	CH3NO2	---	---	---	---	---
3513	methylnonacosylamine	C30H63N	8.92886	4403.89	273.15	334.005	505
3514	2-methylnonadecane	C20H42	7.01251	1946.44	132.1	191.632	490.064
3515	3-methylnonadecane	C20H42	7.01404	1951.3	132.1	192.357	491.311
3516	methylnonadecylamine	C20H43N	7.55403	2442.39	163.637	240.113	500.25
3517	methyl nonadecyl sulfide	C20H42S	7.18259	2111.53	119.001	321.85	421.85
3518	2-methylnonane	C10H22	7.12921	1599.75	209.553	-74.65	336.85
3519	3-methylnonane	C10H22	7.17549	1649.33	216.241	-84.8	339.85
3520	4-methylnonane	C10H22	7.26574	1726.16	227.957	-98.7	336.85
3521	5-methylnonane	C10H22	7.17032	1641.14	217.443	-87.7	336.85
3522	methylnonatriacontylamine	C40H83N	8.985	4859.85	273.15	375.518	573
3523	methylnonylamine	C10H23N	7.1562	1601.18	167.513	114.432	376.25
3524	methyl nonyl sulfide	C10H22S	7.16824	1809.06	195.094	176.85	276.85
3525	methyloctacosylamine	C29H61N	6.056	1450	9.66667	331.378	497
3526	2-methyloctadecane	C19H40	7.04321	1929.69	137.6	181.715	478.491
3527	3-methyloctadecane	C19H40	7.04474	1934.56	137.6	182.44	479.746
3528	methyloctadecylamine	C19H41N	7.59025	2435.39	170.13	230.559	491.35
3529	methyl octadecyl sulfide	C19H40S	7.20937	2103.03	124	311.85	411.85
3530	2-methyloctane	C9H20	7.13732	1553.89	221.781	-80.37	313.6
3531	3-methyloctane	C9H20	7.17567	1594.94	227.131	-107.6	317

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3532	4-methyloctane	C9H20	7.18954	1601.06	229.145	-113.2	314.5
3533	methyloctatriacontylamine	C39H81N	8.99068	4827.71	273.15	377.431	567
3534	methyloctylamine	C9H21N	7.11847	1516.17	171.085	97.6753	357.45
3535	methyl octyl sulfate	C9H20O4S	---	---	---	---	---
3536	methyl octyl sulfide	C9H20S	7.15298	1737.33	199.813	156.85	256.85
3537	methyl oleate	C19H36O2	7.84266	2556.27	171.334	19.9	490.85
3538	methylpentacosylamine	C26H55N	5.90641	1300	8.66667	319.028	471
3539	2-methylpentadecane	C16H34	7.07426	1828.55	154.45	146.583	439.899
3540	3-methylpentadecane	C16H34	7.07487	1830.5	154.45	146.872	440.413
3541	methylpentadecylamine	C16H35N	7.5557	2283.57	181.476	197.194	461.15
3542	methyl pentadecyl sulfide	C16H34S	7.22342	2014.32	140	273.85	373.85
3543	2-methylpentanal	C6H12O	7.18264	1398.09	208	37.0423	295.899
3544	3-methylpentanal	C6H12O	7.18968	1421.93	208	40.9122	303.192
3545	4-methylpentanal	C6H12O	7.18968	1421.93	208	40.9122	303.192
3546	2-methylpentane	C6H14	7.07893	1274.64	243.362	-153.6	224.35
3547	3-methylpentane	C6H14	7.07774	1282.36	242.278	-162.9	231.28
3548	2-methylpentanenitrile	C6H11N	6.9354	1309.08	175.865	63.9697	332.292
3549	3-methylpentanenitrile	C6H11N	6.93341	1326.1	174.222	68.8184	340.938
3550	4-methylpentanenitrile	C6H11N	6.93308	1328.93	173.948	69.6265	342.379
3551	methylpentatriacontylamine	C36H75N	8.96713	4693.46	273.15	379.934	548
3552	methylpentylamine	C6H15N	7.01922	1248.59	184.309	40.9838	287.85
3553	methyl pentyl ether	C6H14O	7.03909	1284.91	210	21.0166	269.474
3554	methyl tert-pentyl ether	C6H14O	7.0937	1361.9	236.97	-113.15	260.85

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3555	methyl pentyl sulfate	C6H14O4S	---	---	---	---	---
3556	methyl pentyl sulfide	C6H14S	6.96487	1321.44	195.551	76.505	314.83
3557	methyl phenyl sulfide	C7H8S	7.11404	1673.52	202.33	124.911	437.613
3558	methyl propanoate	C4H8O2	7.22919	1333.79	227.283	-87.5	257.45
3559	methyl propyl ether	C4H10O	6.98441	1084.66	225.749	0	203.05
3560	methylpropylisopropylamine	C7H17N	6.86278	1184.95	184.729	35.2904	285.638
3561	methyl propyl ketone	C5H10O	7.3543	1548.1	243.751	-76.86	287.93
3562	methyl propyl sulfate	C4H10O4S	7.16586	1780.2	204.905	160.54	260.54
3563	methyl propyl sulfide	C4H10S	7.08299	1355.32	226.969	7.73	289.85
3564	2-methylpyridine	C6H7N	7.15496	1505.99	222.949	-66.71	347.85
3565	3-methylpyridine	C6H7N	7.10475	1521.86	216.154	-18.14	371.85
3566	4-methylpyridine	C6H7N	7.24381	1612.96	224.341	3.58	373
3567	N-methylpyrrole	C5H7N	6.99512	1345.77	214.356	-56.24	336.85
3568	N-methylpyrrolidine	C5H11N	7.09753	1339.57	238.53	-90	276.85
3569	2-methylquinoline	C10H9N	6.64644	1496.63	150.846	-1	499.85
3570	3-methylquinoline	C10H9N	7.3893	2057	203.951	127.12	497.837
3571	4-methylquinoline	C10H9N	7.20782	1899.06	173.224	141.622	517.44
3572	5-methylquinoline	C10H9N	7.00516	1659.08	142.265	157.856	509.135
3573	6-methylquinoline	C10H9N	7.37567	2090.93	200.092	137.179	516.603
3574	7-methylquinoline	C10H9N	7.25586	1924.93	182.249	134.365	505.804
3575	8-methylquinoline	C10H9N	7.31931	1960.24	193.724	125.367	491.41
3576	methyl salicylate	C8H8O3	7.55785	1854.43	175.998	-8	427.85
3577	methyl silane	CH6Si	7.10688	873.39	263.567	-156.81	79.35

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3578	alpha-methylstyrene	C9H10	7.12904	1641.01	220.782	-23.2	380.85
3579	m-methylstyrene	C9H10	7.23895	1742.14	228.144	-86.34	383.85
3580	p-methylstyrene	C9H10	7.09	1630.34	214.55	-34.13	391.85
3581	3-methyl sulfolane	C5H10O2S	7.40961	2174.62	204.177	0.5	543.85
3582	methyltetracosylamine	C25H53N	6.15815	1369.86	6.97904	312.909	564.542
3583	2-methyltetradecane	C15H32	7.07676	1789.91	161.38	133.169	425.83
3584	3-methyltetradecane	C15H32	7.07838	1795.22	161.38	133.964	427.258
3585	methyltetradecylamine	C15H33N	7.35711	2020.65	158.411	185.741	449.55
3586	methyl tetradecyl sulfide	C15H32S	7.22529	1980.43	146	259.85	359.85
3587	2-methyltetrahydrofuran	C5H10O	7.13891	1339.48	234.353	-9.71251	263.85
3588	3-methyltetrahydrofuran	C5H10O	6.99166	1430.57	210	49.4187	365.86
3589	methyltetraatriacontylamine	C35H73N	8.95511	4647.75	273.15	380.213	542
3590	2-methylthiacyclohexane	C6H12S	6.98269	1520.9	217.742	36.4751	387.444
3591	3-methylthiacyclohexane	C6H12S	6.98187	1537.93	216.969	40.1299	395.194
3592	4-methylthiacyclohexane	C6H12S	6.97811	1536.36	216.33	40.6683	396.124
3593	2-methylthiacyclopentane	C5H10S	6.95471	1415.7	215.026	22.7176	363.853
3594	3-methylthiacyclopentane	C5H10S	6.95225	1433.83	213.832	27.0558	373.051
3595	2-methylthiacyclopropane	C3H6S	6.99497	1231.22	224.864	21.6277	287.954
3596	2-methylthiophene	C5H6S	7.05816	1392.74	220.843	9	336.85
3597	3-methylthiophene	C5H6S	7.09187	1423.77	222.653	11	341.85
3598	m-methylthiophenol	C7H8S	7.20546	1762.66	212.484	71.5652	443.189
3599	p-methylthiophenol	C7H8S	7.25212	1811.83	219.582	70.2123	442.883
3600	methyltriacontylamine	C31H65N	8.94116	4461.32	273.15	372.746	513

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3601	methyl trichlorosilane	CH3Cl3Si	7.18818	1370.66	251.814	-77.8	243.85
3602	methyltricosylamine	C24H51N	6.37075	1512.68	31.4414	307.258	553.505
3603	2-methyltridecane	C14H30	7.0684	1740.45	167.72	119.085	410.934
3604	3-methyltridecane	C14H30	7.06957	1744.28	167.72	119.661	411.985
3605	methyltridecylamine	C14H31N	7.11758	1741.4	134.021	172.275	437.05
3606	methyl tridecyl sulfide	C14H30S	7.78265	2485.95	211.297	245.85	345.85
3607	methyltritriacontylamine	C34H71N	8.93872	4592.8	273.15	379.206	535
3608	2-methylundecane	C12H26	7.03727	1632.18	181.835	88.1122	377.561
3609	3-methylundecane	C12H26	7.04629	1632.18	181.835	88.1122	377.561
3610	4-methylundecane	C12H26	7.04488	1627.46	181.835	87.3949	376.214
3611	5-methylundecane	C12H26	7.04061	1613.32	181.835	85.2431	372.174
3612	6-methylundecane	C12H26	7.04061	1613.32	181.835	85.2431	372.174
3613	methylundecylamine	C12H27N	6.79909	1370.45	105.758	144.97	409.15
3614	methyl undecyl sulfide	C12H26S	7.61843	2223.04	205.383	213.85	313.85
3615	methyl vinyl ether	C3H6O	7.08447	1016.34	236.276	-122	163.85
3616	monoethanolamine	C2H7NO	8.36214	2117.92	215.389	10.5	364.85
3617	morpholine	C4H9NO	7.40162	1593.63	224.51	-3.1	344.85
3618	N,N-diethylaniline	C10H15N	7.19346	1811.59	203.794	-38	428.85
3619	N,N-dimethylacetamide	C4H9NO	7.29998	1703.98	219.488	-20	384.85
3620	N,N-dimethylaniline	C8H11N	7.40583	1907.55	228.017	2.45	414
3621	N,N-dimethylformamide	C3H7NO	7.24128	1597.92	213.457	-60.43	373.85
3622	N,N'-diphenyl-p-phenylenediamine	C18H16N2	7.75195	2747.44	149.175	135.85	632.85
3623	naphthalene	C10H8	7.17709	1858.77	214.657	80.28	475.2

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3624	neopentane	C5H12	6.98736	1079.25	253.312	-16.57	160.63
3625	neopentyl acetate	C7H14O2	6.8226	1219.07	181.269	46.7878	303.85
3626	neopentyl glycol	C5H12O2	8.29043	2021.78	163.889	126.85	369.85
3627	1-nitro-2,2-dimethylbutane	C6H13NO2	6.97792	1387.51	169.657	82.5815	364.963
3628	1-nitro-2,2-dimethylpropane	C5H11NO2	6.90098	1305.5	174.239	66.4578	340.85
3629	1-nitro-2,3-dimethylbutane	C6H13NO2	7.0407	1433.59	168.623	89.0515	370.406
3630	2-nitro-2,3-dimethylbutane	C6H13NO2	6.91939	1364	168.742	81.8882	369.781
3631	1-nitro-2-ethylbutane	C6H13NO2	7.10167	1445.48	170.611	86.3835	359.941
3632	1-nitro-2-methylbutane	C5H11NO2	6.97386	1365.35	171.579	76.8147	354.85
3633	2-nitro-2-methylbutane	C5H11NO2	6.9087	1304.43	174.049	66.1072	341.85
3634	1-nitro-2-methylpentane	C6H13NO2	7.10135	1448.45	170.341	87.1965	361.364
3635	2-nitro-2-methylpentane	C6H13NO2	6.97674	1398.56	168.601	85.6999	370.519
3636	3-nitro-2-methylpentane	C6H13NO2	7.0426	1415.62	170.297	84.06	361.594
3637	1-nitro-2-methylpropane	C4H9NO2	6.93045	1283.37	175.189	60.1475	335.85
3638	2-nitro-2-methylpropane	C4H9NO2	6.8715	1219.47	178.419	47.6441	318.85
3639	1-nitro-3,3-dimethylbutane	C6H13NO2	6.97705	1395.69	168.876	84.8899	369.076
3640	2-nitro-3,3-dimethylbutane	C6H13NO2	6.92122	1347.07	170.399	77.0371	361.057
3641	1-nitro-3-methylbutane	C5H11NO2	6.97796	1371.72	171.199	78.1668	356.85
3642	2-nitro-3-methylbutane	C5H11NO2	6.94898	1323.12	174.239	67.5667	340.85
3643	1-nitro-3-methylpentane	C6H13NO2	7.10135	1448.45	170.341	87.1965	361.364
3644	2-nitro-3-methylpentane	C6H13NO2	7.04255	1416.06	170.257	84.1818	361.809
3645	3-nitro-3-methylpentane	C6H13NO2	6.97766	1389.95	169.424	83.27	366.19
3646	1-nitro-4-methyl pentane	C6H13NO2	7.10135	1448.45	170.341	87.1965	361.364

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3647	2-nitro-4-methylpentane	C6H13NO2	7.0426	1415.62	170.297	84.06	361.594
3648	m-nitroaniline	C6H6N2O2	8.2219	2845.38	226.884	114	541.85
3649	p-nitroaniline	C6H6N2O2	8.29954	3020.35	221.391	147.5	577.85
3650	nitrobenzene	C6H5NO2	7.53814	2018.37	222.575	5.76	445.85
3651	3-nitrobenzotrifluoride	C7H4F3NO2	7.40372	1847.44	205.683	-1.15	393.85
3652	1-nitrobutane	C4H9NO2	8.15671	2456.1	312.632	86	350.85
3653	2-nitrobutane	C4H9NO2	7.4743	1822.25	257.003	75	341.85
3654	1-nitrodecane	C10H21NO2	7.33358	1873.17	154.675	165.172	443.819
3655	1-nitrododecane	C12H25NO2	7.40645	2023.76	150.177	191.137	467.493
3656	1-nitroeicosane	C20H41NO2	7.33526	2355.91	134.889	267.271	547.955
3657	nitroethane	C2H5NO2	7.52569	1645.15	240.115	-89.52	319.85
3658	nitroglycerine	C3H5N3O9	8.32302	2305.8	173.838	13	406.85
3659	1-nitroheptadecane	C17H35NO2	7.45245	2296.78	140.399	243.979	518.957
3660	1-nitroheptane	C7H15NO2	7.20071	1622.52	162.591	120.888	402.153
3661	1-nitrohexadecane	C16H33NO2	7.46444	2256.61	142.319	234.579	508.848
3662	1-nitrohexane	C6H13NO2	7.15516	1535.04	165.628	104.719	386.17
3663	2-nitrohexane	C6H13NO2	7.10036	1457.81	169.49	89.7577	365.846
3664	3-nitrohexane	C6H13NO2	7.10036	1457.81	169.49	89.7577	365.846
3665	nitromethane	CH3NO2	7.5385	1588.83	239.919	-28.55	315
3666	1-nitrononadecane	C19H39NO2	7.38879	2343.81	136.924	259.547	537.246
3667	1-nitrononane	C9H19NO2	7.29119	1791.47	157.195	150.932	430.552
3668	1-nitrooctadecane	C18H37NO2	7.42753	2326.11	138.602	252.314	528.411
3669	1-nitrooctane	C8H17NO2	7.24631	1709.78	159.657	136.707	417.598

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3670	1-nitropentadecane	C15H31NO2	7.46443	2209.91	144.132	224.967	499.309
3671	1-nitropentane	C5H11NO2	7.11103	1445.16	169.028	87.4832	368.276
3672	2-nitropentane	C5H11NO2	6.9789	1339.29	174.809	68.6198	337.85
3673	3-nitropentane	C5H11NO2	6.9789	1339.29	174.809	68.6198	337.85
3674	1-nitropropane	C3H7NO2	7.52378	1717.69	238.777	-103.99	331.85
3675	2-nitropropane	C3H7NO2	7.49159	1671.27	242.22	-91.32	320.85
3676	1-nitrotetradecane	C14H29NO2	7.45387	2154.28	146.08	214.363	489.052
3677	m-nitrotoluene	C7H7NO2	7.86534	2473.15	264.314	16.05	460.85
3678	p-nitrotoluene	C7H7NO2	8.10268	2714.94	281.417	51.6	462.85
3679	1-nitrotridecane	C13H27NO2	7.43414	2090.77	148.174	202.802	478.031
3680	1-nitroundecane	C11H23NO2	7.37246	1950.9	152.34	178.583	456.109
3681	nonacosane	C29H60	7.12559	2233.6	85.4	215.356	490.798
3682	1-nonacosene	C29H58	5.90038	1362.54	11.2379	186.221	602.334
3683	nonacosylamine	C29H61N	5.86027	1450	9.66667	355.285	527
3684	nonacosylbenzene	C35H64	6.36225	1750	11.6667	227.072	541
3685	nonacosylcyclohexane	C35H70	6.33476	1750	11.6667	226.627	545
3686	nonacosylcyclopentane	C34H68	6.00313	1848.46	105.014	303.393	537
3687	1-nonacosyne	C29H56	7.87158	4049.27	374.353	307.873	597.09
3688	nonadecanal	C19H38O	7.43282	2295.28	154.235	202.573	501.063
3689	nonadecane	C19H40	7.28529	2171.97	163.227	32.18	482.78
3690	1,2-nonadecanediol	C19H40O2	8.79034	4012.58	273.001	292.838	558.632
3691	1,3-nonadecanediol	C19H40O2	8.79036	4077.59	273.001	284.562	572.104
3692	1,4-nonadecanediol	C19H40O2	8.79039	4201.72	273.001	319.506	597.824

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3693	nonadecanenitrile	C19H37N	7.2892	2259.7	138.591	288.638	528.473
3694	1-nonadecanethiol	C19H40S	7.25347	2225.21	136.882	219	532.14
3695	2-nonadecanethiol	C19H40S	7.17271	2103.03	124	245.238	521.85
3696	nonadecanoic acid	C19H38O2	7.93765	2717.94	151.478	176.85	536.85
3697	1-nonadecanol	C19H40O	7.36374	2102.91	111.243	243.766	502.15
3698	2-nonadecanol	C19H40O	6.93991	1741.35	75.0004	243.766	509.65
3699	2-nonadecanone	C19H38O	8.21269	3284.44	273.001	214.625	493.365
3700	1-nonadecene	C19H38	7.42605	2242.82	164.424	23.4	486.85
3701	nonadecyl acetate	C21H42O2	7.59737	2650	190	321.85	421.85
3702	nonadecylamine	C19H41N	7.65358	2568.26	168.107	219.601	513.15
3703	nonadecylbenzene	C25H44	6.89704	2027.16	94.7424	161.956	568.695
3704	nonadecyl butanoate	C23H46O2	5.09928	1150	7.66667	338.632	560.71
3705	nonadecylcyclohexane	C25H50	6.74649	1935.45	88.6746	161.174	570.163
3706	nonadecylcyclopentane	C24H48	6.8985	2045.35	109.086	268.189	556.844
3707	nonadecyl formate	C20H40O2	9.13705	3950	190	391.37	491.37
3708	nonadecyl propanoate	C22H44O2	8.48694	3800	190	437.83	537.83
3709	1-nonadecyne	C19H36	7.63091	2590	218.243	208	485.79
3710	2-nonadecyne	C19H36	7.7364	2796.1	236.852	196.298	502.721
3711	3-nonadecyne	C19H36	7.56665	2526.67	212.214	187.089	487.512
3712	n-nonaheptacontane	C69H140	7.22079	2657.8	-37.6	390.823	699.632
3713	1-nonanal	C9H18O	7.42543	1825.65	206.718	-18	366.85
3714	nonane	C9H20	7.1884	1607.74	222.414	-53.52	322.5
3715	1,19-nonanecanediol	C19H40O2	8.7672	4108.71	273.001	308.291	582.226

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3716	1,2-nonanediol	C9H20O2	9.65882	3653.35	273.001	173.526	411.577
3717	1,3-nonanediol	C9H20O2	9.65885	3727.92	273.001	182.64	425.547
3718	1,4-nonanediol	C9H20O2	9.6589	3870.29	273.001	200.037	452.217
3719	1,9-nonanediol	C9H20O2	9.72045	3816.52	273.001	189.982	433.508
3720	nonanenitrile	C9H17N	7.12671	1641.6	162.232	128.338	404.043
3721	2-nonanethiol	C9H20S	7.13884	1737.33	199.813	83.1934	398.85
3722	nonanoic acid	C9H18O2	7.58695	1969.53	162.903	12.4	429.85
3723	1-nonanol	C9H20O	7.04565	1520.83	152.06	-5	399.85
3724	2-nonanol	C9H20O	7.87942	1966.54	194.918	-35	349.85
3725	3-nonanol	C9H20O	8.57326	2662.36	273	102.184	347.253
3726	4-nonanol	C9H20O	8.57326	2652.68	273	100.82	344.999
3727	5-nonanol	C9H20O	8.57326	2664.64	273	102.505	347.784
3728	2-nonanone	C9H18O	7.38404	1797.86	205.238	76.3799	371.143
3729	nonatriacontane	C39H80	7.16922	2408.8	43.7	278.891	568.423
3730	1-nonatriacontene	C39H78	6.56006	1950	13	243.604	567
3731	nonatriacontylamine	C39H81N	8.74355	4849.36	273.15	404.396	604
3732	1-nonatriacontyne	C39H76	5.64776	1728.04	111.529	427.873	563
3733	1-nonene	C9H18	7.10879	1541.77	217.79	-81.37	320.1
3734	1-nonyl-[1,2,3,4-tetrahydronaphthalene]C19H30		7.3731	2339.95	172.881	288.459	532.303
3735	2-nonyl-[1,2,3,4-tetrahydronaphthalene]C19H30		7.37256	2350.58	172.311	291.174	536.193
3736	nonyl acetate	C11H22O2	5.89477	826.776	64.3161	136.467	405.55
3737	nonylamine	C9H21N	7.54556	1942.47	214.216	0	374.85
3738	nonylbenzene	C15H24	7.4709	2224.93	202.677	-24.15	467.85

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3739	nonyl butanoate	C13H26O2	6.9072	1685.55	156.626	153.784	433.55
3740	nonylcyclohexane	C15H30	7.15013	1965.61	178.895	141	464.64
3741	nonylcyclopentane	C14H28	7.14708	1891.13	181.166	126	443.8
3742	1-nonylcyclopentene	C14H26	7.21891	1929.33	190.74	145.275	434.757
3743	nonyl formate	C10H20O2	6.87363	1502.05	163.618	114.719	396.75
3744	nonyl mercaptan	C9H20S	7.32205	1896.42	207.201	-20.1	407.85
3745	1-nonylnaphthalene	C19H26	7.31648	2456.35	187.922	11	575.85
3746	2-nonylnaphthalene	C19H26	7.46051	2463.38	168.891	308.556	561.07
3747	nonylphenol	C15H24O	7.82454	2412.87	180.216	6	483.85
3748	nonyl propanoate	C12H24O2	7.22297	1816.06	159.21	156.855	419.95
3749	1-nonyne	C9H16	7.32146	1762.38	246.066	50	337.66
3750	2-nonyne	C9H16	7.01825	1534.87	209.071	53.6536	357.163
3751	3-nonyne	C9H16	7.0196	1519.18	209.96	50.0194	350.209
3752	2-norbornene	C7H10	6.94054	1353.53	237.903	46.25	309.85
3753	o,a-dimethylstyrene	C10H12	7.02362	1567.98	206.282	76.4148	381.796
3754	o-chloroaniline	C6H6ClN	7.40423	1879.69	206.706	-2.1	448.85
3755	o-chlorobenzoicacid	C7H5ClO2	7.62541	2162.82	168.849	142	518.85
3756	o-chloronitrobenzene	C6H4ClNO2	7.43046	2007.47	195.387	33	483.85
3757	o-chlorophenol	C6H5ClO	7.95322	2302.63	279.572	8.85	401.85
3758	o-chlorotoluene	C7H7Cl	7.18144	1645.9	223.563	-36.5	382.85
3759	o-cresol	C7H8O	7.36792	1727.17	193.918	31.04	424.4
3760	o-cymene	C10H14	7.11311	1691	221.366	-71.51	388.85
3761	o-dichlorobenzene	C6H4Cl2	6.97294	1596.2	209.647	-17	431.85

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3762	o-diethylbenzene	C10H14	7.04299	1639.33	210.404	-31.22	394.85
3763	o-difluorobenzene	C6H4F2	7.08993	1298.09	216.889	31	281.31
3764	o-dinitrobenzene	C6H4N2O4	7.67129	2326.99	166.904	116.93	557.85
3765	o-ethylaniline	C8H11N	7.43607	1922.54	212.549	-46.6	430.85
3766	o-ethylphenol	C8H10O	7.407	1816.05	196.712	94.7482	429.85
3767	o-ethylstyrene	C10H12	7.06735	1635.7	203.415	89.185	399.631
3768	o-ethylthiophenol	C8H10S	7.16724	1753.58	199.1	140.264	449.5
3769	o-ethyltoluene	C9H12	7.04815	1615.2	222.406	-80.8	378
3770	o-methylstyrene	C9H10	7.17481	1668.05	218.652	-68.57	385.85
3771	o-methylthiophenol	C7H8S	7.23715	1793.05	217.395	70.0833	441.812
3772	o-nitroaniline	C6H6N2O2	8.28978	2810.04	234.666	71.5	510.85
3773	o-nitroanisole	C7H7NO3	7.55875	2185.16	194.121	10.45	508.85
3774	o-nitrotoluene	C7H7NO2	7.69137	2219.18	238.825	-3.17	446.85
3775	o-phenylenediamine	C6H8N2	7.51273	2028.77	186.147	103.8	507.85
3776	o-terphenyl	C18H14	7.42184	2386.78	189.753	56.2	617.8
3777	o-toluic acid	C8H8O2	7.58639	2036.9	174.019	103.7	477.85
3778	o-toluidine	C7H9N	7.27584	1747.7	197.253	-23.68	421
3779	o-xylene	C8H10	7.14914	1566.59	222.596	-25.17	357.22
3780	octacosane	C28H58	7.12084	2211.6	90	207.998	481.642
3781	1-octacosene	C28H56	6.06147	1451.26	26.2781	179.24	588.548
3782	octacosylamine	C28H59N	5.81377	1400	9.33333	351.623	518
3783	octacosylbenzene	C34H62	6.31285	1700	11.3333	221.607	534
3784	octacosylcyclohexane	C34H68	6.28535	1700	11.3333	221.122	538

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3785	octacosylcyclopentane	C33H66	6.14116	1910	105.826	303.689	530
3786	1-octacosyne	C28H54	8.13913	4324.82	394.473	295.873	585.336
3787	octadecanal	C18H36O	7.49719	2305.85	162.493	192.406	489.16
3788	octadecane	C18H38	7.34072	2172.97	170.513	28.18	472.11
3789	1,2-octadecanediol	C18H38O2	8.96257	4044.37	273.001	283.799	541.182
3790	1,3-octadecanediol	C18H38O2	8.96258	4111.28	273.001	276.235	554.649
3791	1,4-octadecanediol	C18H38O2	8.96262	4239.02	273.001	310.593	580.359
3792	1,18-octadecanediol	C18H38O2	8.94776	4149.8	273.001	299.48	564.477
3793	octadecanenitrile	C18H35N	7.31707	2229.94	140.663	278.73	517.568
3794	1-octadecanethiol	C18H38S	7.31342	2245.85	146.655	209	522.21
3795	2-octadecanethiol	C18H38S	7.19784	2085.13	129	235.486	513.85
3796	octadecanoic acid	C18H36O2	7.86912	2572.31	140.468	176.85	525.85
3797	1-octadecanol	C18H38O	7.03073	1877.62	117.448	57.9	503.85
3798	2-octadecanol	C18H38O	6.90963	1696.13	80.0004	232.219	500.75
3799	2-octadecanone	C18H36O	8.23053	3241.93	273.001	207.043	485.324
3800	1-octadecene	C18H36	7.31231	2093.33	157.556	17.61	474.85
3801	octadecyl acetate	C20H40O2	7.63532	2600	190	306.85	406.85
3802	octadecylamine	C18H39N	7.60988	2483.32	168.118	211.579	504.25
3803	octadecylbenzene	C24H42	7.00426	2092.43	107.447	153.968	559.566
3804	octadecyl butanoate	C22H44O2	5.1023	1100	7.33333	337.632	537.83
3805	octadecylcyclohexane	C24H48	6.85652	2002.83	101.767	153.159	560.782
3806	octadecylcyclopentane	C23H46	6.94665	2039.99	112.741	260.234	546.545
3807	octadecyl formate	C19H38O2	9.12578	3800	190	368.49	468.49

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3808	octadecyl propanoate	C21H42O2	8.37742	3600	190	414.95	514.95
3809	1-octadecyne	C18H34	7.15065	1981.93	151.16	196	474.18
3810	2-octadecyne	C18H34	7.36684	2286.35	184.66	184.659	491.433
3811	3-octadecyne	C18H34	7.36877	2246.54	186.572	176.204	477.372
3812	octafluoro-2-butene	C4F8	6.96659	994.3	246.147	-135	118.85
3813	octafluorocyclobutane	C4F8	7.06892	970.741	237.765	-40.19	115.22
3814	octafluorocyclopentene	C5F8	6.19304	681.29	178.69	0	192.08
3815	octafluoropropane	C3F8	7.20679	959.438	258.535	-147.69	71.9
3816	n-octahexacontane	C68H138	7.21987	2652.9	-35.6	388.223	696.658
3817	octamethylcyclotetrasiloxane	C8H24O4Si4	6.90464	1445.51	184.239	17.65	313.35
3818	1-octanal	C8H16O	7.38945	1738.96	211.697	-27.15	347.85
3819	octane	C8H18	7.14462	1498.96	225.874	-56.77	295.68
3820	"1,2-octanediol"	C8H18O2	9.65382	3555.83	273	161.873	399.641
3821	"1,3-octanediol"	C8H18O2	9.65385	3630.35	273	170.985	413.734
3822	"1,4-octanediol"	C8H18O2	9.6539	3772.61	273.001	188.381	440.638
3823	"1,8-octanediol"	C8H18O2	9.72125	3721.2	273.001	178.375	421.556
3824	octanenitrile	C8H15N	7.08062	1555.96	165.285	112.392	387.977
3825	2-octanethiol	C8H18S	7.05078	1609.48	199.569	66.4262	379.85
3826	octanoic acid	C8H16O2	7.50163	1856.28	161.821	16.5	418.85
3827	1-octanol	C8H18O	7.16033	1536.79	163.905	-15.5	379.35
3828	2-octanol	C8H18O	6.99299	1420.06	165.53	-31.6	364
3829	3-octanol	C8H18O	8.10218	2103.25	228.117	68.0253	328.569
3830	4-octanol	C8H18O	7.9921	2007.41	216.139	70.9566	331.122

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3831	2-octanone	C8H16O	7.08502	1475.8	178.43	-20.3	350.85
3832	octatriacontane	C38H78	7.16932	2394.7	47.4	273.445	561.863
3833	1-octatriacontene	C38H76	6.51602	1900	12.6667	238.757	560
3834	octatriacontylamine	C38H79N	8.73859	4804.26	273.15	405.995	597
3835	1-octatriacontyne	C38H74	5.69192	1749.46	115.337	415.873	557
3836	1-octene	C8H16	7.09965	1461.11	225.041	-101.7	293.45
3837	cis-2-octene	C8H16	7.16218	1527.15	231.058	16.7689	302.913
3838	trans-2-octene	C8H16	7.09038	1501.41	231.665	-87.7	303.85
3839	cis-3-octene	C8H16	7.15222	1507.87	230.115	14.9789	298.955
3840	trans-3-octene	C8H16	7.11187	1509.58	233.486	-110	300.85
3841	cis-4-octene	C8H16	7.15021	1504.72	229.904	14.758	298.435
3842	trans-4-octene	C8H16	7.05997	1464	228.05	-93.78	299.85
3843	1-octyl-[1,2,3,4-tetrahydronaphthalene]	C18H28	7.34473	2278.16	175.351	276.334	524.162
3844	2-octyl-[1,2,3,4-tetrahydronaphthalene]	C18H28	7.34399	2292.25	174.591	279.953	529.407
3845	octyl acetate	C10H20O2	6.91213	1517.31	165.081	114.093	389.05
3846	octylamine	C8H19N	7.54133	1879.97	223.783	-0.4	353.85
3847	octylbenzene	C14H22	7.34646	2082.73	201.988	-36	455.85
3848	octyl butanoate	C12H24O2	6.85659	1604.05	159.457	138.724	418.65
3849	octylcyclohexane	C14H28	7.12617	1901.79	184.361	126	450.46
3850	octylcyclopentane	C13H26	7.12421	1827.14	186.873	112	428.91
3851	1-octylcyclopentene	C13H24	7.17999	1852.82	193.97	130.922	421.735
3852	octyl formate	C9H18O2	7.73249	2151.95	244.747	-39.1	371.85
3853	octyl mercaptan	C8H18S	7.26085	1796.44	211.103	-49.2	390.85

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3854	tert-octyl mercaptan	C8H18S	7.02083	1591.27	228.513	-74.15	353.85
3855	1-octylnaphthalene	C18H24	7.4322	2385.48	172.121	292.778	548.114
3856	2-octylnaphthalene	C18H24	7.43167	2396.25	171.551	295.498	552.055
3857	p-tert-octylphenol	C14H22O	7.38595	2115.6	179.147	85.4	491.85
3858	octyl propanoate	C11H22O2	6.60773	1312.32	124.12	136.176	404.05
3859	1-octyne	C8H14	7.2556	1537.1	225.155	27.6799	301.05
3860	2-octyne	C8H14	6.86715	1339.47	198.286	37.08	334.296
3861	3-octyne	C8H14	6.85797	1316.63	197.909	33.8175	327.51
3862	oleic acid	C18H34O2	8.0641	2729.09	166.667	13.38	507.85
3863	oxalic acid	C2H2O4	8.20735	2370.64	149.212	189.5	530.85
3864	oxazole	C3H3NO	7.28388	1352.11	237.583	-84	280.85
3865	p,a-dimethylstyrene	C10H12	7.01987	1612.82	203.66	87.3191	402.09
3866	paraldehyde	C6H12O3	7.26159	1471.15	211.721	12.6	305.85
3867	pentachlorobenzene	C6HCl5	7.1273	1826.04	154.012	152.825	518.023
3868	pentachloroethane	C2HCl5	6.92727	1495.9	209.802	-29	391.85
3869	pentachlorofluoroethane	C2Cl5F	6.68077	1162.78	168.097	100	356.95
3870	pentacosane	C25H52	7.10352	2138.8	104.6	184.239	451.866
3871	1-pentacosene	C25H50	6.53579	1732.58	73.0336	156.88	553.015
3872	pentacosylamine	C25H53N	6.37987	1636.53	28.7065	335.999	598.818
3873	pentacosylbenzene	C31H56	6.38649	1722.73	29.4097	203.817	512
3874	pentacosylcyclohexane	C31H62	6.2602	1660.59	25.3884	203.337	516
3875	pentacosylcyclopentane	C30H60	6.52704	2063.1	109.816	298.724	506
3876	1-pentacosyne	C25H48	8.49456	4420.58	388.456	259.873	552.068

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3877	pentadecanal	C15H30O	7.65123	2325.09	190.397	159.175	455.332
3878	pentadecane	C15H32	7.29987	1985.73	178.677	9.95	433.65
3879	1,2-pentadecanediol	C15H32O2	9.36666	4040.69	273.001	253.975	492.926
3880	1,3-pentadecanediol	C15H32O2	9.36669	4112.05	273.001	248.2	506.449
3881	1,4-pentadecanediol	C15H32O2	9.36673	4248.28	273.001	281.044	532.266
3882	1,15-pentadecanediol	C15H32O2	9.37932	4172.04	273.001	270.21	515.513
3883	pentadecanenitrile	C15H29N	7.32676	2085.98	147.187	209.413	483.227
3884	1-pentadecanethiol	C15H32S	7.42034	2243.94	173.602	176	491.62
3885	2-pentadecanethiol	C15H32S	7.19548	1980.43	146	200.329	483.85
3886	pentadecanoic acid	C15H30O2	7.64964	2187.3	119.766	52.53	492.85
3887	1-pentadecanol	C15H32O	8.12423	2621.38	195.077	195.785	449.38
3888	2-pentadecanol	C15H32O	6.86263	1576.8	97.0003	195.785	470.05
3889	2-pentadecanone	C15H30O	7.54693	2221.04	183.994	155.256	450.57
3890	1-pentadecene	C15H30	7.29191	1986.27	181.83	-3.73	434.85
3891	pentadecyl acetate	C17H34O2	7.76275	2450	190	261.85	361.85
3892	pentadecylamine	C15H33N	7.41658	2173.34	166.157	175.127	473.35
3893	pentadecylbenzene	C21H36	7.77891	2645.34	174.066	216	526.85
3894	pentadecyl butanoate	C19H38O2	5.11336	950	6.33333	334.632	469.19
3895	pentadecylcyclohexane	C21H42	7.02845	2045.58	126.182	213	530.31
3896	pentadecylcyclopentane	C20H40	6.89767	1871.14	113.972	203	506.85
3897	1-pentadecylcyclopentene	C20H38	7.35504	2283.42	175.351	213.124	494.02
3898	pentadecyl formate	C16H32O2	8.79736	3239.51	197.685	248.248	474.15
3899	pentadecyl propanoate	C18H36O2	7.99756	3000	190	346.31	446.31

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3900	1-pentadecyne	C15H28	7.3573	2093.13	199.573	140	438.26
3901	2-pentadecyne	C15H28	7.32145	2119.41	197.277	147.605	456.553
3902	3-pentadecyne	C15H28	7.31941	2082.66	198.216	140.798	444.68
3903	1,2-pentadiene	C5H8	6.88699	1126.51	236.335	-137.26	226.85
3904	cis-1,3-pentadiene	C5H8	6.8682	1119.38	236.661	-140.8	225.85
3905	trans-1,3-pentadiene	C5H8	6.73433	1039.11	227.633	-87.44	226.85
3906	1,4-pentadiene	C5H8	6.75043	1022.71	238.334	-148.29	205.85
3907	2,3-pentadiene	C5H8	6.99884	1168.69	235.549	-125.65	223.85
3908	pentaerythritol	C5H12O4	10.673	4244.33	186.84	261	506.85
3909	pentaerythritol tetranitrate	C5H8N4O12	8.50487	2380.81	153.477	140.5	402.85
3910	pentaethylbenzene	C16H26	7.56363	2346.39	224.053	86	450.49
3911	pentafluoroethane	C2HF5	6.99473	811.133	245.168	-103	68.85
3912	1,1,1,2,2-pentafluoropropane	C3H3F5	6.59647	695.465	207.172	-23.15	112.041
3913	1,1,1,2,3-pentafluoropropane	C3H3F5	6.74066	785.524	206.662	-23.15	130.69
3914	1,1,1,3,3-pentafluoropropane	C3H3F5	6.74066	785.524	206.662	-23.15	130.69
3915	1,1,2,2,3-pentafluoropropane	C3H3F5	6.77934	893.656	203.229	-23.15	174.29
3916	1,1,2,3,3-pentafluoropropane	C3H3F5	6.83643	915.725	204.65	-23.15	168.231
3917	n-pentahexacontane	C65H132	7.22221	2637.4	-29.5	380.231	687.492
3918	2,2,3,4,4-pentamethyl-3-ethylpentane	C12H26	6.63414	1485.7	181.835	81.8605	415.456
3919	2,2,3,4,4-pentamethyl-3-pentanol	C10H22O	8.04589	2414.16	273	94.5204	364.762
3920	pentamethylbenzene	C11H16	7.09984	1800.5	194.958	138.415	441.689
3921	2,2,3,3,4-pentamethylheptane	C12H26	6.72029	1466.05	181.835	74.4538	386.915
3922	2,2,3,3,5-pentamethylheptane	C12H26	6.71238	1440.04	181.835	70.2553	378.544

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3923	2,2,3,3,6-pentamethylheptane	C12H26	6.71104	1435.7	181.835	69.5556	377.149
3924	2,2,3,4,4-pentamethylheptane	C12H26	6.72289	1474.72	181.835	75.8535	389.705
3925	2,2,3,4,5-pentamethylheptane	C12H26	6.76683	1460.5	181.835	71.4238	374.477
3926	2,2,3,4,6-pentamethylheptane	C12H26	6.75853	1434.12	181.835	67.2068	366.159
3927	2,2,3,5,5-pentamethylheptane	C12H26	6.70288	1409.71	181.835	65.3578	368.779
3928	2,2,3,5,6-pentamethylheptane	C12H26	6.75965	1437.63	181.835	67.769	367.268
3929	2,2,3,6,6-pentamethylheptane	C12H26	6.70011	1401.05	181.835	63.9587	365.989
3930	2,2,4,4,5-pentamethylheptane	C12H26	6.71504	1448.7	181.835	71.6548	381.334
3931	2,2,4,4,6-pentamethylheptane	C12H26	6.70094	1403.65	181.835	64.3784	366.826
3932	2,2,4,5,5-pentamethylheptane	C12H26	6.7015	1405.38	181.835	64.6583	367.384
3933	2,2,4,5,6-pentamethylheptane	C12H26	6.7543	1420.93	181.835	65.0986	362
3934	2,2,4,6,6-pentamethylheptane	C12H26	6.69016	1370.55	181.835	59.0274	356.154
3935	2,2,5,5,6-pentamethylheptane	C12H26	6.7015	1405.38	181.835	64.6583	367.384
3936	2,3,3,4,4-pentamethylheptane	C12H26	6.72418	1479.06	181.835	76.5533	391.1
3937	2,3,3,4,5-pentamethylheptane	C12H26	6.77492	1486.91	181.835	75.6414	382.795
3938	2,3,3,4,6-pentamethylheptane	C12H26	6.76819	1464.9	181.835	72.1267	375.864
3939	2,3,3,5,5-pentamethylheptane	C12H26	6.72029	1466.05	181.835	74.4538	386.915
3940	2,3,3,5,6-pentamethylheptane	C12H26	6.76409	1451.7	181.835	70.0181	371.705
3941	2,3,4,4,5-pentamethylheptane	C12H26	6.77492	1486.91	181.835	75.6414	382.795
3942	2,3,4,4,6-pentamethylheptane	C12H26	6.76132	1442.91	181.835	68.6124	368.932
3943	2,3,4,5,5-pentamethylheptane	C12H26	6.7709	1473.7	181.835	73.5325	378.636
3944	2,3,4,5,6-pentamethylheptane	C12H26	6.82308	1485.58	181.835	73.2848	371.931
3945	2,4,4,5,5-pentamethylheptane	C12H26	6.71504	1448.7	181.835	71.6548	381.334

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3946	3,3,4,4,5-pentamethylheptane	C12H26	6.72801	1492.08	181.835	78.6529	395.285
3947	3,3,4,5,5-pentamethylheptane	C12H26	6.7318	1505.1	181.835	80.7526	399.47
3948	2,2,3,3,4-pentamethylhexane	C11H24	6.69644	1418.27	187.7	61.2745	375.737
3949	2,2,3,3,5-pentamethylhexane	C11H24	6.67883	1360.45	187.7	51.8651	356.575
3950	2,2,3,4,4-pentamethylhexane	C11H24	6.69896	1426.84	187.7	62.6687	378.576
3951	2,2,3,4,5-pentamethylhexane	C11H24	6.73839	1395.29	187.7	55.4492	357.271
3952	2,2,3,5,5-pentamethylhexane	C11H24	6.67272	1341.2	187.7	48.7293	350.187
3953	2,2,4,4,5-pentamethylhexane	C11H24	6.68613	1384	187.7	55.6982	364.381
3954	2,3,3,4,4-pentamethylhexane	C11H24	6.70021	1431.13	187.7	63.3658	379.995
3955	2,3,3,4,5-pentamethylhexane	C11H24	6.74771	1425.73	187.7	60.3509	367.14
3956	2,2,3,3,4-pentamethylpentane	C10H22	6.94212	1568.22	220.077	44	370.65
3957	2,2,3,4,4-pentamethylpentane	C10H22	6.97171	1575.01	225.704	38	354.15
3958	pentanal	C5H10O	7.27832	1453.59	227.549	-91.15	280.85
3959	pentane	C5H12	7.00877	1134.15	238.678	-129.73	196.5
3960	1,2-pentanediol	C5H12O2	9.58802	3232.87	273	125.584	364.827
3961	1,3-pentanediol	C5H12O2	9.58805	3313.38	273	135.507	380.706
3962	1,4-pentanediol	C5H12O2	7.55211	1577.57	135.715	137.864	384.477
3963	1,5-pentanediol	C5H12O2	9.21354	2982.19	231.918	-16	399.85
3964	2-pentanethiol	C5H12S	7.05377	1407.84	224.971	7.58408	306.85
3965	3-pentanethiol	C5H12S	7.12107	1455.59	229.378	8.42122	306.85
3966	pentanoic acid	C5H10O2	7.61722	1828.33	200.516	-34	377.85
3967	1-pentanol	C5H12O	7.45784	1516.51	193.53	-77.59	313
3968	2-pentanol	C5H12O	7.61023	1502.48	198.688	-73.15	278.85

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3969	3-pentanol	C5H12O	7.7147	1573.76	210.267	-69	273.85
3970	pentatriacontane	C35H72	7.15799	2348.6	59.1	256.016	540.758
3971	1-pentatriacontene	C35H70	6.37615	1750	11.6667	223.029	539
3972	pentatriacontylamine	C35H73N	8.73939	4681.88	273.15	407.573	576
3973	pentatriacontylbenzene	C41H76	6.66543	2050	13.6667	256.522	578
3974	pentatriacontylcyclohexane	C41H82	6.62397	2050	13.6667	256.179	584
3975	pentatriacontylcyclopentane	C40H80	5.17665	1445.83	103.763	287.052	576
3976	1-pentatriacontyne	C35H68	5.84797	1819.77	127.303	379.873	536
3977	1-pentene	C5H10	7.02741	1132.42	243.136	-163.15	191.63
3978	cis-2-pentene	C5H10	7.05033	1160.24	241.338	-151.4	202.78
3979	trans-2-pentene	C5H10	7.05181	1161.52	242.135	-140.26	202.22
3980	1-pentene-3-yne	C5H6	7.12893	1270.25	239.765	-123.15	246.85
3981	1-pentene-4-yne	C5H6	6.99974	1169.1	241.337	-123.15	229.85
3982	trans-2-pentenoic acid	C5H8O2	6.96646	1459.4	157.202	108.659	430.517
3983	cis-2-pentenoic acid	C5H8O2	6.9705	1416.83	161.44	96.476	408.209
3984	trans-3-pentenoic acid	C5H8O2	6.96831	1439.53	159.18	102.974	420.106
3985	cis-3-pentenoic acid	C5H8O2	6.99194	1229.6	180.09	42.8724	310.054
3986	4-pentenoic acid	C5H8O2	6.9864	1433.1	161.06	99.064	410.209
3987	tert-pentyl-alcohol	C5H12O	7.00538	1125.64	170.91	-8.8	272
3988	1-pentyl-[1,2,3,4-tetrahydronaphthalene]C15H22		7.23511	2062.2	183.97	233.981	494.451
3989	2-pentyl-[1,2,3,4-tetrahydronaphthalene]C15H22		7.23403	2080.62	182.95	238.826	501.773
3990	pentyl acetate	C7H14O2	7.33379	1636	218.395	-70.8	324.85
3991	tert-pentyl acetate	C7H14O2	6.87619	1223.46	182.219	44.3868	298.85

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3992	pentylamine	C5H13N	7.34146	1488.24	229.138	-55	281.85
3993	pentylbenzene	C11H16	7.33675	1937.75	229.409	-75	406.75
3994	pentyl butanoate	C9H18O2	6.80187	1391.68	169.926	91.4357	363.55
3995	pentylcyclohexane	C11H22	7.04049	1683.04	200.89	78	400.86
3996	pentylcyclopentane	C10H20	7.05449	1613.88	206.072	60	374.34
3997	1-pentylcyclopentene	C10H18	7.05949	1604.57	204.99	82.4453	374.321
3998	pentyl formate	C6H12O2	7.46279	1612.1	218.384	-73.5	302.85
3999	pentyl Mercaptan	C5H12S	7.15741	1514.57	227.513	-75.7	324.85
4000	1-pentyl-naphthalene	C15H18	7.46457	2337.72	203	185	520.17
4001	2-pentyl-naphthalene	C15H18	7.48938	2381.4	206.724	190	524.33
4002	pentyl propanoate	C8H16O2	6.89741	1374.75	173.517	80.1132	344.65
4003	1-pentyne	C5H8	7.2117	1223.32	242.283	-105.7	208.05
4004	2-pentyne	C5H8	6.80954	1078.84	218.534	-33	248.84
4005	alpha-phellandrene	C10H16	7.16911	1695.59	220.401	-53.15	375.85
4006	beta-phellandrene	C10H16	7.14903	1675.74	218.609	-53.15	374.85
4007	phenanthrene	C14H10	7.5004	2565.81	215.12	99.23	596.1
4008	p-phenetidine	C8H11NO	7.51883	2094.46	196.735	3.85	480.85
4009	phenetole	C8H10O	7.30227	1706.4	215.935	-29.52	374
4010	phenol	C6H6O	7.54098	1801.28	204.687	40.91	421.1
4011	1-phenyl-2,2-dimethylpropane	C11H16	6.97145	1593.96	203.66	98.6564	394.501
4012	1-phenyl-2-methylbutane	C11H16	7.08478	1675.58	201.57	109.539	400.495
4013	2-phenyl-2-methylbutane	C11H16	6.96979	1614.44	202.448	103.85	403.778
4014	2-phenyl-2-propanol	C9H12O	8.03839	2245.56	233.391	36	386.85

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4015	1-phenyl-3-methylbutane	C11H16	7.08428	1681.85	201.209	111.093	403.218
4016	2-phenyl-3-methylbutane	C11H16	7.03158	1624.11	203.28	101.282	392.452
4017	phenylbenzene (biphenyl)	C12H10	7.1367	1883.14	187.48	69.22	516.11
4018	m-phenylenediamine	C6H8N2	7.92349	2597.74	228.301	60.85	550.85
4019	p-phenylenediamine	C6H8N2	7.5568	2078.94	177.749	139.85	522.85
4020	2-phenylethanol	C8H10O	8.25639	2462.01	239.1	-26.15	410.85
4021	1-phenylhexadecane	C22H38	7.84553	2723.46	170.552	227	534.85
4022	phenylhydrazine	C6H8N2	7.69242	2180.88	209.754	19.2	487.85
4023	phenyl isocyanate	C7H5NO	7.6215	1942.05	244.056	-30	374.85
4024	phenyl mercaptan	C6H6S	7.06085	1549.9	201.647	-14.89	415.85
4025	1-phenylnaphthalene	C16H12	7.34289	2325.7	187.214	45	575.85
4026	2-phenylpentane	C11H16	7.08665	1652.48	202.9	103.813	390.465
4027	3-phenylpentane	C11H16	7.08638	1655.78	202.71	104.631	391.898
4028	1-phenyltetradecane	C20H34	7.75362	2611.34	181.89	205	518.85
4029	phosgene	CCl2O	7.13083	1060.08	241.87	-127.78	181.85
4030	phthalic acid	C8H6O4	8.16112	2473.61	143.61	191	526.85
4031	phthalic anhydride	C8H4O3	9.30387	4271.98	380.602	131	517.85
4032	alpha-pinene	C10H16	7.06153	1621.22	231.645	-64	358.85
4033	beta-pinene	C10H16	7.01375	1583.34	217.063	-61.54	369.85
4034	piperazine	C4H10N2	7.37904	1564.9	201.893	106	364.85
4035	piperidine	C5H11N	7.13925	1427.24	228.756	-10.5	320.9
4036	propane	C3H8	7.01887	889.864	257.084	-187.69	96.67
4037	1,2-propanediamine	C3H10N2	7.56852	1579.22	217.586	-36.62	313.85

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4038	1,3-propanediol	C3H8O2	9.73868	3368.78	276.828	-26.7	384.85
4039	1,2-propanediol(propylene glycol)	C3H8O2	9.18762	2651.27	232.783	-60	352.85
4040	propanoic acid	C3H6O2	7.66944	1727.17	219.512	-20.7	330.85
4041	propargyl alcohol	C3H4O	8.03112	1838.05	243.282	-51.8	306.85
4042	propargyl chloride	C3H3Cl	7.02798	1230.74	238.915	19.85	267.85
4043	cis-1-propenylbenzene	C9H10	6.97224	1510.68	199.22	18	391.45
4044	trans-1-propenylbenzene	C9H10	6.9217	1462.53	191.924	105	391.45
4045	2-propenylbenzene	C9H10	7.01198	1490.6	205.019	50.4025	367.769
4046	beta-propiolactone	C3H4O2	7.49489	1754.89	218.335	-33.4	412.85
4047	propionaldehyde	C3H6O	7.30641	1285.88	242.556	-80	222.85
4048	propionic anhydride	C6H10O3	7.88478	2020.68	234.815	-45	344.85
4049	propionitrile	C3H5N	7.29327	1480.58	238.197	-92.89	291.25
4050	2-propyl-1,3-propanediol	C6H14O2	9.61598	3192.54	273	119.258	346.885
4051	2-propyl-1,4-butanediol	C7H16O2	9.6387	3279.47	273	128.818	354.832
4052	2-propyl-1-heptanol	C10H22O	8.6188	2816.78	273	121.414	370.248
4053	2-propyl-1-hexanol	C9H20O	8.57324	2629.05	273	97.4908	339.496
4054	3-propyl-1-hexanol	C9H20O	8.57324	2629.05	273	97.4908	339.496
4055	2-propyl-1-pentanol	C8H18O	7.58795	1653.77	172.332	78.6971	334.347
4056	2-propyl-1-pentene	C8H16	7.07147	1435.25	224.788	11.6045	293.066
4057	4-propyl-4-heptanol	C10H22O	8.47465	2612.32	273	100.32	344.536
4058	1-propyl-[1,2,3,4-tetrahydronaphthalene]C13H18		7.15315	1908.39	190.284	203.025	472.824
4059	2-propyl-[1,2,3,4-tetrahydronaphthalene]C13H18		7.15217	1923.86	189.41	207.169	479.304
4060	propyl acetate	C5H10O2	7.22305	1408.02	222.76	-95	276.25

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4061	propyl acrylate	C6H10O2	7.21702	1440.91	213.296	0	295.85
4062	propyl alcohol	C3H8O	7.77374	1518.16	213.076	-73.15	263.56
4063	propylamine	C3H9N	7.27675	1257.56	237.574	-83	223.8
4064	propylbenzene	C9H12	7.18167	1655.21	225.615	-99.48	365.23
4065	propyl butanoate	C7H14O2	7.36547	1681.07	231.55	-95.2	320.85
4066	propyl butyl sulfide	C7H16S	7.15241	1575.03	210.873	107.85	207.85
4067	propylcyclohexane	C9H18	6.92797	1529.11	221.073	-94.87	366
4068	propylcyclopentane	C8H16	7.01197	1485.23	228.559	-117.34	329.85
4069	1-propylcyclopentene	C8H14	6.98716	1417.81	214.072	43.2412	329.564
4070	propylcyclopropane	C6H12	7.00721	1217.33	225.862	17.2547	246.997
4071	propyl decyl sulfide	C13H28S	7.13871	1863.9	157.9	229.85	329.85
4072	propyl dodecyl sulfide	C15H32S	7.22529	1980.43	146	259.85	359.85
4073	propylene	C3H6	7.01672	860.992	255.895	-184.15	91.61
4074	propyleneimine	C3H7N	7.20945	1270	232.545	-44.15	255.85
4075	1,2-propylene oxide	C3H6O	7.16778	1158	236.22	-111.93	209.1
4076	1,3-propylene oxide	C3H6O	7.17849	1240.34	240.757	-43.15	246.85
4077	propyl formate	C4H8O2	7.21129	1355.8	232.264	-92.9	264.85
4078	propyl heptadecyl sulfide	C20H42S	7.18259	2111.53	119.001	321.85	421.85
4079	4-propylheptane	C10H22	7.08282	1541.67	209.378	44	327.85
4080	propyl heptyl sulfide	C10H22S	7.16824	1809.06	195.094	176.85	276.85
4081	propyl hexadecyl sulfide	C19H40S	7.20937	2103.03	124	311.85	411.85
4082	propyl hexyl sulfide	C9H20S	7.15298	1737.33	199.813	156.85	256.85
4083	propyl isocyanide	C4H7N	6.91079	1147.02	185.622	25.4728	280.937

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4084	propylisopropylamine	C6H15N	6.94736	1166.58	188.573	24.6869	265.407
4085	propyl isopropyl ether	C6H14O	6.95564	1181.7	210	5.69693	245.808
4086	propyl mercaptan	C3H8S	7.11863	1284.31	235.338	-113.2	262.85
4087	propyl methacrylate	C7H12O2	7.17755	1547.39	219.281	-50.15	325.85
4088	1-propylnaphthalene	C13H14	7.34885	2130.42	204.003	155	498.3
4089	2-propylnaphthalene	C13H14	7.34066	2123.5	202.627	160	499.29
4090	propyl nitrate	C3H7NO3	7.72383	1721.67	245.486	-10	120
4091	4-propylnonane	C12H26	7.03045	1580.33	181.835	80.2228	362.746
4092	5-propylnonane	C12H26	7.02749	1570.91	181.835	78.7885	360.052
4093	propyl nonyl sulfide	C12H26S	7.61843	2223.04	205.383	213.85	313.85
4094	4-propyloctane	C11H24	7.00737	1517.34	187.7	64.8789	346.048
4095	propyl octyl sulfide	C11H24S	7.09661	1759.04	170.4	196.85	296.85
4096	propyl pentadecyl sulfide	C18H38S	7.13143	2069.41	135	301.85	401.85
4097	propyl pentyl sulfide	C8H18S	7.09805	1717.84	220.489	136.85	236.85
4098	2-propylphenol	C9H12O	7.17613	1651.12	165	136.455	443.218
4099	3-propylphenol	C9H12O	7.19073	1698.11	165	144.21	457.18
4100	4-propylphenol	C9H12O	7.19739	1720.16	165	147.845	463.725
4101	propyl phenyl sulfide	C9H12S	7.18304	1794.89	197.2	149.1	447.043
4102	propyl propanoate	C6H12O2	7.20119	1501.07	224.94	-75.9	304.85
4103	propyl tetradecyl sulfide	C17H36S	7.25728	2069.41	135	287.85	387.85
4104	2-propylthiophene	C7H10S	7.10723	1552.72	208.885	95.1393	376.082
4105	3-propylthiophene	C7H10S	7.10649	1561.01	208.41	97.2808	379.842
4106	propyl tridecyl sulfide	C16H34S	7.22342	2014.32	140	273.85	373.85

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4107	propyl undecyl sulfide	C14H30S	7.78265	2485.95	211.297	245.85	345.85
4108	pyrene	C16H10	7.4202	2698	199.552	150.66	662.85
4109	pyridine	C5H5N	7.1874	1463.63	224.598	-41.64	346.8
4110	pyrocatechol	C6H6O2	8.71149	3032.88	274.659	104.45	490.85
4111	pyromellitic acid	C10H6O8	9.19171	3487.92	103.832	280.85	619.85
4112	pyrrole	C4H5N	7.20345	1451.6	205.963	-23.41	366.6
4113	pyrrolidine	C4H9N	7.15003	1291.56	215.958	-57.84	295.4
4114	2-pyrrolidone	C4H7NO	7.5694	2089.39	200.634	25	518.85
4115	pyruvic acid	C3H4O3	8.30281	2241.01	248.318	13.6	361.37
4116	quinoline	C9H7N	7.23233	1909.9	201.305	-14.9	509
4117	resorcinol	C6H6O2	7.96913	2282.29	172.036	108.85	536.85
4118	salicylaldehyde	C7H6O2	8.34867	2565.85	272.761	-7	406.85
4119	salicylic acid	C7H6O3	7.97042	2114.97	159.697	158.6	465.85
4120	sebacic acid	C10H18O4	8.44589	2959.84	162.919	134.5	541.85
4121	sorbitol	C6H14O6	10.2336	4586.45	119.915	97.7	685.85
4122	spiropentane	C5H8	7.22104	1250.41	249.058	3	226.59
4123	cis-stilbene	C14H12	7.20754	1941.61	186.898	-5	483.85
4124	trans-stilbene	C14H12	7.14773	2030.21	169.302	124.2	546.85
4125	styrene	C8H8	6.94579	1443.88	210.039	-30.61	374.85
4126	succinic acid	C4H6O4	8.14478	2441.39	145.942	188	532.85
4127	succinic anhydride	C4H4O3	8.03192	2582.17	237.855	119.85	537.85
4128	succinonitrile	C4H4N2	7.4738	2086.17	187.208	58.15	496.85
4129	sulfolane	C4H8O2S	7.415	2207.21	201.794	27.6	575.85

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4130	t-butyl hydroperoxide	C4H10O2	8.0104	1874.75	233.128	4.3	302.85
4131	tartaric acid	C4H6O6	9.67704	3399.75	113.391	206	554.85
4132	terephthalic acid	C8H6O4	8.13159	3394.38	87.6035	427	839.85
4133	m-terphenyl	C18H14	7.56576	2631.92	184.933	86.85	651.7
4134	p-terphenyl	C18H14	7.34905	2408.68	163.067	211.85	652.8
4135	alpha-terpinene	C10H16	7.13456	1673.54	216.227	-53.15	378.85
4136	gamma-terpinene	C10H16	7.13775	1703.3	217.124	-53.15	387.85
4137	terpinolene	C10H16	6.92978	1574.26	203.804	-73.15	398.85
4138	1,1,2,2-tetrabromoethane	C2H2Br4	7.52538	1775.96	138.874	193.5	293.5
4139	1,1,1,2-tetrabromoethane	C2H2Br4	7.44775	1775.96	138.874	158.576	526.978
4140	1,1,1,2-tetrabromopropane	C3H4Br4	7.41161	1771.5	140.991	157.518	515.839
4141	1,1,1,3-tetrabromopropane	C3H4Br4	7.47343	1834.39	139.421	166.498	524.101
4142	1,1,2,2-tetrabromopropane	C3H4Br4	7.41523	1724.39	145.289	145.105	493.217
4143	1,1,2,3-tetrabromopropane	C3H4Br4	7.54518	1885.55	139.245	171.488	525.026
4144	1,1,3,3-tetrabromopropane	C3H4Br4	7.5429	1918.11	136.427	179.791	539.858
4145	1,2,2,3-tetrabromopropane	C3H4Br4	7.47578	1802.43	142.262	158.21	509.148
4146	1,1,2,2-tetrachloro-1,2-difluoroethane	C2Cl4F2	6.95599	1269.97	218.785	26	277.85
4147	1,1,2,2-tetrachloro-1-fluoroethane	C2HCl4F	6.71849	1118.2	174.776	26.9803	324.85
4148	1,1,1,2-tetrachloro-2,2-difluoroethane	C2Cl4F2	7.0158	1308.4	224.923	45.4268	287.35
4149	1,1,1,2-tetrachloro-2-fluoroethane	C2HCl4F	6.71775	1118.69	174.559	27.3119	325.45
4150	1,2,3,4-tetrachlorobenzene	C6H2Cl4	7.49767	2230.43	229.006	123.824	499.728
4151	1,2,3,5-tetrachlorobenzene	C6H2Cl4	7.69517	2438.36	260.377	113.66	488.001
4152	1,2,4,5-tetrachlorobenzene	C6H2Cl4	7.3799	2054.22	211.487	139	486.535

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4153	1,1,1,2-tetrachloroethane	C2H2Cl4	7.03897	1467.16	222.34	-70.21	350.85
4154	1,1,2,2-tetrachloroethane	C2H2Cl4	6.91043	1378.88	197.086	-43.8	371.85
4155	tetrachloroethylene	C2Cl4	7.06892	1458.45	226.986	-22.35	346.85
4156	1,1,1,2-tetrachloropropane	C3H4Cl4	6.68611	1210.06	167.994	64.3084	373.715
4157	1,1,1,3-tetrachloropropane	C3H4Cl4	6.73939	1255.93	166.49	72.1766	381.632
4158	1,1,2,2-tetrachloropropane	C3H4Cl4	6.68465	1223.09	166.542	68.3282	381.358
4159	1,1,2,3-tetrachloropropane	C3H4Cl4	6.7963	1331.75	162.123	88.2442	404.618
4160	1,1,3,3-tetrachloropropane	C3H4Cl4	6.79941	1301.58	165.305	79.2479	387.867
4161	1,2,2,3-tetrachloropropane	C3H4Cl4	6.73796	1269.2	165.051	76.203	389.208
4162	tetrachlorothiophene	C4Cl4S	7.16956	1850.87	198.174	28.82	479.85
4163	tetracontane	C40H82	7.16731	2422.3	40.1	284.165	574.764
4164	1-tetracontene	C40H80	6.60984	2000	13.3333	248.354	573
4165	tetracontylamine	C40H83N	8.7483	4888.5	273.15	401.462	610
4166	1-tetracontyne	C40H78	5.59858	1705.07	107.38	439.873	570
4167	tetracosane	C24H50	7.09722	2112	109.6	175.858	441.255
4168	1-tetracosene	C24H48	6.66817	1804.88	86.5542	148.819	540.962
4169	tetracosylamine	C24H51N	6.61038	1808.03	55.782	329.614	586.572
4170	tetracosylbenzene	C30H54	6.52691	1814.28	43.5948	197.444	504
4171	tetracosylcyclohexane	C30H60	6.39756	1750.45	39.7485	196.877	508
4172	tetracosylcyclopentane	C29H58	6.49	1957.3	95.3121	295.143	608.885
4173	1-tetracosyne	C24H46	8.46927	4238.07	369.361	247.873	541.96
4174	tetradecanal	C14H28O	7.70907	2346.17	202.924	146.777	444.174
4175	tetradecane	C14H30	7.26165	1914.86	183.519	5.86	419.25

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4176	1,2-tetradecanediol	C14H30O2	9.4614	4007.58	273.001	243.279	478.073
4177	1,3-tetradecanediol	C14H30O2	9.46142	4079.98	273.001	238	491.639
4178	1,4-tetradecanediol	C14H30O2	9.46147	4218.2	273.001	270.407	517.537
4179	1,14-tetradecanediol	C14H30O2	9.48335	4146.4	273.001	259.655	500.483
4180	tetradecanenitrile	C14H27N	7.30909	2025.17	149.326	197.927	471.969
4181	1-tetradecanethiol	C14H30S	7.4252	2211.27	180.384	164	480.65
4182	2-tetradecanethiol	C14H30S	7.16278	1926.46	151.9	186.927	472.85
4183	tetradecanoic acid	C14H28O2	7.91297	2450.62	160.791	54.4	482.85
4184	1-tetradecanol	C14H30O	6.91214	1670.73	127.436	37.5	467.85
4185	2-tetradecanol	C14H30O	6.85008	1536.11	103	182.896	458.25
4186	2-tetradecanone	C14H28O	7.41282	2035.25	171.083	146.289	439.505
4187	1-tetradecene	C14H28	7.2715	1926.44	187.657	-12.85	418.85
4188	2-tetradecene	C14H28	7.11328	1903.65	186.773	133.86	443.122
4189	tetradecyl acetate	C16H32O2	7.81046	2400	190	246.85	346.85
4190	tetradecylamine	C14H31N	8.14238	2767.92	234.764	38.19	449.15
4191	tetradecylbenzene	C20H34	6.84018	1873.51	119.183	211.588	520.75
4192	tetradecyl butanoate	C18H36O2	7.26007	2458.53	165.094	304.466	446.85
4193	tetradecylcyclohexane	C20H40	7.0646	2043.82	134.499	203	519.67
4194	tetradecylcyclopentane	C19H38	6.97952	1918.14	128.976	192	498.85
4195	1-tetradecylcyclopentene	C19H36	7.35067	2237.75	177.63	203.357	484.833
4196	tetradecyl formate	C15H30O2	7.95491	2424.89	150.926	223.413	463.55
4197	tetradecyl propanoate	C17H34O2	7.85038	2800	190	323.43	423.43

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4198	1-tetradecyne	C14H26	7.5873	2229.71	221.754	126.032	416.75
4199	3-tetradecyne	C14H26	7.27867	2002.64	200.367	127.798	432.434
4200	1,2,3,4-tetraethylbenzene	C14H22	7.52422	2245.91	232.668	66	435.05
4201	1,2,3,5-tetraethylbenzene	C14H22	7.42588	2131.99	218.567	174	434.37
4202	1,2,4,5-tetraethylbenzene	C14H22	7.41784	2121.02	217.48	174	433.7
4203	tetraethylene glycol	C8H18O5	9.07325	2968.08	171.457	-5	448.85
4204	tetraethylene glycol dimethyl ether	C10H22O5	8.25962	2682.07	222.836	-29.7	431.85
4205	tetraethylenepentamine	C8H23N5	8.5453	2903.29	179.543	-30.15	500.85
4206	1,1,1,2-tetrafluoroethane	C2H2F4	7.01019	902.327	244.514	-101	106.85
4207	1,1,2,2-tetrafluoroethane	C2H2F4	7.19118	954.119	241.404	-65.49	107.847
4208	tetrafluoroethylene	C2F4	7.00263	714.849	249.07	-131.15	33.3
4209	1,1,1,2-tetrafluoropropane	C3H4F4	6.67947	782.252	206.929	-34.06	141.659
4210	1,1,1,3-tetrafluoropropane	C3H4F4	6.74258	889.782	201.008	-19.06	183.953
4211	1,1,2,2-tetrafluoropropane	C3H4F4	6.71557	884.505	203.805	-34.06	184.108
4212	1,1,2,3-tetrafluoropropane	C3H4F4	6.83792	919.456	205.506	-33.9908	176.287
4213	1,1,3,3-tetrafluoropropane	C3H4F4	6.83792	919.456	205.506	-33.9908	176.287
4214	1,2,2,3-tetrafluoropropane	C3H4F4	6.73926	880.26	201.288	-19.06	180.101
4215	n-tetrahexacontane	C64H130	7.21871	2631.8	-27.3	377.346	684.183
4216	tetrahydrofuran	C4H8O	7.10537	1256.68	232.621	-108.5	267
4217	tetrahydrofurfuryl alcohol	C5H10O2	8.29744	2297.33	246.126	-80.15	365.85
4218	1,2,3,4-tetrahydronaphthalene	C10H12	7.16735	1806.14	213.732	-35.75	447
4219	tetrahydrothiophene	C4H8S	7.11636	1491.31	230.974	-96.16	358.8
4220	1,1,1,2-tetraiodoethane	C2H2I4	6.60592	1667.17	106.211	218.851	698.892

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4221	1,1,2,2-tetraiodoethane	C2H2I4	6.65667	1713.42	107.813	222.992	690.461
4222	1,1,1,2-tetraiodopropane	C3H4I4	6.59045	1729.35	102.399	235.806	718.955
4223	1,1,1,3-tetraiodopropane	C3H4I4	6.64454	1762.36	104.03	237.023	710.37
4224	1,1,2,2-tetraiodopropane	C3H4I4	6.59045	1729.35	102.399	235.806	718.955
4225	1,1,2,3-tetraiodopropane	C3H4I4	6.70479	1803.36	105.023	239.942	705.145
4226	1,1,3,3-tetraiodopropane	C3H4I4	6.70479	1803.36	105.023	239.942	705.145
4227	1,2,2,3-tetraiodopropane	C3H4I4	6.64454	1762.36	104.03	237.023	710.37
4228	2,2,3,3-tetramethyl-1-butanol	C8H18O	8.14756	2348.03	272.971	150	343.37
4229	2,3,4,4-tetramethyl-2-hexanol	C10H22O	8.1911	2458.66	273	93.2004	351.777
4230	3,3,5,5-tetramethyl-2-hexanol	C10H22O	8.1911	2457.87	273	93.0818	351.575
4231	2,3,3,4-tetramethyl-2-pentanol	C9H20O	8.13449	2379.13	273	84.3675	347.083
4232	2,3,4,4-tetramethyl-2-pentanol	C9H20O	8.13449	2379.13	273	84.3675	347.083
4233	3,3,4,4-tetramethyl-2-pentanol	C9H20O	8.13449	2379.92	273	84.4859	347.289
4234	2,2,3,4-tetramethyl-3-ethylhexane	C12H26	6.72546	1483.4	181.835	77.2531	392.495
4235	2,2,3,5-tetramethyl-3-ethylhexane	C12H26	6.71238	1440.04	181.835	70.2553	378.544
4236	2,2,4,4-tetramethyl-3-ethylhexane	C12H26	6.72029	1466.05	181.835	74.4538	386.915
4237	2,2,4,5-tetramethyl-3-ethylhexane	C12H26	6.76132	1442.91	181.835	68.6124	368.932
4238	2,2,5,5-tetramethyl-3-ethylhexane	C12H26	6.69309	1379.41	181.835	60.4612	359.014
4239	2,3,4,4-tetramethyl-3-ethylhexane	C12H26	6.73054	1500.76	181.835	80.0527	398.075
4240	2,3,4,5-tetramethyl-3-ethylhexane	C12H26	6.77625	1491.31	181.835	76.3443	384.182
4241	2,2,3,4-tetramethyl-3-ethylpentane	C11H24	6.69896	1426.84	187.7	62.6687	378.576
4242	2,2,4,4-tetramethyl-3-ethylpentane	C11H24	6.69133	1401.13	187.7	58.4862	370.059
4243	2,2,3,4-tetramethyl-3-hexanol	C10H22O	8.1911	2469.29	273	94.7824	354.476

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4244	2,2,3,5-tetramethyl-3-hexanol	C10H22O	8.19122	2725.99	273	133.01	419.687
4245	2,2,4,4-tetramethyl-3-hexanol	C10H22O	8.1911	2458.66	273	93.2004	351.777
4246	2,2,5,5-tetramethyl-3-hexanol	C10H22O	8.19104	2352.43	273	77.381	324.791
4247	2,3,4,4-tetramethyl-3-hexanol	C10H22O	8.19113	2517.09	273	101.901	366.62
4248	2,3,5,5-tetramethyl-3-hexanol	C10H22O	8.19113	2521.61	273	102.573	367.766
4249	2,4,4,5-tetramethyl-3-hexanol	C10H22O	8.26755	2557.89	273	103.691	364.403
4250	3,4,4,5-tetramethyl-3-hexanol	C10H22O	8.19113	2522.4	273	102.692	367.969
4251	3,4,5,5-tetramethyl-3-hexanol	C10H22O	8.19111	2485.22	273	97.1553	358.524
4252	2,2,3,4-tetramethyl-3-isopropylpentane	C12H26	6.67599	1464.31	181.835	76.1485	396.86
4253	2,2,4,4-tetramethyl-3-isopropylpentane	C12H26	6.66317	1421.54	181.835	69.1802	382.818
4254	2,2,3,4-tetramethyl-3-pentanol	C9H20O	8.13448	2349.44	273	79.9086	339.348
4255	2,2,4,4-tetramethyl-3-pentanol	C9H20O	8.13446	2311.6	273	74.2264	329.49
4256	2,2,3,3-tetramethyl-4-ethylhexane	C12H26	6.72159	1470.39	181.835	75.1536	388.31
4257	2,2,3,4-tetramethyl-4-ethylhexane	C12H26	6.73054	1500.76	181.835	80.0527	398.075
4258	2,2,3,5-tetramethyl-4-ethylhexane	C12H26	6.76271	1447.31	181.835	69.3152	370.318
4259	2,2,4,5-tetramethyl-4-ethylhexane	C12H26	6.71636	1453.04	181.835	72.3545	382.729
4260	2,3,3,4-tetramethyl-4-ethylhexane	C12H26	6.73054	1500.76	181.835	80.0527	398.075
4261	2,3,3,5-tetramethyl-4-ethylhexane	C12H26	6.7709	1473.7	181.835	73.5325	378.636
4262	1,2,3,4-tetramethylbenzene	C10H14	7.00693	1655.57	196.141	80	421.95
4263	1,2,3,5-tetramethylbenzene	C10H14	7.27117	1818.38	216.175	-23.69	405.85
4264	1,2,4,5-tetramethylbenzene	C10H14	7.27724	1809.75	214.802	79.23	402
4265	2,2,3,3-tetramethylbutane	C8H18	6.83046	1278.39	217.222	103	294.65
4266	1,1,2,2-tetramethylcyclopentane	C9H18	6.83789	1372.04	213.73	42.2103	336.232

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4267	1,1,cis-2,trans-3-tetramethylcyclopentane	C9H18	6.82902	1359.37	214.3	39.6971	324.729
4268	1,1,cis-2,cis-4-tetramethylcyclopentane	C9H18	6.82902	1359.37	214.3	39.6971	324.729
4269	1,1,cis-2,trans-4-tetramethylcyclopentane	C9H18	6.82902	1359.37	214.3	39.6971	324.729
4270	1,1,3,3-tetramethylcyclopentane	C9H18	6.8428	1325.47	216.588	30.4404	313.666
4271	1,1,cis-3,cis-4-tetramethylcyclopentane	C9H18	6.82806	1368.63	213.73	42.0435	329.178
4272	1,1,cis-3,trans-4-tetramethylcyclopentane	C9H18	6.83178	1333.44	215.896	33.1274	312.272
4273	1,2,2,cis-3-tetramethylcyclopentane	C9H18	6.82649	1384.06	212.78	45.9541	336.593
4274	1,2,2,trans-3-tetramethylcyclopentane	C9H18	6.82649	1384.06	212.78	45.9541	336.593
4275	1,cis-2,cis-3,cis-4-tetramethylcyclopentane	C9H18	6.81586	1402.65	211.45	51.2801	340.066
4276	1,cis-2,cis-3,trans-4-tetramethylcyclopentane	C9H18	6.81802	1381.09	212.78	45.8081	329.8
4277	1,cis-2,trans-3,cis-4-tetramethylcyclopentane	C9H18	6.82025	1359.54	214.11	40.3362	319.535
4278	1,cis-2,trans-3,trans-4-tetramethylcyclopentane	C9H18	6.81802	1381.09	212.78	45.8081	329.8
4279	1,trans-2,cis-3,trans-4-tetramethylcyclopentane	C9H18	6.82143	1348.46	214.794	37.522	314.255
4280	1,trans-2,trans-3,cis-4-tetramethylcyclopentane	C9H18	6.82025	1359.54	214.11	40.3362	319.535
4281	1,1,cis-2,cis-3-tetramethylcyclopentane	C9H18	6.82649	1384.06	212.78	45.9541	336.593
4282	2,2,3,3-tetramethylheptane	C11H24	6.74142	1419.55	187.7	59.5463	365.671
4283	2,2,3,4-tetramethylheptane	C11H24	6.79151	1422.32	187.7	57.887	355.892
4284	2,2,3,5-tetramethylheptane	C11H24	6.78876	1413.5	187.7	56.4807	353.091
4285	2,2,3,6-tetramethylheptane	C11H24	6.78318	1395.88	187.7	53.6683	347.489
4286	2,2,4,4-tetramethylheptane	C11H24	6.72797	1376.13	187.7	52.547	351.574
4287	2,2,4,5-tetramethylheptane	C11H24	6.78177	1391.47	187.7	52.9653	346.089
4288	2,2,4,6-tetramethylheptane	C11H24	6.77202	1361.53	187.7	48.185	336.565
4289	2,2,5,5-tetramethylheptane	C11H24	6.72242	1358.78	187.7	49.7477	345.935

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4290	2,2,5,6-tetramethylheptane	C11H24	6.78177	1391.47	187.7	52.9653	346.089
4291	2,2,6,6-tetramethylheptane	C11H24	6.71819	1345.77	187.7	47.6484	341.706
4292	2,3,3,4-tetramethylheptane	C11H24	6.79961	1448.78	187.7	62.1062	364.295
4293	2,3,3,5-tetramethylheptane	C11H24	6.79151	1422.32	187.7	57.887	355.892
4294	2,3,3,6-tetramethylheptane	C11H24	6.79014	1417.91	187.7	57.1838	354.492
4295	2,3,4,4-tetramethylheptane	C11H24	6.79423	1431.14	187.7	59.2933	358.693
4296	2,3,4,5-tetramethylheptane	C11H24	6.85155	1456.07	187.7	61.1347	356.071
4297	2,3,4,6-tetramethylheptane	C11H24	6.84457	1433.69	187.7	57.603	349.113
4298	2,3,5,5-tetramethylheptane	C11H24	6.78598	1404.69	187.7	55.0745	350.29
4299	2,3,5,6-tetramethylheptane	C11H24	6.84598	1438.17	187.7	58.3093	350.505
4300	2,4,4,5-tetramethylheptane	C11H24	6.78876	1413.5	187.7	56.4807	353.091
4301	2,4,4,6-tetramethylheptane	C11H24	6.77463	1369.46	187.7	49.4503	339.086
4302	2,4,5,5-tetramethylheptane	C11H24	6.79151	1422.32	187.7	57.887	355.892
4303	3,3,4,4-tetramethylheptane	C11H24	6.74664	1436.93	187.7	62.3465	371.31
4304	3,3,4,5-tetramethylheptane	C11H24	6.79827	1444.37	187.7	61.403	362.895
4305	3,3,5,5-tetramethylheptane	C11H24	6.74142	1419.55	187.7	59.5463	365.671
4306	3,4,4,5-tetramethylheptane	C11H24	6.80358	1462.02	187.7	64.2161	368.497
4307	2,2,3,3-tetramethylhexane	C10H22	7.11854	1638.45	226.305	41	349.85
4308	2,2,3,4-tetramethylhexane	C10H22	6.98343	1543.35	217.378	41	347.25
4309	2,2,3,5-tetramethylhexane	C10H22	6.91187	1438.42	208.425	35	328.15
4310	2,2,4,4-tetramethylhexane	C10H22	7.02641	1579.53	227.203	35	337.05
4311	2,2,4,5-tetramethylhexane	C10H22	6.94875	1468.9	213.201	34	325.35
4312	2,2,5,5-tetramethylhexane	C10H22	6.93252	1408.45	210.14	26.85	308.25

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4313	2,3,3,4-tetramethylhexane	C10H22	6.98015	1562.45	216.548	45	359.95
4314	2,3,3,5-tetramethylhexane	C10H22	6.94751	1488.3	212.864	37	336.95
4315	2,3,4,4-tetramethylhexane	C10H22	6.98091	1552.99	217.16	42	353.45
4316	2,3,4,5-tetramethylhexane	C10H22	6.97175	1504.09	211.454	40	340.05
4317	3,3,4,4-tetramethylhexane	C10H22	6.98334	1603.4	220.822	47	373.55
4318	1,2,3,4-tetramethylnaphthalene	C14H16	7.95793	3085.24	295.413	148	537.389
4319	1,2,3,6-tetramethylnaphthalene	C14H16	7.86278	2949.66	279.805	150	537.389
4320	1,2,4,6-tetramethylnaphthalene	C14H16	7.95793	3085.24	295.413	148	537.389
4321	1,2,4,7-tetramethylnaphthalene	C14H16	7.95793	3085.24	295.413	148	537.389
4322	1,2,4,8-tetramethylnaphthalene	C14H16	7.86278	2949.66	279.805	150	537.389
4323	1,2,5,6-tetramethylnaphthalene	C14H16	7.95793	3085.24	295.413	148	537.389
4324	1,2,5,8-tetramethylnaphthalene	C14H16	7.7702	2820.59	264.619	152	537.389
4325	1,2,6,8-tetramethylnaphthalene	C14H16	7.38271	2310.92	201.059	161	537.389
4326	1,3,5,8-tetramethylnaphthalene	C14H16	7.38271	2310.92	201.059	161	537.389
4327	1,3,6,7-tetramethylnaphthalene	C14H16	7.38271	2310.92	201.059	161	537.389
4328	1,4,5,8-tetramethylnaphthalene	C14H16	7.38271	2310.92	201.059	161	537.389
4329	1,4,6,7-tetramethylnaphthalene	C14H16	7.38271	2310.92	201.059	161	537.389
4330	2,3,6,7-tetramethylnaphthalene	C14H16	7.35979	2282.32	197.3	191	537.389
4331	2,2,3,3-tetramethyloctane	C12H26	6.76997	1485.02	181.835	75.5347	382.739
4332	2,2,3,4-tetramethyloctane	C12H26	6.81806	1483.69	181.835	73.1799	371.877
4333	2,2,3,5-tetramethyloctane	C12H26	6.81387	1470.32	181.835	71.0627	367.744
4334	2,2,3,6-tetramethyloctane	C12H26	6.81667	1479.23	181.835	72.4741	370.499
4335	2,2,3,7-tetramethyloctane	C12H26	6.81667	1479.23	181.835	72.4741	370.499

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4336	2,2,4,4-tetramethyloctane	C12H26	6.75915	1449.86	181.835	69.9135	371.649
4337	2,2,4,5-tetramethyloctane	C12H26	6.80677	1448.03	181.835	67.5343	360.855
4338	2,2,4,6-tetramethyloctane	C12H26	6.80389	1439.12	181.835	66.123	358.099
4339	2,2,4,7-tetramethyloctane	C12H26	6.8036	1438.23	181.835	65.9819	357.823
4340	2,2,5,5-tetramethyloctane	C12H26	6.74795	1414.74	181.835	64.2934	360.56
4341	2,2,5,6-tetramethyloctane	C12H26	6.81105	1461.4	181.835	69.6513	364.988
4342	2,2,5,7-tetramethyloctane	C12H26	6.80389	1439.12	181.835	66.123	358.099
4343	2,2,6,6-tetramethyloctane	C12H26	6.74937	1419.12	181.835	64.9958	361.946
4344	2,2,6,7-tetramethyloctane	C12H26	6.81247	1465.86	181.835	70.3569	366.366
4345	2,2,7,7-tetramethyloctane	C12H26	6.74937	1419.12	181.835	64.9958	361.946
4346	2,3,3,4-tetramethyloctane	C12H26	6.82628	1510.46	181.835	77.4148	380.144
4347	2,3,3,5-tetramethyloctane	C12H26	6.81667	1479.23	181.835	72.4741	370.499
4348	2,3,3,6-tetramethyloctane	C12H26	6.81944	1488.15	181.835	73.8857	373.255
4349	2,3,3,7-tetramethyloctane	C12H26	6.81944	1488.15	181.835	73.8857	373.255
4350	2,3,4,4-tetramethyloctane	C12H26	6.81944	1488.15	181.835	73.8857	373.255
4351	2,3,4,5-tetramethyloctane	C12H26	6.87605	1513.54	181.835	75.742	370.824
4352	2,3,4,6-tetramethyloctane	C12H26	6.87323	1504.48	181.835	74.3242	368.085
4353	2,3,4,7-tetramethyloctane	C12H26	6.87181	1499.96	181.835	73.6153	366.715
4354	2,3,5,5-tetramethyloctane	C12H26	6.81806	1483.69	181.835	73.1799	371.877
4355	2,3,5,6-tetramethyloctane	C12H26	6.87323	1504.48	181.835	74.3242	368.085
4356	2,3,5,7-tetramethyloctane	C12H26	6.86607	1481.86	181.835	70.7801	361.236
4357	2,3,6,6-tetramethyloctane	C12H26	6.81527	1474.77	181.835	71.7684	369.122
4358	2,3,6,7-tetramethyloctane	C12H26	6.87464	1509.01	181.835	75.0331	369.454

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4359	2,4,4,5-tetramethyloctane	C12H26	6.81247	1465.86	181.835	70.3569	366.366
4360	2,4,4,6-tetramethyloctane	C12H26	6.80389	1439.12	181.835	66.123	358.099
4361	2,4,4,7-tetramethyloctane	C12H26	6.80244	1434.67	181.835	65.4174	356.721
4362	2,4,5,5-tetramethyloctane	C12H26	6.81387	1470.32	181.835	71.0627	367.744
4363	2,4,5,6-tetramethyloctane	C12H26	6.87181	1499.96	181.835	73.6153	366.715
4364	2,4,5,7-tetramethyloctane	C12H26	6.86068	1465.13	181.835	68.1577	356.168
4365	2,4,6,6-tetramethyloctane	C12H26	6.80677	1448.03	181.835	67.5343	360.855
4366	2,5,5,6-tetramethyloctane	C12H26	6.81667	1479.23	181.835	72.4741	370.499
4367	2,5,6,6-tetramethyloctane	C12H26	6.81944	1488.15	181.835	73.8857	373.255
4368	3,3,4,4-tetramethyloctane	C12H26	6.77261	1493.81	181.835	76.9401	385.512
4369	3,3,4,5-tetramethyloctane	C12H26	6.8222	1497.08	181.835	75.2973	376.011
4370	3,3,4,6-tetramethyloctane	C12H26	6.81944	1488.15	181.835	73.8857	373.255
4371	3,3,5,5-tetramethyloctane	C12H26	6.76595	1471.83	181.835	73.4266	378.581
4372	3,3,5,6-tetramethyloctane	C12H26	6.81527	1474.77	181.835	71.7684	369.122
4373	3,3,6,6-tetramethyloctane	C12H26	6.75597	1439.76	181.835	68.2976	368.461
4374	3,4,4,5-tetramethyloctane	C12H26	6.82628	1510.46	181.835	77.4148	380.144
4375	3,4,4,6-tetramethyloctane	C12H26	6.81806	1483.69	181.835	73.1799	371.877
4376	3,4,5,5-tetramethyloctane	C12H26	6.82082	1492.61	181.835	74.5915	374.633
4377	3,4,5,6-tetramethyloctane	C12H26	6.87885	1522.59	181.835	77.1598	373.563
4378	4,4,5,5-tetramethyloctane	C12H26	6.76997	1485.02	181.835	75.5347	382.739
4379	2,2,3,3-tetramethylpentane	C9H20	6.92311	1455.54	219.789	-9.89	337.7
4380	2,2,3,4-tetramethylpentane	C9H20	7.01955	1500.49	229.518	-121.09	319
4381	2,2,4,4-tetramethylpentane	C9H20	6.9758	1436.93	228.61	-66.2	298.2

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4382	2,3,3,4-tetramethylpentane	C9H20	7.02486	1518.1	224.762	26.85	334.35
4383	2,3,4,5-tetramethylphenol	C10H14O	7.23935	1852.38	165	169.341	484.769
4384	2,3,4,6-tetramethylphenol	C10H14O	7.22548	1803.04	165	161.252	470.553
4385	2,3,5,6-tetramethylphenol	C10H14O	7.22265	1793.18	165	159.635	467.71
4386	tetramethylsilane	C4H12Si	6.8719	1060.66	239.108	-99.08	177.25
4387	tetranitromethane	CN4O8	6.98372	1345.1	202.141	13.9	266.85
4388	tetraphenylethylene	C26H20	7.90699	2818.91	140.795	223	722.85
4389	tetratriacontane	C34H70	7.15874	2331.9	63.1	249.939	533.347
4390	1-tetratriacontene	C34H68	6.33376	1700	11.3333	217.429	531
4391	tetratriacontylamine	C34H71N	8.74438	4638.96	273.15	406.21	568
4392	tetratriacontylbenzene	C40H74	6.6168	2000	13.3333	252.066	572
4393	tetratriacontylcyclohexane	C40H80	6.58223	2000	13.3333	251.703	577
4394	tetratriacontylcyclopentane	C39H78	5.30825	1513.57	103.528	291.545	570
4395	1-tetratriacontyne	C34H66	5.90859	1845.26	131.445	367.873	528
4396	thiacyclobutane	C3H6S	7.12433	1379.92	230.202	-5	329.85
4397	thiacyclodecane	C9H18S	6.90921	1742.64	193.59	161.384	497.884
4398	thiacyclododecane	C11H22S	6.89464	1830.63	188.08	185.926	523.289
4399	thiacycloeicosane	C19H38S	6.87331	2121.65	170.41	264.952	592.752
4400	thiacycloheneicosane	C20H40S	6.87156	2153.05	168.511	273.453	599.599
4401	thiacycloheptadecane	C16H32S	6.8778	2023.68	176.3	238.574	571.572
4402	thiacycloheptane	C6H12S	10.1272	4808.53	490.023	78	366.92
4403	thiacyclohexadecane	C15H30S	6.87969	1989	178.39	229.218	563.799
4404	thiacyclohexane	C5H10S	7.01195	1486.57	218.096	29	383.97

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4405	thiacyclononadecane	C18H36S	6.87479	2090.09	172.31	256.444	586.033
4406	thiacyclononane	C8H16S	6.9198	1685.07	197.2	145.307	478.23
4407	thiacyclooctadecane	C17H34S	6.87618	2058.45	174.21	247.934	579.441
4408	thiacyclooctane	C7H14S	6.93308	1618.39	201.38	126.69	453.693
4409	thiacyclopentadecane	C14H28S	6.88218	1951.35	180.67	219.017	554.692
4410	thiacyclotetradecane	C13H26S	6.88528	1913.94	182.95	208.826	545.645
4411	thiacyclotridecane	C12H24S	6.88937	1873.68	185.42	197.795	535.195
4412	thiacycloundecane	C10H20S	6.90111	1787.99	190.74	174.073	511.358
4413	2-thianonadecane	C18H38S	8.40367	3442.11	250.247	199	516.85
4414	(1-thiapropyl)-benzene	C8H10S	7.14722	1728.11	200.05	135.686	439.812
4415	thioacetic-acid	C2H4OS	6.87681	1022.59	168.894	40	304.19
4416	thiophene	C4H4S	7.06944	1296.79	225.437	-38.21	306.2
4417	threo-4,4-dimethyl-2,3-pentanediol	C7H16O2	9.33007	3480.41	273	170.197	437.153
4418	p-tolualdehyde	C8H8O	7.3225	1813.93	204.386	16.7	424.85
4419	toluene	C7H8	7.1362	1457.29	231.827	-94.97	318.64
4420	m-toluenediamine	C7H10N2	7.61109	2208.99	182.99	98.1	530.85
4421	toluene diisocyanate	C9H6N2O2	7.39464	1984.39	189.623	13.89	463.85
4422	p-toluic acid	C8H8O2	7.57616	2079.93	167.977	179.6	499.85
4423	m-toluidine	C7H9N	7.41381	1909.19	217.775	-30.4	436
4424	p-toluidine	C7H9N	7.52469	1948.19	219.268	43.75	420
4425	tri-o-cresyl phosphate	C21H21O4P	9.9896	3914.38	237.263	154.6	292.7
4426	triacontane	C30H62	7.12997	2254.6	80.9	222.487	499.646
4427	1-triacontene	C30H60	6.14834	1535.5	21.9262	192.878	498

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4428	triacontylamine	C30H63N	8.73528	4444.42	273.15	358.41	536
4429	triacontylbenzene	C36H66	6.41023	1800	12	232.442	548
4430	triacontylcyclohexane	C36H72	6.38276	1800	12	232.041	552
4431	triacontylcyclopentane	C35H70	5.86298	1784.39	104.352	302.498	544
4432	1-triacontyne	C30H58	6.16544	1949.02	147.377	319.873	496
4433	1,1,1-tribromo-2-methylpropane	C4H7Br3	7.15269	1556.78	151.845	122.45	458.712
4434	1,1,2-tribromo-2-methylpropane	C4H7Br3	7.14839	1608.27	146.858	136.724	484.959
4435	1,1,3-tribromo-2-methylpropane	C4H7Br3	7.28257	1623.03	153.354	126.217	450.768
4436	1,2,3-tribromo-2-methylpropane	C4H7Br3	7.2122	1606.57	150.914	129.217	463.609
4437	1,1,1-tribromobutane	C4H7Br3	7.21452	1579.5	153.469	121.83	450.163
4438	1,1,2-tribromobutane	C4H7Br3	7.28235	1625.58	153.121	126.899	451.998
4439	1,1,3-tribromobutane	C4H7Br3	7.28257	1623.03	153.354	126.217	450.768
4440	1,1,4-tribromobutane	C4H7Br3	7.3454	1652.53	154.333	127.272	445.617
4441	1,2,2-tribromobutane	C4H7Br3	7.21379	1587.93	152.674	124.128	454.347
4442	1,2,3-tribromobutane	C4H7Br3	7.28135	1637.22	152.051	130.023	457.629
4443	1,2,4-tribromobutane	C4H7Br3	7.34561	1650.01	154.559	126.605	444.426
4444	1,3,3-tribromobutane	C4H7Br3	7.22176	1501.31	160.849	100.492	411.32
4445	2,3,3-tribromobutane	C4H7Br3	7.1544	1537.33	153.729	117.058	448.798
4446	1,1,1-tribromodecane	C10H19Br3	7.46968	2080.51	141.381	205.8	513.784
4447	1,1,1-tribromododecane	C12H23Br3	7.54903	2232.04	138.136	264.104	530.865
4448	1,1,1-tribromoeicosane	C20H39Br3	7.54245	2609.68	124.82	346.033	600.95
4449	1,1,1-tribromoethane	C2H3Br3	7.15514	1415.73	158.218	91.1179	425.169
4450	1,1,2-tribromoethane	C2H3Br3	7.28093	1517.82	156.019	105.502	436.745

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4451	1,1,1-tribromoheptadecane	C17H33Br3	7.63001	2530.59	129.846	319.636	574.496
4452	1,1,1-tribromoheptane	C7H13Br3	7.33624	1831.58	147.09	165.514	483.739
4453	1,1,1-tribromohexadecane	C16H31Br3	7.63313	2483.51	131.589	309.286	565.323
4454	1,1,1-tribromohexane	C6H11Br3	7.2928	1747.58	149.098	151.397	473.171
4455	1,1,1-tribromononadecane	C19H37Br3	7.58584	2591.07	126.702	337.162	591.043
4456	1,1,1-tribromononane	C9H17Br3	7.42577	2000.28	143.11	193.148	504.685
4457	1,1,1-tribromooctadecane	C18H35Br3	7.61463	2566.77	128.22	328.937	583.058
4458	1,1,1-tribromooctane	C8H15Br3	7.38088	1917.06	145.008	179.711	494.694
4459	1,1,1-tribromopentadecane	C15H29Br3	7.6251	2430.09	133.214	298.794	556.774
4460	1,1,1-tribromopentane	C5H9Br3	7.25169	1665.45	151.034	137.377	462.979
4461	1,1,1-tribromopropane	C3H5Br3	7.18195	1496.2	155.862	106.407	437.569
4462	1,1,2-tribromopropane	C3H5Br3	7.24838	1552.44	154.448	114.548	445.011
4463	1,1,3-tribromopropane	C3H5Br3	7.30976	1592.12	154.48	118.487	444.845
4464	1,2,2-tribromopropane	C3H5Br3	7.18223	1493.24	156.152	105.586	436.041
4465	1,2,3-tribromopropane	C3H5Br3	7.30522	1644.74	149.584	132.626	470.613
4466	1,1,1-tribromotetradecane	C14H27Br3	7.60732	2371.39	134.721	288.188	548.839
4467	1,1,1-tribromotridecane	C13H25Br3	7.58147	2305.01	136.359	276.616	540.218
4468	1,1,1-tribromoundecane	C11H21Br3	7.51129	2156.92	139.81	251.554	522.055
4469	tributylamine	C12H27N	7.68482	2143.4	232.171	-70.15	370.85
4470	tributyl borate	C12H27BO3	6.73482	1805.5	234.973	-70	470
4471	1,2,2-trichloro-1,1-difluoroethane	C2HCl3F2	7.07112	1253.9	227.337	-14.632	255.85
4472	1,1,2-trichloro-1,2,2-trifluoroethane	C2Cl3F3	6.97091	1142.27	231.677	-35	214.1
4473	1,1,2-trichloro-1,2-difluoroethane	C2HCl3F2	7.07039	1256.05	227.304	-14.2065	256.85

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4474	1,1,2-trichloro-1-fluoroethane	C2H2Cl3F	6.87891	1171.53	205.022	0.409212	286.63
4475	1,1,1-trichloro-2,2,2-trifluoroethane	C2Cl3F3	7.25611	1310.37	253.615	13.99	214.55
4476	1,1,1-trichloro-2,2-difluoroethane	C2HCl3F2	7.07365	1259.97	227.506	-13.8616	257.55
4477	1,1,1-trichloro-2-fluoroethane	C2H2Cl3F	7.12634	1403.6	237.758	-100.15	291.85
4478	1,1,2-trichloro-2-fluoroethane	C2H2Cl3F	7.61234	1625.36	241.516	14.6014	279.781
4479	1,1,1-trichloro-2-methylpropane	C4H7Cl3	6.64561	1177.41	170.892	56.9135	358.465
4480	1,1,2-trichloro-2-methylpropane	C4H7Cl3	6.64481	1184.25	170.126	59.0386	362.498
4481	1,1,3-trichloro-2-methylpropane	C4H7Cl3	6.76281	1221.99	172.935	58.2541	347.71
4482	1,2,3-trichloro-2-methylpropane	C4H7Cl3	6.69453	1256.96	165.589	75.3273	386.372
4483	trichloroacetaldehyde	C2HCl3O	7.25772	1419.91	226.71	-57.15	291.85
4484	trichloroacetyl chloride	C2Cl4O	7.24512	1488.96	223.167	0	316.85
4485	1,2,4-trichlorobenzene	C6H3Cl3	7.39117	2027.84	236.596	17	451.85
4486	1,2,3-trichlorobenzene	C6H3Cl3	7.42844	2063.53	235.161	94.8825	461.097
4487	1,3,5-trichlorobenzene	C6H3Cl3	7.42973	2022.18	236.142	87.221	445.867
4488	1,1,1-trichlorobutane	C4H7Cl3	6.70357	1178.13	174.189	51.2282	341.111
4489	1,1,2-trichlorobutane	C4H7Cl3	6.76123	1235.39	171.514	62.2785	355.191
4490	1,1,3-trichlorobutane	C4H7Cl3	7.04181	1439.39	192.925	62.2785	355.191
4491	1,1,4-trichlorobutane	C4H7Cl3	6.81814	1257.39	172.501	62.9203	349.997
4492	1,2,2-trichlorobutane	C4H7Cl3	6.69374	1264.45	164.773	77.6167	390.672
4493	1,2,3-trichlorobutane	C4H7Cl3	6.75553	1286.68	166.071	77.6922	383.84
4494	1,2,4-trichlorobutane	C4H7Cl3	6.81206	1311.91	166.863	79.0459	379.671
4495	1,3,3-trichlorobutane	C4H7Cl3	6.69954	1211.89	170.506	61.5506	360.498
4496	2,3,3-trichlorobutane	C4H7Cl3	6.64526	1180.38	170.559	57.8357	360.215

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4497	1,1,1-trichlorodecane	C10H19Cl3	6.98001	1702.41	153.303	156.063	451.038
4498	1,1,1-trichlorododecane	C12H23Cl3	7.06565	1862.69	148.104	185.202	478.403
4499	1,1,1-trichloroeicosane	C20H39Cl3	7.12066	2281.47	131.102	273.16	567.885
4500	1,1,1-trichloroethane	C2H3Cl3	7.00718	1253.2	229.624	-30.4	271.85
4501	1,1,2-trichloroethane	C2H3Cl3	7.14357	1457.65	228.099	-36.65	328.85
4502	trichloroethylene	C2HCl3	7.19536	1419.51	242.056	-84.75	297.85
4503	trichlorofluoromethane	CCl3F	6.99349	1081.98	239.265	-111.11	198.05
4504	1,1,1-trichloroheptadecane	C17H33Cl3	7.17639	2178.91	137.245	245.069	535.553
4505	1,1,1-trichloroheptane	C7H13Cl3	6.83774	1445.91	162.413	107.316	403.092
4506	1,1,1-trichlorohexadecane	C16H31Cl3	7.1713	2129.05	139.225	234.674	525.132
4507	1,1,1-trichlorohexane	C6H11Cl3	6.79092	1356.95	166.036	89.3272	384.024
4508	1,1,1-trichlorononadecane	C19H37Cl3	7.15205	2256.02	133.189	264.353	556.905
4509	1,1,1-trichlorononane	C9H17Cl3	6.93315	1620.69	155.94	141.106	437.161
4510	1,1,1-trichlorooctadecane	C18H35Cl3	7.17027	2222.6	135.156	255.244	546.552
4511	1,1,1-trichlorooctane	C8H15Cl3	6.88547	1534	159.055	124.581	420.763
4512	1,1,1-trichloropentadecane	C15H29Cl3	7.15641	2070.85	141.341	223.29	513.995
4513	1,1,1-trichloropentane	C5H9Cl3	6.74621	1264.88	170.231	69.8251	361.941
4514	1,1,1-trichloropropane	C3H5Cl3	6.66582	1081.25	179.666	28.7192	312.285
4515	1,1,2-trichloropropane	C3H5Cl3	6.71828	1170.83	173.106	50.2862	346.81
4516	1,1,3-trichloropropane	C3H5Cl3	6.77034	1228.3	170.246	61.8049	361.864
4517	1,2,2-trichloropropane	C3H5Cl3	6.65996	1124.97	174.679	42.3784	338.534

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4518	1,2,3-trichloropropane	C3H5Cl3	7.15238	1612.2	220.575	-14.7	378.85
4519	1,1,1-trichlorotetradecane	C14H27Cl3	7.13302	2005.35	143.603	210.957	502.093
4520	1,1,1-trichlorotridecane	C13H25Cl3	7.10226	1936.68	145.772	198.518	490.674
4521	1,1,1-trichloroundecane	C11H21Cl3	7.02449	1784.3	150.609	171.04	465.216
4522	tricosane	C23H48	7.09051	2083.8	114.8	167.094	430.131
4523	1-tricosene	C23H46	6.79262	1874.14	100.097	140.404	529.571
4524	tricosylamine	C23H49N	6.82295	1964.06	80.2225	321.981	573.842
4525	tricosylbenzene	C29H52	6.32876	1661.43	35.8622	190.838	607.299
4526	tricosylcyclohexane	C29H58	6.18522	1582.73	29.9755	190.3	611.064
4527	tricosylcyclopentane	C28H56	6.59359	1991.78	97.4654	291.822	598.722
4528	1-tricosyne	C23H44	8.37255	3958.14	342.745	235.873	531.273
4529	1-tridecanal	C13H26O	7.61338	2142.83	185.784	15	426.85
4530	tridecane	C13H28	7.342	1958.01	203.429	-5.39	402.65
4531	1,2-tridecanediol	C13H28O2	9.53625	3959.99	273.001	232.275	463.778
4532	1,3-tridecanediol	C13H28O2	9.53627	4033.21	273.001	227.451	477.398
4533	1,4-tridecanediol	C13H28O2	9.53632	4173.01	273.001	259.451	503.401
4534	1,13-tridecanediol	C13H28O2	9.56724	4105.47	273.001	248.775	486.038
4535	tridecanenitrile	C13H25N	7.28335	1957.46	151.621	185.51	459.894
4536	1-tridecanethiol	C13H28S	7.41106	2158.27	185.603	151	468.98
4537	2-tridecanethiol	C13H28S	7.1179	1863.9	157.9	172.532	460.85
4538	tridecanoic acid	C13H26O2	7.67341	2209.93	149.014	182.141	473.437

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4539	1-tridecanol	C13H28O	6.92012	1653.37	135.32	30.6	457.85
4540	2-tridecanol	C13H28O	6.8296	1488.69	109	169.131	445.45
4541	2-tridecanone	C13H26O	7.21343	1868.68	168.725	132.024	434.105
4542	1-tridecene	C13H26	7.35746	1970.61	207.417	-23.07	401.85
4543	tridecyl acetate	C15H30O2	7.75524	2300	190	231.85	331.85
4544	tridecylamine	C13H29N	7.2686	1944.23	163.1	148.981	448.55
4545	tri-N-decylamine	C30H63N	9.42857	4446.91	273.15	295.064	456
4546	tridecylbenzene	C19H32	7.57877	2386.94	166.8	10	509.85
4547	tridecyl butanoate	C17H34O2	12.3594	8223.72	494.177	276.127	481.65
4548	tridecylcyclohexane	C19H38	7.12823	2079.95	148.187	191	510.23
4549	tridecylcyclopentane	C18H36	7.12123	2006.63	147.806	180	493.32
4550	1-tridecylcyclopentene	C18H34	7.33709	2187.63	179.91	193.408	476.186
4551	tridecyl formate	C14H28O2	7.62665	2169.62	153.073	199.738	452.25
4552	tridecyl propanoate	C16H32O2	7.69073	2600	190	300.55	400.55
4553	1-tridecyne	C13H24	7.2687	1918.85	203.295	120	410.96
4554	2-tridecyne	C13H24	7.22602	1935.6	200.455	119.483	428.67
4555	3-tridecyne	C13H24	7.22981	1913.47	201.978	114.104	419.189
4556	tridodecylamine	C36H75N	9.45922	4744.02	273.15	340.626	498
4557	trieicosylamine	C60H123N	9.27854	5381.45	273.15	347.636	618
4558	triethanolamine	C6H15NO3	8.44235	2922.52	185.639	21.2	513.85
4559	triethyl aluminum	C6H15Al	14.835	12972.3	891.17	-52.5	405

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4560	triethylamine	C6H15N	7.15625	1403.04	239.392	-114.7	262
4561	1,2,3-triethylbenzene	C12H18	7.22336	1839.35	206.055	146	411.22
4562	1,2,4-triethylbenzene	C12H18	7.3066	1926.97	217.886	46	411.22
4563	1,3,5-triethylbenzene	C12H18	7.20241	1812.07	203.296	145	409.13
4564	triethylenediamine	C6H12N2	7.14935	1499.93	177.393	161.1	381.85
4565	triethylene glycol	C6H14O4	10.2245	4208.28	295.198	-7.36	426.85
4566	triethylene glycol dimethyl ether	C8H18O4	7.7215	2009.47	199.12	-43.8	377.85
4567	triethylene tetramine	C6H18N4	8.10228	2320.5	177.916	12	444.85
4568	3,3,4-triethylhexane	C12H26	6.88335	1552.33	181.835	82.0153	383.099
4569	triethyl phosphate	C6H15O4P	7.87023	2317.27	249.437	-56.5	483.15
4570	1,1,1-trifluoro-2-methylpropane	C4H7F3	6.68903	839.927	208.647	-47.4913	159.755
4571	1,1,2-trifluoro-2-methylpropane	C4H7F3	6.68903	839.927	208.647	-47.4913	159.755
4572	1,1,3-trifluoro-2-methylpropane	C4H7F3	6.80672	879.193	209.246	-44.2823	156.598
4573	trifluoroacetic acid	C2HF3O2	7.50596	1399.76	230.84	-15.25	218.1
4574	1,1,1-trifluorobutane	C4H7F3	7.14988	1081.14	236.55	-45.9653	152.65
4575	1,1,2-trifluorobutane	C4H7F3	6.80672	879.193	209.246	-44.2823	156.598
4576	1,1,3-trifluorobutane	C4H7F3	6.80672	879.193	209.246	-44.2823	156.598
4577	1,1,4-trifluorobutane	C4H7F3	6.86451	896.064	209.793	-43.4667	153.722
4578	1,2,2-trifluorobutane	C4H7F3	6.72945	846.993	207.726	-39.94	156.666
4579	1,2,3-trifluorobutane	C4H7F3	6.80672	879.193	209.246	-44.2823	156.598
4580	1,2,4-trifluorobutane	C4H7F3	6.86451	896.064	209.793	-43.4667	153.722

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4581	1,3,3-trifluorobutane	C4H7F3	6.72945	846.993	207.726	-39.94	156.666
4582	2,3,3-trifluorobutane	C4H7F3	6.68903	839.927	208.647	-47.4913	159.755
4583	1,1,1-trifluorodecane	C10H19F3	7.22905	1659.07	212.55	75.887	326.95
4584	1,1,1-trifluorododecane	C12H23F3	7.27574	1813.13	204.55	139.122	365.05
4585	1,1,1-trifluoroicosane	C20H39F3	7.2509	2169.97	172.551	240.706	470.25
4586	1,1,1-trifluoroethane	C2H3F3	7.07645	846.165	249.078	-111.3	73.1
4587	1,1,2-trifluoroethane	C2H3F3	6.77457	841.127	212.319	-62.0763	157.761
4588	trifluoroethene	C2HF3	8.70142	1858.36	371.413	-93	74.07
4589	1,1,1-trifluoroheptadecane	C17H33F3	7.30378	2085.65	184.551	208.688	437.45
4590	1,1,1-trifluoroheptane	C7H13F3	7.16566	1394.93	224.55	20.6679	254.75
4591	1,1,1-trifluorohexadecane	C16H31F3	7.28321	2027.53	188.551	195.217	425.05
4592	1,1,1-trifluorohexane	C6H11F3	7.14603	1294.71	228.55	-0.162853	225.05
4593	1,1,1-trifluorononadecane	C19H37F3	7.26495	2141.87	176.551	230.267	460.05
4594	1,1,1-trifluorononane	C9H17F3	7.21462	1579.89	216.55	58.8119	305.25
4595	1,1,1-trifluorooctadecane	C18H35F3	7.17133	2044.65	180.551	214.831	449.15
4596	1,1,1-trifluorooctane	C8H15F3	7.1781	1484.93	220.55	39.9188	281.35
4597	1,1,1-trifluoropentadecane	C15H29F3	7.27457	1975.21	192.551	181.928	411.65
4598	1,1,1-trifluoropentane	C5H9F3	7.13634	1189.63	232.55	-22.3386	191.35
4599	1,1,1-trifluoropropane	C3H5F3	7.05706	950.305	240.55	-70.2427	118.85
4600	1,1,2-trifluoropropane	C3H5F3	6.77248	801.11	214.032	-62.7473	131.408
4601	1,1,3-trifluoropropane	C3H5F3	6.82998	816.858	214.583	-61.9809	128.511

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4602	1,2,2-trifluoropropane	C3H5F3	6.67704	760.712	210.916	-51.21	131.431
4603	1,2,3-trifluoropropane	C3H5F3	6.82998	816.858	214.583	-61.9809	128.511
4604	1,1,1-trifluorotetradecane	C14H27F3	7.28945	1933.41	196.55	168.971	397.25
4605	1,1,1-trifluorotridecane	C13H25F3	7.27102	1868.25	200.55	153.888	381.75
4606	1,1,1-trifluoroundecane	C11H21F3	7.25173	1737.66	208.55	122.323	346.85
4607	triheptadecylamine	C51H105N	9.32726	5177.46	273.15	423.35	580
4608	triheptylamine	C21H45N	6.44215	1318.59	40.2525	248.821	471.571
4609	n-trihexacontane	C63H128	7.21503	2626.1	-25.1	374.449	680.85
4610	trihexadecylamine	C48H99N	9.35545	5109.46	273.15	358.393	566
4611	trihexylamine	C18H39N	6.64438	1299.04	81.161	160.788	400.593
4612	1,1,1-triiodoheptadecane	C17H33I3	7.13088	2868.24	83.4698	475.546	818.584
4613	1,1,1-triiodo-2-methylpropane	C4H7I3	6.57065	1543.38	124.758	178.249	601.274
4614	1,1,2-triiodo-2-methylpropane	C4H7I3	6.57065	1543.38	124.758	178.249	601.274
4615	1,1,3-triiodo-2-methylpropane	C4H7I3	6.68462	1609.82	126.902	182.232	589.992
4616	1,2,3-triiodo-2-methylpropane	C4H7I3	6.62467	1572.8	126.14	179.402	593.999
4617	1,1,1-triiodobutane	C4H7I3	6.62467	1572.8	126.14	179.402	593.999
4618	1,1,2-triiodobutane	C4H7I3	6.68462	1609.82	126.902	182.232	589.992
4619	1,1,3-triiodobutane	C4H7I3	6.68462	1609.82	126.902	182.232	589.992
4620	1,1,4-triiodobutane	C4H7I3	6.74014	1639.98	128.189	183.415	583.218
4621	1,2,2-triiodobutane	C4H7I3	6.62467	1572.8	126.14	179.402	593.999
4622	1,2,3-triiodobutane	C4H7I3	6.68462	1609.82	126.902	182.232	589.992

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4623	1,2,4-triiodobutane	C4H7I3	6.74014	1639.98	128.189	183.415	583.218
4624	1,3,3-triiodobutane	C4H7I3	6.62467	1572.8	126.14	179.402	593.999
4625	2,2,3-triiodobutane	C4H7I3	6.57065	1543.38	124.758	178.249	601.274
4626	1,1,1-triiododecane	C10H19I3	6.90804	2172.56	108.227	291.808	688.28
4627	1,1,1-triiodododecane	C12H23I3	6.99806	2382.47	101.656	375.023	722.865
4628	1,1,1-triiododononadecane	C19H37I3	7.12052	3020.83	75.3491	514.597	861.325
4629	1,1,1-triiodoeicosane	C20H39I3	7.09709	3082.59	71.0763	533.698	883.814
4630	1,1,1-triiodoethane	C2H3I3	6.54774	1392.91	131.659	143.044	564.952
4631	1,1,2-triiodoethane	C2H3I3	6.66064	1455.13	133.982	146.74	552.725
4632	1,1,1-triiodoheptane	C7H13I3	6.76211	1863.33	117.48	235.091	639.581
4633	1,1,1-triiodohexadecane	C16H31I3	7.11994	2780.25	87.3342	455.69	798.245
4634	1,1,1-triiodohexane	C6H11I3	6.71429	1763.96	120.425	216.39	624.079
4635	1,1,1-triiodononane	C9H17I3	6.85986	2068.09	111.386	272.822	671.653
4636	1,1,1-triiodooctadecane	C18H35I3	7.13145	2948.91	79.4775	495.196	839.597
4637	1,1,1-triiodooctane	C8H15I3	6.81091	1964.84	114.469	253.908	655.429
4638	1,1,1-triiodopentadecane	C15H29I3	7.09989	2686.36	91.0781	435.671	778.54
4639	1,1,1-triiodopentane	C5H9I3	6.66824	1667.04	123.31	197.822	608.895
4640	1,1,1-triiodopropane	C3H5I3	6.58428	1481.39	128.922	161.14	579.361
4641	1,1,2-triiodopropane	C3H5I3	6.64366	1517.08	129.745	163.892	575.03
4642	1,1,3-triiodopropane	C3H5I3	6.69856	1546.09	131.105	165	567.871
4643	1,2,2-triiodopropane	C3H5I3	6.58428	1481.39	128.922	161.14	579.361

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4644	1,2,3-triiodopropane	C3H5I3	6.69856	1546.09	131.105	165	567.871
4645	1,1,1-triiodotetradecane	C14H27I3	7.07203	2587.94	94.7086	415.53	759.432
4646	1,1,1-triiodotridecane	C13H25I3	7.03766	2486.26	98.2324	395.303	740.885
4647	1,1,1-triiodoundecane	C11H21I3	6.95447	2277.61	104.986	354.721	705.341
4648	trimellitic anhydride	C9H4O5	8.21048	2807.76	136.967	165	616.85
4649	2,2,3-trimethyl-1-butanol	C7H16O	8.24244	2305.5	273	45.3319	323.695
4650	2,3,3-trimethyl-1-butanol	C7H16O	8.24245	2321.59	273	47.5529	327.858
4651	2,3,3-trimethyl-1-butene	C7H14	6.95371	1268.94	233.668	-109.85	257.85
4652	3,3,5-trimethyl-1-hexanol	C9H20O	8.35372	2549.56	273	97.7579	354.279
4653	3,4,4-trimethyl-1-hexanol	C9H20O	8.35372	2539.43	273	96.2855	351.788
4654	3,5,5-trimethyl-1-hexanol	C9H20O	8.35372	2550.38	273	97.8773	354.481
4655	4,5,5-trimethyl-1-hexanol	C9H20O	8.35375	2599.65	273	105.041	366.599
4656	2,2,3-trimethyl-1-pentanol	C8H18O	7.50271	1653.16	183.18	71.0463	338.338
4657	2,2,4-trimethyl-1-pentanol	C8H18O	7.68641	1793.29	204.867	63.3322	329.869
4658	2,3,3-trimethyl-1-pentanol	C8H18O	8.29874	2431.84	273	60.1856	340.182
4659	2,3,4-trimethyl-1-pentanol	C8H18O	8.37849	2506.94	273	66.7633	346.445
4660	2,4,4-trimethyl-1-pentanol	C8H18O	7.8087	1917.64	218.14	63.5052	333.557
4661	3,3,4-trimethyl-1-pentanol	C8H18O	8.29872	2404.74	273	56.4738	333.352
4662	3,4,4-trimethyl-1-pentanol	C8H18O	8.29872	2404.74	273	56.4738	333.352
4663	2,3,3-trimethyl-1-pentene	C8H16	6.73853	1209.83	205.304	5.52249	292.563
4664	2,3,4-trimethyl-1-pentene	C8H16	6.82685	1255.61	210.194	5.29225	284.607

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4665	2,4,4-trimethyl-1-pentene	C8H16	6.91487	1333.24	229.057	-93.45	279.85
4666	3,3,4-trimethyl-1-pentene	C8H16	6.7161	1184.86	203.936	3.3485	288.473
4667	3,4,4-trimethyl-1-pentene	C8H16	6.71291	1179.17	203.71	2.69523	286.988
4668	2,3,3-trimethyl-2-butanol	C7H16O	8.09015	2104.57	273	23.8303	294.871
4669	1,3,5-trimethyl-2-ethylbenzene	C11H16	7.11252	1739.42	198.644	122.664	415.068
4670	2,4,6-trimethyl-2-heptanol	C10H22O	8.33676	2541.66	273	97.5228	349.101
4671	2,5,6-trimethyl-2-heptanol	C10H22O	8.33676	2542.47	273	97.6421	349.301
4672	4,6,6-trimethyl-2-heptanol	C10H22O	8.33676	2541.66	273	97.5228	349.101
4673	2,3,4-trimethyl-2-hexanol	C9H20O	8.28295	2516.59	273	96.7691	357.7
4674	2,4,4-trimethyl-2-hexanol	C9H20O	8.205	2480.28	273	95.6559	361.201
4675	2,4,5-trimethyl-2-hexanol	C9H20O	8.28295	2516.59	273	96.7691	357.7
4676	2,5,5-trimethyl-2-hexanol	C9H20O	8.205	2480.28	273	95.6559	361.201
4677	2,3,3-trimethyl-2-pentanol	C8H18O	7.94246	2073.58	249.666	49.0156	325.607
4678	2,3,4-trimethyl-2-pentanol	C8H18O	8.22674	2304.1	273	45.829	319.281
4679	2,4,4-trimethyl-2-pentanol	C8H18O	7.62622	1717.78	215.589	43.6514	306.808
4680	3,3,4-trimethyl-2-pentanol	C8H18O	8.22677	2341.53	273	51.0075	328.9
4681	3,4,4-trimethyl-2-pentanol	C8H18O	7.4639	1587.97	188.484	57.1828	319.281
4682	2,3,4-trimethyl-2-pentene	C8H16	6.85304	1305.1	212.295	10.6821	300.97
4683	2,4,4-trimethyl-2-pentene	C8H16	6.88636	1320.64	224.794	-106.31	284.85
4684	3,4,4-trimethyl-cis-2-pentene	C8H16	6.72445	1217.28	204.7	7.94578	300.098
4685	3,4,4-trimethyl-trans-2-pentene	C8H16	6.72672	1219.14	204.998	7.88918	300.098

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4686	2,2,4-trimethyl-3,3-diethylpentane	C12H26	6.72801	1492.08	181.835	78.6529	395.285
4687	2,2,4-trimethyl-3-ethyl-3-pentanol	C10H22O	8.1911	2463.98	273	93.9914	353.127
4688	1,2,4-trimethyl-3-ethylbenzene	C11H16	7.11147	1753.38	197.846	126.104	421.022
4689	2,2,3-trimethyl-3-ethylheptane	C12H26	6.76997	1485.02	181.835	75.5347	382.739
4690	2,2,4-trimethyl-3-ethylheptane	C12H26	6.81387	1470.32	181.835	71.0627	367.744
4691	2,2,5-trimethyl-3-ethylheptane	C12H26	6.81105	1461.4	181.835	69.6513	364.988
4692	2,2,6-trimethyl-3-ethylheptane	C12H26	6.81105	1461.4	181.835	69.6513	364.988
4693	2,3,4-trimethyl-3-ethylheptane	C12H26	6.82897	1519.39	181.835	78.8265	382.9
4694	2,3,5-trimethyl-3-ethylheptane	C12H26	6.82151	1494.84	181.835	74.9444	375.322
4695	2,3,6-trimethyl-3-ethylheptane	C12H26	6.81944	1488.15	181.835	73.8857	373.255
4696	2,4,4-trimethyl-3-ethylheptane	C12H26	6.81667	1479.23	181.835	72.4741	370.499
4697	2,4,5-trimethyl-3-ethylheptane	C12H26	6.87464	1509.01	181.835	75.0331	369.454
4698	2,4,6-trimethyl-3-ethylheptane	C12H26	6.86752	1486.38	181.835	71.4889	362.606
4699	2,5,5-trimethyl-3-ethylheptane	C12H26	6.81105	1461.4	181.835	69.6513	364.988
4700	3,4,4-trimethyl-3-ethylheptane	C12H26	6.77654	1507.01	181.835	79.0484	389.67
4701	3,4,5-trimethyl-3-ethylheptane	C12H26	6.82763	1514.93	181.835	78.1207	381.522
4702	2,2,3-trimethyl-3-ethylhexane	C11H24	6.74142	1419.55	187.7	59.5463	365.671
4703	2,2,4-trimethyl-3-ethylhexane	C11H24	6.79014	1417.91	187.7	57.1838	354.492
4704	2,2,5-trimethyl-3-ethylhexane	C11H24	6.78318	1395.88	187.7	53.6683	347.489
4705	2,3,4-trimethyl-3-ethylhexane	C11H24	6.8062	1470.84	187.7	65.6227	371.298
4706	2,3,5-trimethyl-3-ethylhexane	C11H24	6.79151	1422.32	187.7	57.887	355.892

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4707	2,4,4-trimethyl-3-ethylhexane	C11H24	6.79423	1431.14	187.7	59.2933	358.693
4708	2,2,3-trimethyl-3-heptanol	C10H22O	8.26031	2469.19	273	91.0158	343.085
4709	2,2,6-trimethyl-3-heptanol	C10H22O	8.33675	2525.28	273	95.1365	345.095
4710	2,3,6-trimethyl-3-heptanol	C10H22O	8.33675	2525.28	273	95.1365	345.095
4711	3,5,5-trimethyl-3-heptanol	C10H22O	8.26033	2520.85	273	98.6296	355.969
4712	2,2,3-trimethyl-3-hexanol	C9H20O	8.20495	2375.1	273	80.0257	334.316
4713	2,2,4-trimethyl-3-hexanol	C9H20O	8.28288	2387.72	273	77.8372	325.413
4714	2,2,5-trimethyl-3-hexanol	C9H20O	8.28286	2339.09	273	70.6931	313.229
4715	2,3,4-trimethyl-3-hexanol	C9H20O	8.28287	2370.7	273	75.3367	321.149
4716	2,3,5-trimethyl-3-hexanol	C9H20O	8.28287	2370.7	273	75.3367	321.149
4717	2,4,4-trimethyl-3-hexanol	C9H20O	8.28289	2398.52	273	79.4248	328.12
4718	2,5,5-trimethyl-3-hexanol	C9H20O	8.28288	2386.91	273	77.7181	325.21
4719	3,4,4-trimethyl-3-hexanol	C9H20O	8.20493	2337.29	273	74.4068	324.651
4720	3,5,5-trimethyl-3-hexanol	C9H20O	8.20493	2336.49	273	74.288	324.447
4721	2,2,3-trimethyl-3-isopropylhexane	C12H26	6.72159	1470.39	181.835	75.1536	388.31
4722	2,2,4-trimethyl-3-isopropylhexane	C12H26	6.75993	1438.51	181.835	67.9096	367.546
4723	2,2,5-trimethyl-3-isopropylhexane	C12H26	6.74712	1398.97	181.835	61.5851	355.069
4724	2,3,4-trimethyl-3-isopropylhexane	C12H26	6.7802	1504.52	181.835	78.4534	388.341
4725	2,3,5-trimethyl-3-isopropylhexane	C12H26	6.76683	1460.5	181.835	71.4238	374.477
4726	2,4,4-trimethyl-3-isopropylhexane	C12H26	6.76409	1451.7	181.835	70.0181	371.705
4727	2,2,4-trimethyl-3-isopropylpentane	C11H24	6.73293	1377.9	187.7	52.6486	351.632

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4728	2,3,4-trimethyl-3-isopropylpentane	C11H24	6.7542	1447.49	187.7	63.8526	374.189
4729	2,2,3-trimethyl-3-pentanol	C8H18O	7.78541	1886.21	232.58	45.4002	314.549
4730	2,2,4-trimethyl-3-pentanol	C8H18O	7.56515	1648.39	200.894	50.1878	309.663
4731	2,3,4-trimethyl-3-pentanol	C8H18O	8.3631	2440.02	288.073	43.3116	317.907
4732	1,2,3-trimethyl-4-ethylbenzene	C11H16	7.11053	1766.01	197.124	129.216	426.408
4733	2,2,3-trimethyl-4-ethylheptane	C12H26	6.81527	1474.77	181.835	71.7684	369.122
4734	2,2,4-trimethyl-4-ethylheptane	C12H26	6.76189	1458.64	181.835	71.3187	374.422
4735	2,2,5-trimethyl-4-ethylheptane	C12H26	6.80533	1443.58	181.835	66.8286	359.477
4736	2,2,6-trimethyl-4-ethylheptane	C12H26	6.79657	1416.86	181.835	62.5952	351.21
4737	2,3,3-trimethyl-4-ethylheptane	C12H26	6.82356	1501.54	181.835	76.0031	377.388
4738	2,3,4-trimethyl-4-ethylheptane	C12H26	6.8222	1497.08	181.835	75.2973	376.011
4739	2,3,5-trimethyl-4-ethylheptane	C12H26	6.87464	1509.01	181.835	75.0331	369.454
4740	2,3,6-trimethyl-4-ethylheptane	C12H26	6.86607	1481.86	181.835	70.7801	361.236
4741	2,4,5-trimethyl-4-ethylheptane	C12H26	6.81806	1483.69	181.835	73.1799	371.877
4742	2,4,6-trimethyl-4-ethylheptane	C12H26	6.80389	1439.12	181.835	66.123	358.099
4743	2,5,5-trimethyl-4-ethylheptane	C12H26	6.81387	1470.32	181.835	71.0627	367.744
4744	3,3,4-trimethyl-4-ethylheptane	C12H26	6.77654	1507.01	181.835	79.0484	389.67
4745	3,3,5-trimethyl-4-ethylheptane	C12H26	6.82082	1492.61	181.835	74.5915	374.633
4746	3,4,5-trimethyl-4-ethylheptane	C12H26	6.83164	1528.32	181.835	80.2384	385.655
4747	2,2,3-trimethyl-4-ethylhexane	C11H24	6.79151	1422.32	187.7	57.887	355.892
4748	2,2,4-trimethyl-4-ethylhexane	C11H24	6.73878	1410.86	187.7	58.1463	362.852

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4749	2,2,5-trimethyl-4-ethylhexane	C11H24	6.77751	1378.26	187.7	50.8562	341.887
4750	2,3,3-trimethyl-4-ethylhexane	C11H24	6.80094	1453.19	187.7	62.8095	365.696
4751	2,3,4-trimethyl-4-ethylhexane	C11H24	6.79693	1439.96	187.7	60.6998	361.494
4752	2,3,5-trimethyl-4-ethylhexane	C11H24	6.84878	1447.12	187.7	59.7219	353.288
4753	3,3,4-trimethyl-4-ethylhexane	C11H24	6.75429	1463.01	187.7	66.5472	379.769
4754	2,2,4-trimethyl-4-heptanol	C10H22O	8.26029	2442.29	273	87.0503	336.374
4755	2,2,5-trimethyl-4-heptanol	C10H22O	8.33673	2481.63	273	88.7733	334.413
4756	2,2,6-trimethyl-4-heptanol	C10H22O	8.33673	2481.63	273	88.7733	334.413
4757	2,4,5-trimethyl-4-heptanol	C10H22O	8.33673	2481.63	273	88.7733	334.413
4758	2,4,6-trimethyl-4-heptanol	C10H22O	8.33673	2482.44	273	88.8926	334.613
4759	3,3,6-trimethyl-4-heptanol	C10H22O	8.33673	2481.63	273	88.7733	334.413
4760	2,2,5-trimethyl-4-isopropylhexane	C12H26	6.74712	1398.97	181.835	61.5851	355.069
4761	2,3,5-trimethyl-4-isopropylhexane	C12H26	6.81606	1463.26	181.835	69.7549	365.041
4762	1,2,3-trimethyl-5-ethylbenzene	C11H16	7.11167	1750.72	197.998	125.449	419.888
4763	1,2,4-trimethyl-5-ethylbenzene	C11H16	7.11237	1741.41	198.53	123.155	415.919
4764	2,2,3-trimethyl-5-ethylheptane	C12H26	6.81387	1470.32	181.835	71.0627	367.744
4765	2,2,4-trimethyl-5-ethylheptane	C12H26	6.80677	1448.03	181.835	67.5343	360.855
4766	2,2,5-trimethyl-5-ethylheptane	C12H26	6.75499	1436.68	181.835	67.8058	367.491
4767	2,2,6-trimethyl-5-ethylheptane	C12H26	6.80677	1448.03	181.835	67.5343	360.855
4768	2,3,3-trimethyl-5-ethylheptane	C12H26	6.81667	1479.23	181.835	72.4741	370.499
4769	2,3,4-trimethyl-5-ethylheptane	C12H26	6.87605	1513.54	181.835	75.742	370.824

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4770	2,3,5-trimethyl-5-ethylheptane	C12H26	6.81667	1479.23	181.835	72.4741	370.499
4771	2,3,6-trimethyl-5-ethylheptane	C12H26	6.87039	1495.43	181.835	72.9065	365.345
4772	2,4,4-trimethyl-5-ethylheptane	C12H26	6.81387	1470.32	181.835	71.0627	367.744
4773	2,4,5-trimethyl-5-ethylheptane	C12H26	6.82082	1492.61	181.835	74.5915	374.633
4774	3,3,4-trimethyl-5-ethylheptane	C12H26	6.82356	1501.54	181.835	76.0031	377.388
4775	3,3,5-trimethyl-5-ethylheptane	C12H26	6.77261	1493.81	181.835	76.9401	385.512
4776	3,4,4-trimethyl-5-ethylheptane	C12H26	6.82763	1514.93	181.835	78.1207	381.522
4777	1,2,4-trimethyl-6-ethylbenzene	C11H16	7.11237	1741.41	198.53	123.155	415.919
4778	trimethylamine	C3H9N	6.94803	981.847	238.535	-117.07	160.1
4779	1,2,3-trimethylbenzene	C9H12	7.29803	1789.65	229.034	-25.36	391.38
4780	1,2,4-trimethylbenzene	C9H12	7.29329	1763.35	230.248	-43.77	375.98
4781	2,3'-trimethylbiphenyl	C14H14	7.29847	2036.27	186.94	220.523	508.55
4782	2,2,3-trimethylbutane	C7H16	6.95435	1285.26	234.634	-24.58	258.02
4783	1,1,2-trimethylcyclohexane	C9H18	6.94273	1506.31	225.636	35.5756	351.716
4784	1,1,3-trimethylcyclohexane	C9H18	6.88664	1423.78	218.801	30.5248	338.909
4785	1,1,4-trimethylcyclohexane	C9H18	6.96341	1488.77	229.663	27.5859	336.481
4786	1,cis-2,cis-3-trimethylcyclohexane	C9H18	7.18023	1775.68	260.004	35.7399	356.105
4787	1,cis-2,trans-3-trimethylcyclohexane	C9H18	7.12655	1712.77	252.409	35.4308	353.152
4788	1,trans-2,cis-3-trimethylcyclohexane	C9H18	7.07006	1628.89	244.827	31.5405	342.816
4789	1,cis-2,cis-4-trimethylcyclohexane	C9H18	7.19435	1769.23	262.158	31.8211	348.722
4790	1,cis-2,trans-4-trimethylcyclohexane	C9H18	7.12513	1699.23	252.355	33.2784	348.722

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4791	1,trans-2,cis-4-trimethylcyclohexane	C9H18	7.12376	1685.77	252.31	31.1246	344.292
4792	1,trans-2,trans-4-trimethylcyclohexane	C9H18	7.12339	1670.16	252.447	28.3818	338.711
4793	cis,cis-1,3,5-trimethylcyclohexane	C9H18	6.50756	1109.19	167.326	78	334.71
4794	1,cis-3,cis-5-trimethylcyclohexane	C9H18	6.91826	1464.01	224.198	30.7612	334.561
4795	cis,trans-1,3,5-trimethylcyclohexane	C9H18	6.74735	1259.42	185.173	80	329.05
4796	1,cis-3,trans-5-trimethylcyclohexane	C9H18	7.14842	1694.9	255.935	27.8591	338.711
4797	1,1,2-trimethylcyclopentane	C8H16	6.89769	1352.09	222.874	6.38404	311.5
4798	1,1,3-trimethylcyclopentane	C8H16	6.90859	1330.51	225.44	-0.257966	298.147
4799	1,cis-2,cis-3-trimethylcyclopentane	C8H16	6.85592	1353.28	217.439	13.6574	318.421
4800	1,cis-2,trans-3-trimethylcyclopentane	C8H16	6.85907	1337.21	218.63	9.59918	310.208
4801	1,trans-2,cis-3-trimethylcyclopentane	C8H16	6.88171	1331.51	222.602	3.77864	299.307
4802	1,cis-2,cis-4-trimethylcyclopentane	C8H16	6.84752	1325.54	217.167	9.51763	309.461
4803	1,cis-2,trans-4-trimethylcyclopentane	C8H16	6.86539	1340.05	219.577	8.88958	309.06
4804	1,trans-2,cis-4-trimethylcyclopentane	C8H16	6.86663	1315.52	220.76	3.47747	297.948
4805	1,1,2-trimethylcyclopropane	C6H12	6.89286	1129.3	229.037	1.76851	231.19
4806	1,cis-2,cis-3-trimethylcyclopropane	C6H12	6.88104	1169.91	226.46	13.2237	246.913
4807	1,cis-2,trans-3-trimethylcyclopropane	C6H12	6.88388	1150.31	227.657	7.87475	237.252
4808	2,2,3-trimethylheptane	C10H22	6.98152	1511.32	210.941	42	338.55
4809	2,2,4-trimethylheptane	C10H22	6.96492	1462.88	209.877	35	321.35
4810	2,2,5-trimethylheptane	C10H22	6.96153	1468.3	209.004	37	324.85
4811	2,2,6-trimethylheptane	C10H22	6.9372	1436.9	205.291	37	320.25

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4812	2,3,3-trimethylheptane	C10H22	6.99216	1531.96	212.408	43	344.35
4813	2,3,4-trimethylheptane	C10H22	7.03388	1550.68	213.471	44	340.55
4814	2,3,5-trimethylheptane	C10H22	7.06065	1577.57	216.713	44	339.65
4815	2,3,6-trimethylheptane	C10H22	6.9979	1501.74	208.748	42	330.95
4816	2,4,4-trimethylheptane	C10H22	6.99734	1501.67	213.781	37	327.15
4817	2,4,5-trimethylheptane	C10H22	7.02361	1528.5	212.444	41	333.75
4818	2,4,6-trimethylheptane	C10H22	6.9716	1445.59	205.766	36	317.15
4819	2,5,5-trimethylheptane	C10H22	6.96672	1480.75	209.595	39	329.75
4820	3,3,4-trimethylheptane	C10H22	7.00517	1552.26	214.453	44	348.95
4821	3,3,5-trimethylheptane	C10H22	7.0502	1556.29	217.567	40	336.35
4822	3,4,4-trimethylheptane	C10H22	7.01159	1554.96	215.323	43	347.75
4823	3,4,5-trimethylheptane	C10H22	7.12971	1626.17	220.217	45	339.65
4824	2,2,3-trimethylhexane	C9H20	6.96485	1433.93	217.506	23	314.85
4825	2,2,4-trimethylhexane	C9H20	6.97344	1412.33	218.55	18	300.35
4826	2,2,5-trimethylhexane	C9H20	7.06137	1478.01	229.455	-105.76	294.9
4827	2,3,3-trimethylhexane	C9H20	6.992	1472.03	220.366	25	322.85
4828	2,3,4-trimethylhexane	C9H20	7.0358	1496.67	221.16	26.85	321.35
4829	2,3,5-trimethylhexane	C9H20	6.99147	1429.28	216.351	22	306.05
4830	2,4,4-trimethylhexane	C9H20	7.01244	1463.45	223.546	20	308.35
4831	3,3,4-trimethylhexane	C9H20	7.00502	1492.7	221.465	26.85	329.15
4832	1,2,3-trimethylindene	C12H14	7.36551	2064.49	224.491	71.5	452.85

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4833	1,2,3-trimethylnaphthalene	C13H14	6.63966	1408.87	91.8152	158	510.801
4834	1,2,4-trimethylnaphthalene	C13H14	7.02335	1804.25	153.543	146	509.392
4835	1,2,5-trimethylnaphthalene	C13H14	7.31087	2125.64	199.822	137	506.573
4836	1,2,6-trimethylnaphthalene	C13H14	6.96852	1738.22	145.232	146	506.573
4837	1,2,7-trimethylnaphthalene	C13H14	7.20694	1996.82	183.573	143	503.753
4838	1,2,8-trimethylnaphthalene	C13H14	7.33601	2175.03	203.202	144	513.621
4839	1,3,5-trimethylnaphthalene	C13H14	7.2452	2065.09	188.668	142	512.916
4840	1,3,6-trimethylnaphthalene	C13H14	7.07844	1858.53	162.758	143	506.573
4841	1,3,7-trimethylnaphthalene	C13H14	7.35135	2173.92	206.276	136	506.573
4842	1,3,8-trimethylnaphthalene	C13H14	7.76864	2726.48	272.811	130	513.621
4843	1,4,5-trimethylnaphthalene	C13H14	7.25977	2084.1	190.936	142	513.621
4844	1,4,6-trimethylnaphthalene	C13H14	7.13496	1914.95	172.137	140	503.753
4845	2,3,6-trimethylnaphthalene	C13H14	7.14454	1922.26	173.84	139	502.344
4846	1,6,7-trimethylnaphthalene	C13H14	7.27091	2078.49	193.449	138	506.573
4847	2,2,3-trimethylnonane	C12H26	6.87515	1525.18	181.835	77.763	374.881
4848	2,2,4-trimethylnonane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
4849	2,2,5-trimethylnonane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
4850	2,2,6-trimethylnonane	C12H26	6.861	1479.97	181.835	70.677	361.185
4851	2,2,7-trimethylnonane	C12H26	6.86815	1502.57	181.835	74.2198	368.033
4852	2,2,8-trimethylnonane	C12H26	6.86815	1502.57	181.835	74.2198	368.033
4853	2,3,3-trimethylnonane	C12H26	6.87791	1534.23	181.835	79.1803	377.62

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4854	2,3,4-trimethylnonane	C12H26	6.9307	1546.39	181.835	78.9079	371.186
4855	2,3,5-trimethylnonane	C12H26	6.925	1528.04	181.835	76.0611	365.738
4856	2,3,6-trimethylnonane	C12H26	6.92786	1537.21	181.835	77.4845	368.462
4857	2,3,7-trimethylnonane	C12H26	6.93211	1550.98	181.835	79.6196	372.547
4858	2,3,8-trimethylnonane	C12H26	6.9307	1546.39	181.835	78.9079	371.186
4859	2,4,4-trimethylnonane	C12H26	6.861	1479.97	181.835	70.677	361.185
4860	2,4,5-trimethylnonane	C12H26	6.92356	1523.45	181.835	75.3495	364.377
4861	2,4,6-trimethylnonane	C12H26	6.9192	1509.69	181.835	73.2146	360.291
4862	2,4,7-trimethylnonane	C12H26	6.92211	1518.86	181.835	74.6378	363.015
4863	2,4,8-trimethylnonane	C12H26	6.91773	1505.11	181.835	72.503	358.929
4864	2,5,5-trimethylnonane	C12H26	6.861	1479.97	181.835	70.677	361.185
4865	2,5,6-trimethylnonane	C12H26	6.925	1528.04	181.835	76.0611	365.738
4866	2,5,7-trimethylnonane	C12H26	6.92211	1518.86	181.835	74.6378	363.015
4867	2,5,8-trimethylnonane	C12H26	6.9192	1509.69	181.835	73.2146	360.291
4868	2,6,6-trimethylnonane	C12H26	6.861	1479.97	181.835	70.677	361.185
4869	2,6,7-trimethylnonane	C12H26	6.92928	1541.8	181.835	78.1962	369.824
4870	2,7,7-trimethylnonane	C12H26	6.87097	1511.61	181.835	75.637	370.772
4871	3,3,4-trimethylnonane	C12H26	6.87791	1534.23	181.835	79.1803	377.62
4872	3,3,5-trimethylnonane	C12H26	6.861	1479.97	181.835	70.677	361.185
4873	3,3,7-trimethylnonane	C12H26	6.86815	1502.57	181.835	74.2198	368.033
4874	3,3,6-trimethylnonane	C12H26	6.87237	1516.13	181.835	76.3456	372.142

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4875	3,4,4-trimethylnonane	C12H26	6.87515	1525.18	181.835	77.763	374.881
4876	3,4,5-trimethylnonane	C12H26	6.9307	1546.39	181.835	78.9079	371.186
4877	3,4,6-trimethylnonane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
4878	3,4,7-trimethylnonane	C12H26	6.9307	1546.39	181.835	78.9079	371.186
4879	3,5,5-trimethylnonane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
4880	3,5,6-trimethylnonane	C12H26	6.92643	1532.62	181.835	76.7728	367.1
4881	3,5,7-trimethylnonane	C12H26	6.92356	1523.45	181.835	75.3495	364.377
4882	3,6,6-trimethylnonane	C12H26	6.861	1479.97	181.835	70.677	361.185
4883	4,4,5-trimethylnonane	C12H26	6.87237	1516.13	181.835	76.3456	372.142
4884	4,4,6-trimethylnonane	C12H26	6.86245	1484.49	181.835	71.3855	362.554
4885	4,5,5-trimethylnonane	C12H26	6.87237	1516.13	181.835	76.3456	372.142
4886	4,5,6-trimethylnonane	C12H26	6.92786	1537.21	181.835	77.4845	368.462
4887	2,2,3-trimethyloctane	C11H24	6.84644	1454.19	187.7	61.0316	356.016
4888	2,2,4-trimethyloctane	C11H24	6.83592	1420.68	187.7	55.7362	345.58
4889	2,2,5-trimethyloctane	C11H24	6.83521	1418.44	187.7	55.3832	344.884
4890	2,2,6-trimethyloctane	C11H24	6.83947	1431.85	187.7	57.5012	349.059
4891	2,2,7-trimethyloctane	C11H24	6.83378	1413.98	187.7	54.6772	343.493
4892	2,3,3-trimethyloctane	C11H24	6.85054	1467.61	187.7	63.15	360.191
4893	2,3,4-trimethyloctane	C11H24	6.90417	1479.39	187.7	62.8666	353.519
4894	2,3,5-trimethyloctane	C11H24	6.89993	1465.77	187.7	60.7389	349.37
4895	2,3,6-trimethyloctane	C11H24	6.90417	1479.39	187.7	62.8666	353.519

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4896	2,3,7-trimethyloctane	C11H24	6.90276	1474.85	187.7	62.1573	352.136
4897	2,4,4-trimethyloctane	C11H24	6.83521	1418.44	187.7	55.3832	344.884
4898	2,4,5-trimethyloctane	C11H24	6.89851	1461.24	187.7	60.0297	347.987
4899	2,4,6-trimethyloctane	C11H24	6.89564	1452.17	187.7	58.6113	345.221
4900	2,4,7-trimethyloctane	C11H24	6.8913	1438.56	187.7	56.4839	341.073
4901	2,5,5-trimethyloctane	C11H24	6.83663	1422.91	187.7	56.0892	346.276
4902	2,5,6-trimethyloctane	C11H24	6.90135	1470.31	187.7	61.4481	350.753
4903	2,6,6-trimethyloctane	C11H24	6.84227	1440.78	187.7	58.9133	351.842
4904	3,3,4-trimethyloctane	C11H24	6.85054	1467.61	187.7	63.15	360.191
4905	3,3,5-trimethyloctane	C11H24	6.83947	1431.85	187.7	57.5012	349.059
4906	3,3,6-trimethyloctane	C11H24	6.84367	1445.25	187.7	59.6194	353.233
4907	3,4,4-trimethyloctane	C11H24	6.84918	1463.14	187.7	62.4438	358.799
4908	3,4,5-trimethyloctane	C11H24	6.90557	1483.93	187.7	63.5758	354.902
4909	3,4,6-trimethyloctane	C11H24	6.90276	1474.85	187.7	62.1573	352.136
4910	3,5,5-trimethyloctane	C11H24	6.83378	1413.98	187.7	54.6772	343.493
4911	4,4,5-trimethyloctane	C11H24	6.84781	1458.67	187.7	61.7377	357.408
4912	trimethylolpropane	C6H14O3	10.529	4294.67	272.635	58	435.85
4913	2,2,3-trimethylpentane	C8H18	7.02209	1416.58	232.214	-112.26	290.35
4914	2,2,4-trimethylpentane	C8H18	6.99021	1358.75	231.405	-107.37	270.81
4915	2,3,3-trimethylpentane	C8H18	7.03244	1443.86	233.013	-100.93	300.35
4916	2,3,4-trimethylpentane	C8H18	7.07131	1452.82	233.223	-109.2	293.15

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4917	2,3,4-trimethylphenol	C9H12O	7.18231	1729.2	165	150.355	466.811
4918	2,3,5-trimethylphenol	C9H12O	7.17999	1721.39	165	149.064	464.49
4919	2,3,6-trimethylphenol	C9H12O	7.18209	1728.47	165	150.234	466.593
4920	2,4,5-trimethylphenol	C9H12O	7.17999	1721.39	165	149.064	464.49
4921	2,4,6-trimethylphenol	C9H12O	7.15816	1650.2	165	137.279	443.313
4922	3,4,5-trimethylphenol	C9H12O	7.20306	1801.52	165	162.304	488.278
4923	trimethyl phosphate	C3H9O4P	7.62138	2069.63	243.878	-46.15	490.85
4924	2,4,6-trimethylpyridine	C8H11N	7.27424	1741.56	225.55	-44.15	379.85
4925	trimethyl silane	C3H10Si	6.90193	1030.41	249.55	-135.89	158.85
4926	2,2,3-trimethylthiacyclopropane	C5H10S	6.92835	1265.02	221.75	34.9317	296.569
4927	2,3,4-trimethylthiophene	C7H10S	7.26221	1660.06	206.187	109.28	381.394
4928	2,3,5-trimethylthiophene	C7H10S	7.08675	1565.64	207.745	100.043	383.113
4929	1,3,5-trinitrobenzene	C6H3N3O6	9.85104	6399.03	443.202	125.25	731.85
4930	2,4,6-trinitrotoluene	C7H5N3O6	7.35106	2010.84	149.978	80.85	521.85
4931	trinonadecylamine	C57H117N	9.28913	5313.45	273.15	490.97	606
4932	trinonylamine	C27H57N	6.3335	1350	9	284.12	432
4933	trioctadecylamine	C54H111N	9.30789	5245.46	273.15	340.294	593
4934	trioctylamine	C24H51N	6.16848	1200	8	268.77	407
4935	trioxane	C3H6O3	7.34399	1484.18	218.039	61.5	330.85
4936	tripentadecylamine	C45H93N	9.4015	5041.47	273.15	365.637	550
4937	tripentylamine	C15H33N	6.83325	1403.73	112.154	143.791	390.116

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4938	triphenylethylene	C20H16	7.347	2553.77	175.95	69	634.85
4939	triphenylphosphate	C18H15O4P	8.18951	3328.64	213.517	50	413.5
4940	triphenylphosphine	C18H15P	7.72816	2717.52	183.621	81.25	734.85
4941	tripropylamine	C9H21N	7.59939	1754.25	215.275	-93.5	304.35
4942	tritetradecylamine	C42H87N	9.44949	4973.47	273.15	370.753	534
4943	tritriacontane	C33H68	7.14856	2314.4	67.3	243.557	525.555
4944	1-tritriacontene	C33H66	6.2899	1650	11	211.627	523
4945	tritriacontylamine	C33H69N	8.72458	4582.39	273.15	405.187	561
4946	tritriacontylbenzene	C39H72	6.56701	1950	13	247.327	566
4947	tritriacontylcyclohexane	C39H78	6.5325	1950	13	247.04	571
4948	tritriacontylcyclopentane	C38H76	5.44368	1582.39	103.432	295.502	564
4949	1-tritriacontyne	C33H64	5.96393	1869.19	135.266	355.873	521
4950	tritridecylamine	C39H81N	9.46483	4873.16	273.15	339.994	517
4951	triundecylamine	C33H69N	9.4483	4604.79	273.15	336.7	478
4952	undecanal	C11H22O	7.64132	2112.13	210.678	0	398.85
4953	undecane	C11H24	7.18058	1706.26	200.897	-25.58	365.61
4954	1,2-undecanediol	C11H24O2	9.6299	3826.74	273.001	209.507	436.736
4955	1,3-undecanediol	C11H24O2	9.62993	3900.99	273.001	205.484	450.505
4956	1,4-undecanediol	C11H24O2	9.62998	4042.76	273.001	236.74	476.79
4957	1,11-undecanediol	C11H24O2	9.67757	3982.9	273.001	226.198	458.779
4958	undecanenitrile	C11H21N	7.25467	1822.67	156.721	158.755	433.051

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4959	1-undecanethiol	C11H24S	7.22678	1845.59	167.267	-3	436.85
4960	2-undecanethiol	C11H24S	7.09207	1759.04	170.4	142.878	432.85
4961	undecanoic acid	C11H22O2	7.57033	2016.72	145.848	161.095	451.851
4962	1-undecanol	C11H24O	6.91093	1551.12	139.882	15.9	430.85
4963	2-undecanol	C11H24O	6.8416	1417.96	123	141.324	416.55
4964	2-undecanone	C11H22O	7.10455	1672.11	168.055	105.858	404.855
4965	1-undecene	C11H22	7.17524	1699.83	203.153	-49.16	364.85
4966	undecylacetate	C13H26O2	7.91687	2200	190	196.85	296.85
4967	undecylamine	C11H25N	7.1033	1698.33	159.211	118.427	419.25
4968	undecylbenzene	C17H28	7.48314	2272.37	180.494	-5.15	490.85
4969	undecylbutanoate	C15H30O2	5.1353	750	5	224.879	377.67
4970	undecylcyclohexane	C17H34	7.16018	2045.12	164.793	167	488.59
4971	undecylcyclopentane	C16H32	7.16056	1978.5	166.683	154	470.15
4972	1-undecylcyclopentene	C16H30	7.28818	2067.23	185.04	170.701	456.546
4973	undecylformate	C12H24O2	7.16557	1783.44	157.899	155.621	426.85
4974	1-undecylnaphthalene	C21H30	7.49911	2566.44	164.711	329.017	573.193
4975	2-undecylnaphthalene	C21H30	7.49828	2584.68	163.761	333.555	579.564
4976	undecylpropanoate	C14H28O2	7.68048	2201.69	153.928	200.992	447.75
4977	1-undecyne	C11H20	7.12695	1685.36	201.907	80	377.84
4978	2-undecyne	C11H20	7.1278	1746.01	205.117	88.2471	396.351
4979	3-undecyne	C11H20	7.12408	1720.43	205.45	83.7978	387.967

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4980	valeronitrile	C5H9N	7.36051	1665.31	230.446	-96.2	329.85
4981	vanillin	C8H8O3	7.81755	2260.06	172.954	81.85	503.85
4982	vinyl acetate	C4H6O2	7.34453	1393.85	239.762	-92.8	250.85
4983	vinylacetic acid	C4H6O2	6.87443	1288.84	153.724	65.6735	396.543
4984	vinylacetonitrile	C4H5N	7.4065	1617.88	238.968	-87	310.85
4985	vinylacetylene	C4H4	6.77495	901.122	226.305	-93.2	180.85
4986	vinyl bromide	C2H3Br	7.67449	1403.35	276.951	-137.8	199.85
4987	vinyl chloride	C2H3Cl	6.89716	897.722	236.887	-153.79	158.85
4988	vinylcyclohexene	C8H12	7.16585	1528.42	228.837	-109.15	325.85
4989	vinyl fluoride	C2H3F	7.24752	857.669	268.611	-160.5	54.65
4990	vinyl formate	C3H4O2	7.18214	1177.3	226.856	-73.15	224.85
4991	vinyl iodide	C2H3I	6.60168	911.131	188.871	-11.0737	263.84
4992	vinyl propionate	C5H8O2	6.6846	993.683	170.035	88.85	272.85
4993	m-xylene	C8H10	7.18115	1573.02	226.671	-47.85	343.9
4994	p-xylene	C8H10	7.15471	1553.95	225.23	13.26	343.11
4995	2,3-xylenol	C8H10O	7.61977	2001.18	205.363	72.56	449.8
4996	2,4-xylenol	C8H10O	7.50567	1885.49	196.705	72.56	434.5
4997	2,5-xylenol	C8H10O	7.80247	2106.55	216.837	74.84	433.9
4998	2,6-xylenol	C8H10O	7.45107	1874	208.973	45.61	427.9
4999	3,4-xylenol	C8H10O	7.67221	2014.61	193.464	65.1	456.8
5000	3,5-xylenol	C8H10O	7.19633	1689	169.638	63.44	442.5