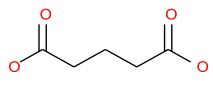
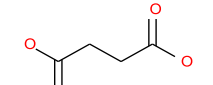
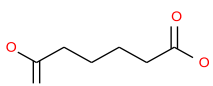
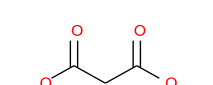
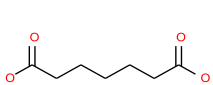
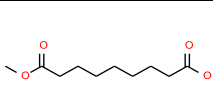
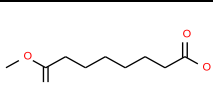
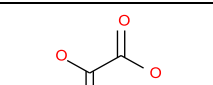
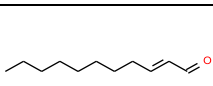
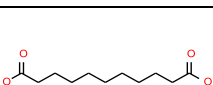
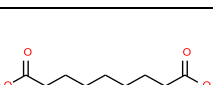
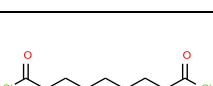
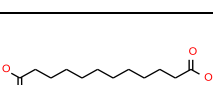
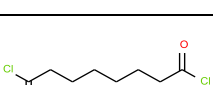
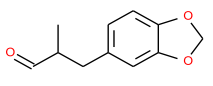
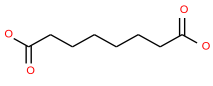
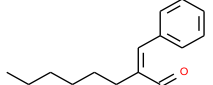
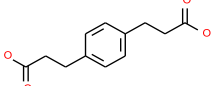
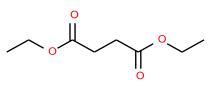
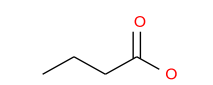
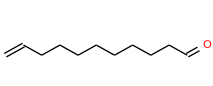
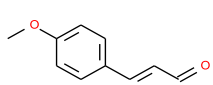
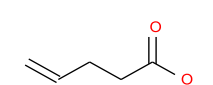
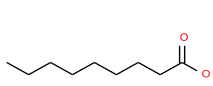
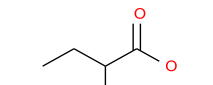
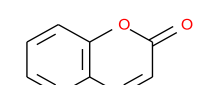
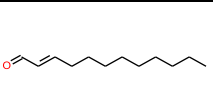
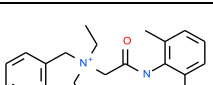
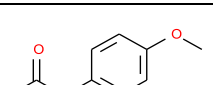
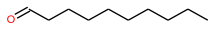
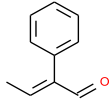
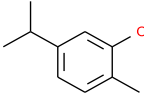
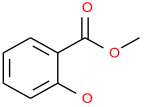
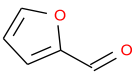
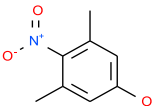
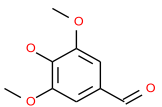
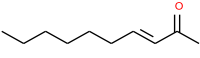
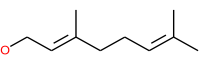
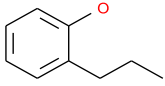
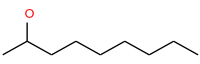
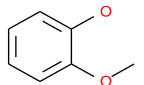
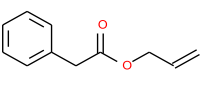
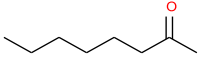
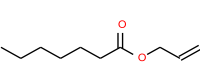


Rank	mol	Name	formula	molWeight	Score	molLogP	molPSA	molVolume	Natom	Nflex	Hbond	Hphob	Vwint	Eintl	Dsolv	SolEI	mfScore
1		glutaric acid	C5H8O4	132.042	-42.01	-0.05	57.28	121.52	15	4	-13.27	-1.49	-4.45	0.81	8.75	-18.1	-11.49
2		succinic acid	C4H6O4	118.027	-40.81	-0.53	57.28	103.62	12	3	-13.21	-1.21	-8.03	0	8.75	-10.45	-25.76
3		adipic acid	C6H10O4	146.058	-40.15	0.43	57.28	139.43	18	5	-12.18	-1.87	-8.76	5.58	8.68	-13.4	-20.05
4		malonic acid	C3H4O4	104.011	-36.55	-0.96	57.28	85.29	9	2	-9.82	-0.74	-12.03	0.65	8.67	-10.43	-18.27
5		heptanedioic acid	C7H12O4	160.074	-35.61	0.92	57.28	157.34	21	6	-12.42	-2.19	-2.57	7.58	8.73	-15.59	-4.98
6		9-methoxy-9-oxononanoic acid	C10H18O4	202.121	-32.99	2.23	49.47	216.15	31	8	-10.57	-4.8	-14.41	0.51	12.26	-3.95	-76.98
7		8-methoxy-8-oxooctanoic acid	C9H16O4	188.105	-30.2	1.75	49.47	198.25	28	7	-9.31	-4.27	-17.49	2.66	12.59	0.08	-98.29
8		oxalic acid	C2H2O4	89.995	-29.72	-0.54	57.33	67.91	6	1	-10.84	-0.3	-7.21	0.01	8.63	-2.99	-30.76
9		undec-2-enal	C11H20O	168.151	-28.66	4.35	14.61	215.74	32	7	-7.02	-5.31	-21.55	8.39	8.05	6.01	-103.73
10		undecanedioic acid	C11H20O4	216.136	-27.67	2.84	57.28	228.96	33	10	-10.3	-4.45	-15.11	4.96	13.15	0.95	-104.3
11		nonanedioic acid	C9H16O4	188.105	-27.5	1.88	57.28	193.15	27	8	-9.26	-3.6	-15.77	4.6	11.98	0.51	-97.71
12		nonanedioyl chloride	C9H14Cl2O2	224.037	-26.89	3.41	27.2	215.39	27	8	-7.95	-5.2	-15.22	0.97	8.86	0.73	-84.05
13		dodecanedioic acid	C12H22O4	230.152	-26.78	3.33	57.28	246.87	36	11	-10.29	-4.75	-14.3	8.79	13.02	0.55	-105.11
14		octanedioyl chloride	C8H12Cl2O2	210.021	-26.75	2.93	27.2	197.48	24	7	-6.86	-4.86	-20.67	0	8.89	5.54	-88.72

15		3-(7,9-dioxabicyclo[4.3.0]nona-1,3,5-trien-3-yl)-2-methylpropanal	C11H12O3	192.079	-26	2.44	30.69	198.9	26	3	-5.39	-4.55	-20.01	0.86	10.5	1.56	-89.87
16		octanedioic acid	C8H14O4	174.089	-25.29	1.4	57.28	175.24	24	7	-11.44	-2.58	3.33	4.63	8.46	-12.88	-10.78
17		alpha-hexyl cinnamaldehyde	C15H22O	216.151	-25.24	4.98	14.4	255.25	36	6	-7.27	-5.93	-16.17	1.27	8.88	4.58	-53.42
18		3-(4-(2-carboxy-ethyl)-phenyl)-propanoic acid	C12H14O4	222.089	-24.98	1.81	57.01	214.27	28	6	-9.94	-3.99	-14.31	1.73	12.95	5.83	-102.9
19		1,4-diethyl butanedioate	C8H14O4	174.089	-24.57	1.12	40.83	183.64	26	5	-7.23	-4.17	-11.23	3.13	7.92	-1.83	-41.03
20		butyric acid	C4H8O2	88.052	-24.49	0.87	28.89	91.05	13	2	-6.83	-2.04	-6.89	0.68	5.02	-5.93	-5.17
21		undec-10-enal	C11H20O	168.151	-24.27	3.96	14.61	216.02	32	9	-5	-5.39	-22.33	3.14	7.65	4.81	-88.66
22		3-(4-methoxy-phenyl)-acrylaldehyde	C10H10O2	162.068	-24.26	2.38	21.89	175.81	22	0	-4.93	-4.14	-17.57	0.81	8.48	3.33	-84.61
23		pent-4-enoic acid	C5H8O2	100.052	-24.2	0.97	28.89	112.8	14	3	-6.32	-2.4	-10.29	2.04	5.2	-3.03	-8.3
24		nonanoic acid	C9H18O2	158.131	-24.19	3.28	28.89	180.58	28	7	-6.56	-4.62	-16.34	3.58	9.51	0.77	-110.39
25		2-methyl-butanoic acid	C5H10O2	102.068	-24.18	1.19	28.92	106.24	16	2	-6.96	-2.53	-5.95	1.13	5.19	-6.1	-11.79
26		3-oxo-2-oxabicyclo[4.4.0]deca-1(6),4,7,9-tetraene	C9H6O2	146.037	-24.04	1.72	20.65	151.42	17	0	-6.55	-3.41	-13.62	0	7.94	3.75	-64.12
27		dodec-2-enal	C12H22O	182.167	-23.7	4.83	14.61	233.64	35	8	-4.82	-5.71	-21.69	10.21	8.05	4.81	-105.73
28		2-(diethyl-(phenyl-methyl)-amino)-1-(2,6-dimethyl-phenylamino)-ethanone	C21H29N2O	446.257	-23.57	4.91	50.12	461.02	53	6	-2.58	-6.54	-18.89	1.59	1.29	2.49	-71.55
29		4-methoxy-phenyl ethanoate	C9H10O3	166.063	-22.85	1.68	28.53	167.45	22	0	-4.2	-4.36	-18.67	0	9.71	3.16	-97.52

30		phenyl-methyl 2-hydroxy-benzoate	C14H12O3	228.079	-22.84	3.15	37.64	215.23	29	2	-3.09	-4.83	-15.95	0	4.08	-0.15	-56.9
31		(2R,3R,4S)-2,3,4,5-tetrahydroxy-pentanal	C5H10O5	150.053	-22.84	-3	79.77	126.4	20	8	-15.85	-1.21	-6.83	3.44	15.61	12.7	-0.96
32		octanal	C8H16O	128.12	-22.76	2.9	14.61	158.45	25	6	-4.96	-4.17	-17.6	1.71	6.92	2.1	-89.01
33		5-oxo-nonanedioic acid	C9H14O5	202.084	-22.74	0.46	70.03	202.57	26	8	-14.24	-3.12	-0.16	0.38	13.34	1.1	-68.79
34		6-bromo-hexanoic acid	C6H11BrO2	193.994	-22.67	2.16	28.89	146	19	5	-5.67	-3.88	-15.22	1.1	8.89	-0.26	-85.73
35		(S)-3,7-dimethyl-oct-6-enal	C10H18O	154.136	-22.49	3.37	14.61	198.02	29	5	-5.02	-4.9	-19.01	0	7.97	5.37	-91.96
36		(R)-6-oxo-2-pentyl-3,6-dihydro-2H-pyran	C10H16O2	168.115	-22.46	2.78	21.06	205.58	28	4	-4.44	-4.97	-19.67	1.65	8.97	4	-94.46
37		3-(4-hydroxy-3-methoxyphenyl)-acrylaldehyde	C10H10O3	178.063	-22.46	2	38.52	187.24	23	0	-4.06	-3.95	-21.01	0.79	9.74	6.31	-92.1
38		1,9-dimethyl nonanedioate	C11H20O4	216.136	-22.29	2.58	41.67	239.16	35	8	-7.05	-5.69	-16.2	3.49	12.09	2.57	-82.82
39		5-methyl-2-phenyl-hex-2-enal	C13H16O	188.12	-22.18	3.71	14.4	216.98	30	3	-2.61	-4.98	-23.58	1.27	8.07	5.31	-121.47
40		2-hydroxy-benzaldehyde	C7H6O2	122.037	-22.08	1.27	30.95	114.6	15	0	-3.77	-2.46	-15.73	2.78	5.41	1.18	-77.2
41		propionic acid	C3H6O2	74.037	-22.03	0.39	28.89	73.58	10	1	-6.51	-1.68	-9.81	0	4.99	1.55	-12.46
42		2-ethoxy-5-(prop-1-enyl)-phenol	C11H14O2	178.099	-21.67	3.39	24	197.13	27	1	-6.59	-5.22	-11.56	0	9.26	3.81	-77.3
43		2-phenyl-propanal	C9H10O	134.073	-21.63	1.73	14.4	134.9	20	2	-4.85	-3.68	-18.38	0.05	7.1	7.52	-97.73
44		tridec-2-enal	C13H24O	196.183	-21.62	5.31	14.61	251.55	38	9	-6.99	-6.12	-15.25	6.62	8.08	5.99	-104.79

45		nonan-2-one	C9H18O	142.136	-21.58	3.25	13.84	176.66	28	6	-5.07	-5	-15.72	1.19	6.82	2.42	-81.7
46		methyl 2-phenoxyethanoate	C9H10O3	166.063	-21.49	1.55	28.32	161.34	22	3	-5.83	-4.3	-11.89	2.57	7.66	0.72	-44.59
47		2-phenylacetaldehyde	C8H8O	120.058	-21.44	1.51	14.34	124.59	17	2	-4.93	-3.24	-15.5	0.07	6.54	3.92	-66.84
48		(4-methoxyphenyl)methanol	C8H10O2	138.068	-21.18	1.37	24.9	135.9	20	2	-2.65	-3.52	-14.65	1.25	4.27	-2.83	-30.83
49		2-(3-(carboxy-methyl)phenyl)-acetic acid	C10H10O4	194.058	-21.12	0.95	57.01	178.84	22	4	-4.85	-1.82	-10.59	1.02	7.55	-7.74	-50.83
50		11-bromo-undecanoic acid	C11H21BrO2	264.072	-21.09	4.57	28.89	235.53	34	10	-6.91	-5.81	-13.27	9.14	9.7	0.42	-96.19
51		3-phenylallyl 2-methylpropanoate	C13H16O2	204.115	-21	3.42	21.29	224.76	31	4	-3.59	-5.77	-16.45	2.3	5.18	3.22	-29.17
52		2,6-diisopropylphenol	C12H18O	178.136	-20.98	3.59	15.72	195.09	31	2	-2.49	-5.14	-13.1	1.13	1.98	-1.25	-39
53		1-(thiazol-2-yl)ethanone	C5H5NOS	127.009	-20.91	0.76	24.5	109.15	13	0	-7.14	-2.78	-13.62	0.15	4.86	13.64	-4.04
54		2-mercapto-propanoic acid	C3H6O2S	106.009	-20.9	0.37	28.92	89.44	11	2	-7.22	-1.3	-9.84	1.19	6.78	2.71	-27.77
55		(S)-dec-1-en-3-ol	C10H20O	156.151	-20.84	3.77	17.13	193.6	31	8	-3.78	-5.46	-22.15	5.46	9.33	4.13	-97.94
56		furan-2-ylmethyl isopropyl sulfite	C8H12O4S	204.243	-20.8	0.96	39.31	169.25	25	5	-5.86	-4.79	-17.58	1.24	11.54	4.79	-93.2
57		1-(furan-2-yl)ethanone	C6H6O2	110.037	-20.75	0.83	22.64	107.73	14	0	-7.02	-2.71	-13.99	0.22	4.73	14.04	-3.57
58		4-methyl-2,6-ditert-butylphenol	C15H24O	220.183	-20.64	4.99	15.72	277.97	40	2	0	-6.27	-16.37	0	-0.24	-1.66	-70.29
59		propyl hydrogen sulfite	C3H8O3S	124.159	-20.6	-0.24	39.46	95.44	14	3	-7.05	-2.11	-12.39	0.2	6.64	6.46	-6.39

60		decanal	C10H20O	156.151	-20.55	3.87	14.61	194.27	31	8	-4.92	-4.98	-17.85	3.36	7.69	3.83	-89.79
61		2-phenyl-but-2-enal	C10H10O	146.073	-20.51	2.51	14.4	166.87	21	1	-2.67	-4	-19.14	0	7.48	2.82	-83.04
62		5-isopropyl-2-methyl-phenol	C10H14O	150.104	-20.48	3	16.79	160.73	25	1	-2.4	-4.6	-11.89	3.17	2.51	-2.92	-37.03
63		methyl 2-hydroxybenzoate	C8H8O3	152.047	-20.43	1.53	37.96	143.66	19	0	-4.27	-3.5	-14.65	1.53	7.38	2.79	-74.03
64		furan-2-carbaldehyde	C5H4O2	96.021	-20.42	0.87	22.15	90.05	11	0	-6.67	-1.84	-16.48	0.05	5	15.78	-19.42
65		3,5-dimethyl-4-nitrophenol	C8H9NO3	167.162	-20.37	1.83	50.64	153.25	21	1	-2.76	-3.51	-13.73	0	3.16	-0.43	-44.45
66		4-hydroxy-3,5-dimethoxybenzaldehyde	C9H10O4	182.058	-20.35	1.33	45.14	178.02	23	0	-6.48	-3.42	-15.92	0	10.74	9.39	-53.71
67		dec-3-en-2-one	C10H18O	154.136	-20.25	3.47	13.84	201.86	29	5	-2.89	-5.23	-20.24	0	7.38	3.43	-82.71
68		(2E)-3,7-dimethyl-octa-2,6-dien-1-ol	C10H18O	154.136	-20.25	3.33	17.17	210.16	29	5	-2.77	-4.67	-15.46	0	3.19	-0.08	-30.79
69		2-propyl-phenol	C9H12O	136.089	-20.22	2.86	16.79	144.04	22	2	-2.85	-4.09	-12.89	0.75	2.48	-0.66	-35.78
70		nonan-2-ol	C9H20O	144.151	-20.2	3.51	16.99	173.48	30	7	-4.22	-5.03	-18.87	5.2	8.91	2.78	-107.95
71		2-methoxy-phenol	C7H8O2	124.052	-20.1	1.57	24.42	119.09	17	0	-2.36	-3.5	-11.75	0.46	1.1	-1.29	-19.76
72		allyl 2-phenyl-ethanoate	C11H12O2	176.084	-20.08	2.5	20.69	189.42	25	4	-2.05	-5.13	-24.7	1.97	8.65	6.62	-114.24
73		octan-2-one	C8H16O	128.12	-20.06	2.77	13.84	158.75	25	5	-5.3	-4.73	-13.01	0	6.87	2.11	-72.6
74		allyl heptanoate	C10H18O2	170.131	-19.94	3.41	20.96	206.86	30	7	-3.93	-5.59	-20.15	1.06	9.07	4.38	-115.77

75		methyl 4-hydroxybenzoate	C8H8O3	152.047	-19.91	1.65	39.03	143.03	19	0	-5.22	-3.48	-14.83	0.37	10.39	4.06	-66.85
76		2-methoxy-4-vinylphenol	C9H10O2	150.068	-19.85	2.43	24.42	163.95	21	0	-4.67	-4.32	-17.37	0	10.11	7.03	-83.82
77		(S)-(4-isopropenylcyclohex-1-enyl)methanol	C10H16O	152.12	-19.81	2.85	17.55	198.5	27	3	-3.03	-3.96	-13.51	1.2	3.25	-0.33	-26.72
78		(R)-(4-isopropenylcyclohex-1-enyl)methanol	C10H16O	152.12	-19.81	2.85	17.55	198.5	27	3	-3.03	-3.95	-13.48	1.21	3.25	-0.4	-26.58
79		hexanal	C6H12O	100.089	-19.79	1.94	14.61	122.64	19	4	-4.66	-3.29	-14.05	0.41	6.11	1.91	-80.11
80		4-allyl-2-methoxyphenol	C10H12O2	164.084	-19.77	2.61	24.42	181.27	24	2	-1.02	-4.64	-17.56	0.46	3.93	-1.01	-45.95
81		(R)-1-phenylpentan-2-ol	C11H16O	164.12	-19.77	3.12	16.86	173	28	5	-2.65	-4.75	-14.18	1.14	2.92	-1.36	-38.52
82		(7S,11R,E)-3,7,11,15-tetramethylhexadec-2-en-1-ol	C20H40O	296.308	-19.74	8.28	17.17	372.58	61	14	-2.51	-6.05	-22.19	7.04	6.02	-0.09	-75.56
83		pentyl butanoate	C9H18O2	158.131	-19.74	3.14	20.96	185.28	29	6	-3.78	-5.06	-13.73	3.86	5.97	-1.73	-53.8
84		ethyl decanoate	C12H24O2	200.178	-19.7	4.59	20.67	238.5	38	9	-4.05	-6.49	-20.52	5.31	9.25	4.66	-85.31
85		3,7,11-trimethyl-dodeca-2,6,10-trienal	C15H24O	220.183	-19.63	5.48	14.61	309.85	40	6	0	-4.79	-21.92	0	2.65	-0.14	-60.27
86		2-phenyl-ethyl 2-methylbut-2-enoate	C13H16O2	204.115	-19.56	3.51	21.29	230.67	31	3	0	-5.53	-17.44	0	0.66	-1.08	-44.87
87		2-methoxy-pyrazine	C5H6N2O	110.048	-19.55	0.11	26.25	97.1	14	0	-7.37	-2.73	-15.51	0.06	6.09	17.99	-12.82
88		3-phenyl-prop-2-en-1-ol	C9H10O	134.073	-19.53	2.12	16.89	145.12	20	3	-4.14	-4.23	-14.8	0.2	8.72	0.39	-75.8
89		propane-1,2,3-triol	C3H8O3	92.047	-19.53	-1.61	51.36	81.67	14	5	-11.88	-1.54	-10.61	0.68	11.15	16.35	-10.42

90		methyl 2-methylamino-benzoate	C9H11NO2	165.079	-19.5	1.63	31.37	158.05	23	0	-0.76	-4.09	-15.44	0	1.11	-0.37	-43.85
91		resorcinol	C6H6O2	110.037	-19.43	1.34	35.47	97.07	14	0	-4.42	-2.28	-11.63	1.12	5.82	0.85	-32.3
92		dodecanal	C12H24O	184.183	-19.39	4.83	14.61	230.08	37	10	-3.55	-5.83	-22.44	8.5	8.05	5.92	-120.81
93		hex-2-enoic acid	C6H10O2	114.068	-19.39	1.98	28.89	133.84	17	3	-5.49	-2.73	-11.85	3.28	5.25	3.71	-3.02
94		((4-methoxy-phenyl)-methoxy)-methanone	C9H10O3	166.063	-19.3	1.63	30.11	161.45	22	2	-3.23	-3.87	-19.7	0.23	9.85	3.91	-86.62
95		heptan-2-one	C7H14O	114.104	-19.28	2.29	13.84	140.84	22	4	-5	-4.3	-13.42	0	6.82	3.26	-64.9
96		pentanoic acid	C5H10O2	102.068	-19.25	1.35	28.89	108.96	16	3	-5.65	-2.44	-10.56	1.46	5.22	2.33	-5.22
97		1-(2-amino-phenyl)-ethanone	C8H9NO	135.068	-19.21	1.04	34.16	128.19	19	0	-4.05	-3.26	-12.98	0	6.26	2.28	-84.16
98		3,7-dimethyl-octa-2,6-dienal	C10H16O	152.12	-19.21	3.49	14.61	210.36	27	3	0	-4.07	-19.59	0	1.79	-0.07	-39.78
99		allyl 2-methyl-but-2-enoate	C8H12O2	140.084	-19.2	2.34	21.56	180.31	22	2	0	-4.63	-16.42	0	1.19	-2.69	-23.87
100		non-3-en-2-one	C9H16O	140.12	-19.18	2.99	13.84	183.95	26	4	-3.77	-4.84	-14.34	0	4.68	3.08	-62
101		(1R,2R,5R)-5-isopropenyl-2-methyl-cyclohexanol	C10H18O	154.136	-19.14	2.79	16.05	185.65	29	2	-2.75	-4.6	-11.23	0	2.44	-1.36	-29.37
102		heptyl butanoate	C11H22O2	186.162	-19.12	4.11	20.96	221.09	35	8	-3.86	-6.2	-16.73	4.92	8.47	0.57	-69.64
103		(R)-3,7-dimethyl-oct-6-enal	C10H18O	154.136	-19.1	3.37	14.61	198.02	29	5	-2.93	-4.61	-20.04	0	7.63	4.11	-90.23
104		4-vinyl-phenol	C8H8O	120.058	-19.07	2.46	17.86	131.23	17	0	-2.9	-3.23	-12.24	0.55	3.17	0.46	-37.96

105		2-phenyl-ethanol	C8H10O	122.073	-19.03	1.6	16.89	122.59	19	3	-2.86	-3.45	-13.63	0.01	2.91	0.26	-41.49
106		(1R)-(6-methoxyquinolin-4-yl)((2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol	C20H24N2O2	324.184	-19.02	2.41	35.65	339.59	48	4	-2.43	-5.9	-14.63	1.31	3.72	0.79	-52.76
107		4-(hydroxy-methyl)-2-methoxy-phenol	C8H10O3	154.063	-19.02	0.99	41.53	147.33	21	2	-3.1	-3.65	-13.52	1.45	3.55	1.4	-49.39
108		(1R,4R,4aR,6R,8aS)-4,8a,9,9-tetramethyldecahydro-1,6-methanonaphthalen-1-ol	C15H26O	222.366	-19.02	4.33	15.18	288.51	42	1	-2.85	-4.83	-9.72	0	2.58	-2.09	-41.6
109		2-phenyl-ethanamine	C8H11N	121.089	-19.02	1	21.39	124.65	20	3	-2.94	-3.42	-14.57	0.03	3.84	0.89	-39.31
110		3,7-dimethyl-octa-2,6-dienyl ethanoate	C12H20O2	196.146	-19.01	3.9	21.66	257.82	34	5	-3.67	-5.8	-19.06	0	9.57	4.61	-71.09
111		3-(2-methoxy-phenyl)-acrylaldehyde	C10H10O2	162.068	-18.98	2.26	21.97	174.49	22	0	0	-4.22	-16.44	0.42	1.76	-1.55	-39.63
112		3,7-dimethyl-octa-2,6-dienyl 2-phenyl-ethanoate	C18H24O2	272.178	-18.96	5.41	20.69	328.95	44	7	0	-6.09	-22.07	0	1.24	3.11	-98.94
113		hex-4-en-1-ol	C6H12O	100.089	-18.96	1.69	17.17	125.51	19	4	-4.64	-3.65	-14.65	0	7.69	2.57	-67.5
114		4-methyl-phenyl 2-phenyl-ethanoate	C15H14O2	226.099	-18.96	3.51	20.02	227.67	31	2	-2.86	-5.8	-22.17	0	9.63	8.96	-65.82
115		phenol	C6H6O	94.042	-18.96	1.6	17.86	86.44	13	0	-4.36	-2.75	-11.79	0.1	5.16	2.77	-56.38
116		oct-2-en-1-ol	C8H16O	128.12	-18.84	2.74	17.17	163.17	25	6	-3.62	-4.56	-18.59	0.55	8.5	3.04	-86.54
117		(S)-pentan-2-ol	C5H12O	88.089	-18.79	1.58	16.99	101.85	18	3	-4.25	-3.35	-10.44	0.35	5.28	-1.71	-63.84
118		3-phenyl-propan-1-ol	C9H12O	136.089	-18.79	2.08	16.89	140.5	22	4	-2.68	-3.71	-13.61	0.59	2.82	-0.67	-43.49
119		4-methyl-1,2-dinitrobenzene	C7H6N2O4	182.033	-18.77	1.59	76.16	149.24	19	2	0	-3.24	-14.43	0	0	-5.1	-36.24

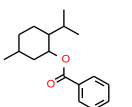
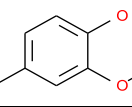
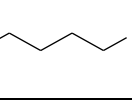
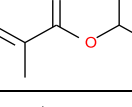
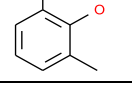
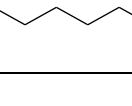
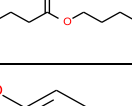
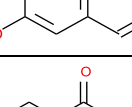
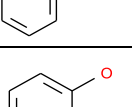
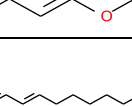
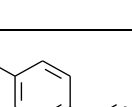
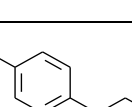
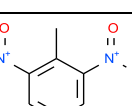
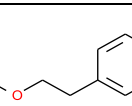

120		5-phenylpentan-1-ol	C11H16O	164.12	-18.74	3.04	16.89	176.31	28	6	-3.89	-5.06	-19.31	2.27	9.17	5.02	-96.16
121		5-isopropenyl-2-methylcyclohexanol	C10H18O	154.136	-18.73	2.79	16.05	185.65	29	2	-2.82	-4.2	-10.88	0	2.84	-1.85	-32.24
122		(S)-ethyl 3-hydroxybutanoate	C6H12O3	132.079	-18.72	0.53	37.15	135.59	21	4	-5.52	-3.53	-13.2	1.63	8.99	2.54	-60.74
123		3-methylbutan-1-amine	C5H13N	87.105	-18.62	0.83	21.67	103.75	19	3	-4.3	-3.1	-13.04	2.52	7.12	0.37	-61.39
124		4-hydroxy-3-methoxybenzaldehyde	C8H8O3	152.047	-18.59	1.36	38.58	147.35	19	0	-5.78	-3.18	-14.32	6.52	11.24	6.16	-72.05
125		(2Z)-3,7-dimethyl-octa-2,6-dien-1-ol	C10H18O	154.136	-18.56	3.33	17.17	210.16	29	5	-4.1	-4.98	-18.25	0	9.27	5.22	-82.02
126		2-methoxy-4-propylphenol	C10H14O2	166.099	-18.52	2.95	24.42	175.79	26	2	-0.99	-4.74	-16.32	0.57	3.88	-0.96	-50.85
127		(Z)-hex-3-en-1-ol	C6H12O	100.089	-18.5	1.61	17.17	128.54	19	4	-4.11	-3.7	-14.78	0	7.85	1.3	-69.86
128		3-phenylpropanal	C9H10O	134.073	-18.49	1.94	14.34	140.86	20	3	-4.36	-3.8	-16.65	0	7.99	6.01	-86.43
129		(R)-1-phenylpropan-1-ol	C9H12O	136.089	-18.46	2.23	16.39	136.46	22	3	-4.47	-4.21	-17.17	0.09	8.91	6.6	-92.95
130		(Z)-non-6-enal	C9H16O	140.12	-18.45	2.92	14.61	182.63	26	6	-3.62	-4.3	-17.98	0.63	7.72	3.29	-90.93
131		2-isopropenyl-5-methylcyclohexanol	C10H18O	154.136	-18.43	2.79	16.05	184.17	29	2	-2.51	-4.57	-11.85	0.45	2.64	-0.53	-33.76
132		3,7-dimethyl-oct-6-en-1-ol	C10H20O	156.151	-18.42	3.51	17.17	199.03	31	6	-2.32	-4.71	-13.75	0	2.87	-2.11	-39.31
133		pentan-2-ol	C5H12O	88.089	-18.39	1.58	16.99	101.85	18	3	-4.26	-3.3	-11.21	0.48	5.64	-0.34	-65.26
134		7-methyl-3-methylene-octa-1,6-diene	C10H16	136.125	-18.39	3.91	0	203.76	26	3	0	-4.75	-15.94	0	0	-1.63	-32.55

135		(R)-6-methyl-hept-5-en-2-ol	C8H16O	128.12	-18.38	2.6	16.99	163.64	25	4	-4.05	-4.7	-15.17	0	8.6	2.02	-89.57
136		3-isopropyl-phenol	C9H12O	136.089	-18.33	2.72	17.86	139.58	22	1	-3.97	-4.22	-16.21	0.76	9	5.15	-94.21
137		4-allyl-2-methoxy-phenyl ethanoate	C12H14O3	206.094	-18.3	2.61	28.71	229.13	29	2	0	-5.51	-16.51	0	2.05	-1.27	-41.52
138		2-phenyl-ethyl propanoate	C11H14O2	178.099	-18.29	2.66	20.69	186.03	27	4	-4.06	-4.82	-12.8	3.84	6.96	0.59	-77.26
139		2-p-tolyl-acetaldehyde	C9H10O	134.073	-18.28	1.91	14.34	145.53	20	2	-3.51	-3.57	-14.14	0	5.26	3.02	-66.78
140		phenyl-methyl butanoate	C11H14O2	178.099	-18.28	2.84	20.77	185.62	27	4	-3.32	-5.06	-13.5	1.56	6.43	-0.34	-61.03
141		5-methyl-furan-2-carbaldehyde	C6H6O2	110.037	-18.28	1.3	21.66	111.07	14	0	-6.43	-2.31	-16.2	0	4.86	18.31	-4.64
142		(R)-nonan-2-ol	C9H20O	144.151	-18.24	3.51	16.99	173.48	30	7	-4.19	-5.14	-16.46	3.94	9.03	1.94	-109.08
143		(R)-heptan-2-ol	C7H16O	116.12	-18.24	2.55	16.99	137.66	24	5	-4.24	-4.34	-15.63	1.96	8.33	2.7	-86.1
144		2-aza-bicyclo[4.4.0]deca-1(10),2,4,6,8-pentaene	C9H7N	129.058	-18.23	2.3	9	120.17	17	0	-3.07	-3.89	-14.97	0	6.57	3.31	-78.07
145		acetophenone	C8H8O	120.058	-18.23	1.61	14.07	122.3	17	1	-2.92	-3.51	-14.25	0	5.22	1.88	-65.7
146		(4-methoxy-phenyl)-methyl 2-phenyl-ethanoate	C16H16O3	256.11	-18.17	3.46	28.04	253.75	35	4	-1.72	-5.6	-17.71	1.89	3.78	3.68	-46.5
147		(4-methoxy-phenyl)-methyl ethanoate	C10H12O3	180.079	-18.12	1.95	29.01	182.62	25	2	-3.57	-4.74	-17.72	0	9.29	5.51	-100.75
148		phenyl-methanol	C7H8O	108.058	-18.11	1.28	17.35	104.06	16	2	-3.68	-3.23	-13.36	0.42	6.56	0.92	-70.17
149		7-aza-bicyclo[4.3.0]nona-1(6),2,4,8-tetraene	C8H7N	117.058	-18.1	2.19	10.02	112.41	16	0	-2.21	-3.39	-13.68	0	3.52	1.23	-65.11

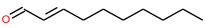
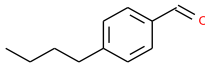
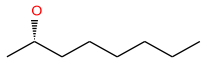
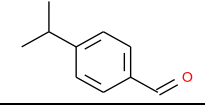
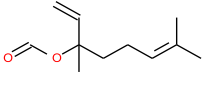
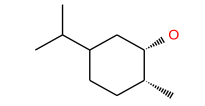
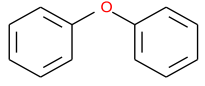
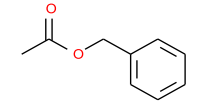
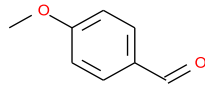

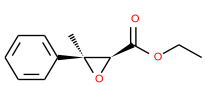
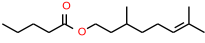

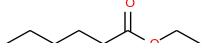
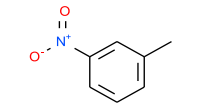
150		3-phenyl-acrylaldehyde	C9H8O	132.058	-18.06	2.29	14.34	143.97	18	1	-2.62	-3.75	-17.24	0	7.25	3.44	-78.17
151		phenyl-methyl propanoate	C10H12O2	164.084	-18.04	2.35	20.77	168.16	24	3	-3.27	-4.7	-12.88	1.49	6.4	-0.51	-59.12
152		dec-9-en-1-ol	C10H20O	156.151	-18.03	3.62	17.17	197.74	31	9	-4.13	-5.4	-20.66	4.26	8.63	7.3	-83.82
153		2,6,10,10-tetramethyl-1-oxa-spiro[4.5]dec-6-ene	C13H22O	194.167	-18.01	4.33	7.79	264.86	36	0	0	-5.1	-14.21	0.05	0.74	-1.44	-55.1
154		2-phenyl-ethyl octanoate	C16H24O2	248.178	-17.99	5.07	20.69	275.12	42	9	0	-5.32	-22.36	6.22	3.58	-0.24	-72.67
155		1-(pyrazin-2-yl)-ethanone	C6H6N2O	122.048	-17.95	-0.38	32.63	112.49	15	0	-8.66	-2.55	-10.28	0.28	6.36	16.93	-12.09
156		7-aza-bicyclo[4.3.0]nona-1,3,5,8-tetraene	C8H7N	117.058	-17.94	2.19	10.02	112.41	16	0	-2.17	-3.41	-13.73	0	3.41	1.53	-64.14
157		2-ethyl-3-hydroxy-4H-pyran-4-one	C7H8O3	140.047	-17.91	0.33	34.44	164.93	18	1	-5.08	-3.47	-14.8	1.4	12.16	3.55	-87.78
158		(S)-3,7-dimethyl-oct-6-en-1-ol	C10H20O	156.151	-17.9	3.51	17.17	199.03	31	6	-1.65	-4.95	-14.02	0	2.36	-2.68	-33.75
159		2-methyl-propyl ethanoate	C6H12O2	116.084	-17.86	1.52	21.74	129.46	20	2	-6.46	-3.41	-13.8	4.86	4.11	15.58	-7.91
160		(R)-4-hydroxy-2,5-dimethyl-2,3-dihydro-furan-3-one	C6H8O3	128.047	-17.85	-0.21	36.87	140.39	17	0	-5.48	-3.2	-13.54	0.02	12.38	3.66	-86.8
161		(3R,7S,11S)-3,7,11,15-tetramethyl-hexadec-1-en-3-ol	C20H40O	296.308	-17.84	8.2	16.84	380.16	61	14	0	-7.93	-20.04	8.69	-2.07	1.01	-134.15
162		octan-3-one	C8H16O	128.12	-17.84	2.78	13.27	159.96	25	5	-3.03	-4.69	-17.88	0.54	7.11	3.8	-91.83
163		octyl ethanoate	C10H20O2	172.146	-17.83	3.61	21.66	204.15	32	7	-3.75	-5.66	-16.21	0.62	8.88	1.21	-79.57
164		(S)-1,5-dimethyl-1-vinyl-hex-4-enyl ethanoate	C12H20O2	196.146	-17.81	3.54	20.24	264.72	34	5	0	-5.63	-16.23	0	1.66	-3.12	-45.31

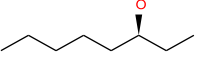
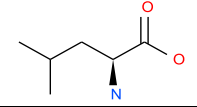
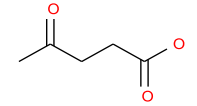
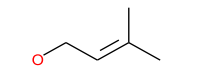
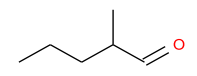
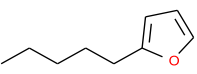
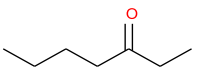
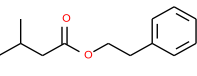
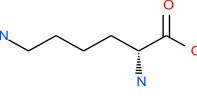
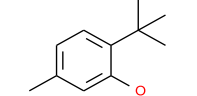
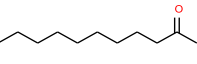
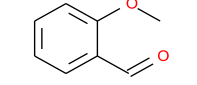
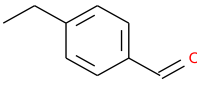
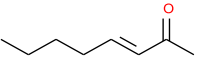
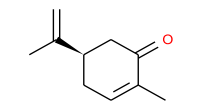
165		4-methoxy-phenol	C7H8O2	124.052	-17.78	1.69	25.4	118.29	17	0	-5.55	-3.53	-12.79	0.51	10.4	5.5	-80.39
166		pentane-2,3-dione	C5H8O2	100.052	-17.78	0.05	27.58	113.02	15	2	-7	-2.42	-14.3	0	5.18	16.32	-16.45
167		(S)-oct-1-en-3-ol	C8H16O	128.12	-17.75	2.81	17.13	157.78	25	6	-3.6	-4.65	-16.82	0.61	8.38	2.15	-75.72
168		hex-2-enal	C6H10O	98.073	-17.72	1.94	14.61	126.21	17	2	-4.43	-3.13	-12.59	0.8	6.59	3.07	-52.65
169		(4-methoxy-phenyl)- methyl propanoate	C11H14O3	194.094	-17.69	2.44	28.32	200	28	3	-3.54	-5.22	-18.01	3.11	9.02	6.38	-109.55
170		pent-3-en-2-one	C5H8O	84.058	-17.62	1.14	13.84	108.71	14	0	-2.9	-3.18	-11.93	0	3.95	1.25	-40.41
171		3-methyl-butanoic acid	C5H10O2	102.068	-17.62	1.19	28.89	105.34	16	2	-5.84	-2.41	-9.41	1.73	5.22	4.64	-13.7
172		1-allyl-4-methoxy- benzene	C10H12O	148.089	-17.61	2.99	7.78	169.84	23	2	-2.7	-5.04	-16.25	0.51	6.72	3.94	-81.75
173		o-cresol	C7H8O	108.058	-17.61	1.88	16.79	107.59	16	0	-2.43	-3.37	-9.72	0	2.31	-1.83	-24.94
174		2-phenyl-ethyl butanoate	C12H16O2	192.115	-17.6	3.14	20.69	203.5	30	5	-3.99	-5.09	-12.44	3.6	6.66	0.52	-80.55
175		octa-2,4-dienal	C8H12O	124.089	-17.59	2.57	14.61	167.67	21	2	-2.59	-4.11	-17.66	0.7	7.7	3.64	-65.01
176		3-mercapto-3-methyl- butan-1-ol	C5H12OS	120.061	-17.56	1.35	17.17	130.24	19	4	-4.54	-2.85	-8.55	0.64	4.01	-1.56	-13.85
177		3,7-dimethyl-octa-1,6- dien-3-ol	C10H18O	154.136	-17.55	3.25	16.84	217.74	29	5	-1.56	-4.99	-14.54	0	2.78	-1.23	-23.14
178		ethyl ethanoate	C4H8O2	88.052	-17.54	0.72	21.37	96.21	14	1	-3.79	-2.89	-8.94	0	4.21	-1.27	-1.68
179		hepta-2,4-dienal	C7H10O	110.073	-17.51	2.09	14.61	149.18	18	1	-2.65	-3.63	-16.43	0.23	6.84	3.51	-56.63

180		(R)-3,7-dimethyl-oct-6-en-1-ol	C10H20O	156.151	-17.5	3.51	17.17	199.03	31	6	-2.89	-4.53	-12.3	0	3.15	-1.22	-38.97
181		hexanoic acid	C6H12O2	116.084	-17.5	1.84	28.89	126.86	19	4	-6.44	-2.82	-4.82	4.27	5.22	-1.23	-15.18
182		bicyclo[4.4.0]deca-1(10),2,4,6,8-pentaen-3-yl)-2-aza-bicyclo[4.4.0]deca-1(10),2,4,6,8-pentaene	C20H12N2O4	344.08	-17.49	3.94	73.44	306.35	36	2	-1.97	-4.72	-14.53	0	5.06	0.29	-71.67
183		4-(2,6,6-trimethyl-cyclohex-2-enyl)-but-3-en-2-one	C13H20O	192.151	-17.48	4.05	13.77	264.15	34	1	0	-5.65	-13.73	0	0.23	-1.12	-36.65
184		(furan-2-yl)-methyl heptanoate	C12H18O3	210.126	-17.46	3.44	28.52	224.58	33	7	0	-5.23	-18.67	2.39	3.17	-2.82	-47.24
185		hexyl 2-phenyl-ethanoate	C14H20O2	220.146	-17.45	4.16	20.69	239.46	36	7	-3.11	-6.53	-19.67	1.46	9.92	4.28	-86.96
186		octan-1-ol	C8H18O	130.136	-17.39	3.04	17.17	158.09	27	7	-4.49	-4.64	-15.79	2.85	8.39	3.59	-84.62
187		(1S,2R,4R)-1,3,3-trimethyl-bicyclo[2.2.1]heptan-2-ol	C10H18O	154.136	-17.38	2.75	16.59	198.5	29	1	-2.64	-4.18	-9.57	0	2.69	-1.42	-35.51
188		methyl non-2-enoate	C10H18O2	170.131	-17.37	3.77	21.09	212.18	30	5	-2.77	-5.52	-20.51	5.05	9.29	5.88	-92.01
189		(R)-2-oxo-6-(pent-2-enyl)-tetrahydro-2H-pyran	C10H16O2	168.115	-17.35	2.16	21.06	199.52	28	3	-3.29	-5	-17.79	2.2	8.96	5.44	-99.02
190		phenyl-methyl 3-phenyl-prop-2-enoate	C16H14O2	238.099	-17.34	4.29	20.5	247.8	32	3	0	-5.57	-17.58	1.6	1.42	1.68	-97.61
191		dec-2-en-1-ol	C10H20O	156.151	-17.34	3.7	17.17	198.98	31	8	-4.46	-5.39	-17.68	4.96	8.56	6.09	-93.87
192		butan-1-amine	C4H11N	73.089	-17.34	0.51	21.67	88.53	16	3	-4.37	-2.81	-10.88	1.32	6.86	-0.7	-50.46
193		1-methyl-2,3-dinitrobenzene	C7H6N2O4	182.033	-17.33	1.47	75.86	149.26	19	2	0	-3.36	-13.6	0	0	-4.06	-34.51
194		(1R,2S,5R)-2-isopropyl-5-methyl-cyclohexanol	C10H20O	156.151	-17.32	2.95	16.05	180.11	31	2	-2.18	-4.55	-11.26	0.43	2.51	-0.86	-39.28

195		2-isopropyl-5-methylcyclohexyl benzoate	C17H24O2	260.178	-17.31	5.04	20.27	278.86	43	3	0	-6.3	-13.16	0.99	0.12	-2.74	-64.52
196		4-ethyl-2-methoxyphenol	C9H12O2	152.084	-17.3	2.47	24.42	158.25	23	1	-4.47	-4.42	-15.14	0.39	10.12	5.94	-87.38
197		butane-1,4-diamine	C4H12N2	88.1	-17.3	-1.25	42.82	98.57	18	5	-6.61	-2.38	-11.25	1.26	11.46	1.02	-47.76
198		1-methyl-ethyl 2-methylbut-2-enoate	C8H14O2	142.099	-17.28	2.33	20.94	173.55	24	1	0	-4.52	-13.36	0	0.02	-2.28	-35.84
199		2,6-dimethylphenol	C8H10O	122.073	-17.28	2.16	15.72	126.7	19	0	-2.62	-3.75	-9.95	0	2.05	0.41	-30.63
200		pentane-1,5-diamine	C5H14N2	102.116	-17.27	-0.76	42.82	116.48	21	6	-6.31	-2.69	-13.24	4.29	12	1.73	-49.69
201		pentyl hexanoate	C11H22O2	186.162	-17.26	4.11	20.96	221.09	35	8	-2.52	-5.43	-21.72	3.14	9.07	4.37	-123.2
202		3,4-dimethoxybenzaldehyde	C9H10O3	166.063	-17.26	1.71	29.66	167.35	22	0	0	-3.64	-17.47	0.09	2.93	0.7	-43.37
203		benzoic acid	C7H6O2	122.037	-17.23	1.56	28.65	109	14	1	-6.26	-2.35	-5.83	0.31	5.22	2.28	0.36
204		2-methoxy-4-methylphenol	C8H10O2	138.068	-17.19	1.97	24.42	140.11	20	0	-4.42	-4.08	-15.32	0	10.12	6.74	-83.98
205		dodeca-2,4-dienal	C12H20O	180.151	-17.18	4.5	14.61	239.29	33	6	-1.69	-5.88	-23.07	0.69	8.38	6.41	-73.62
206		1-methoxy-4-(prop-1-enyl)benzene	C10H12O	148.089	-17.18	3.29	7.78	167.14	23	0	0	-4.58	-13.78	0	0.59	-1.17	-30.8
207		4-ethoxybenzaldehyde	C9H10O2	150.068	-17.16	2.22	21.52	154.49	21	1	-2.82	-3.93	-17.88	0.3	8.87	4.93	-74.48
208		2-methyl-1,3-dinitrobenzene	C7H6N2O4	182.033	-17.16	1.47	76.16	150.2	19	2	0	-3.03	-14.3	0	0	-3.08	-39.5
209		2-phenylethyl ethanoate	C10H12O2	164.084	-17.14	2.17	21.39	168.65	24	3	0	-4.65	-16.53	0	1.04	-0.1	-39.96

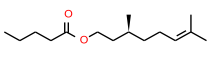
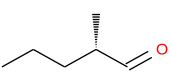
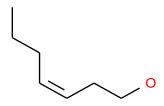
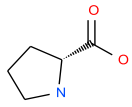
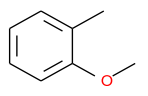
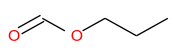
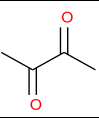
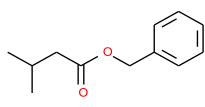
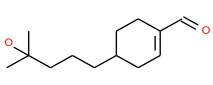
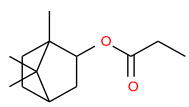
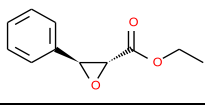
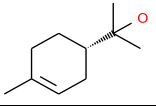
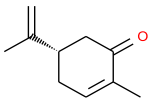
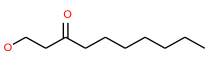
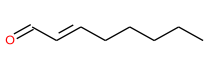
210		(S)-2,6-dimethyl-oct-7-en-2-ol	C10H20O	156.151	-17.12	3.45	16.7	202.43	31	6	-1.38	-5.12	-15.2	1.89	2.87	-1.14	-21.02
211		p-cresol	C7H8O	108.058	-17.1	2	17.86	107.38	16	0	-2.77	-2.87	-10.69	0	3.18	0.2	-31.33
212		allyl furan-2-carboxylate	C8H8O3	152.047	-17.08	1.89	29.86	157	19	2	0	-4.09	-15.97	0.7	1.93	-1.53	-37.87
213		4-propyl-benzaldehyde	C10H12O	148.089	-17.06	3.03	14.4	160.7	23	2	-2.65	-4.11	-17.89	1.23	7.76	4.97	-89.07
214		oct-1-en-3-ol	C8H16O	128.12	-17.03	2.81	17.13	157.78	25	6	-3.45	-4.64	-16.8	1.02	8.38	2.63	-76.39
215		m-cresol	C7H8O	108.058	-16.99	2	17.86	107.46	16	0	-2.18	-3.01	-11.82	0	3.17	-0.02	-39.08
216		diethylamino-m-tolyl-methanone	C12H17NO	191.131	-16.96	2.7	16.17	216.2	31	3	0	-5.49	-14.84	0	1.39	-1.96	-52.1
217		(3S,3aR,7R,8aS)-3,6,8,8-tetramethyl-2,3,4,7,8,8a-hexahydro-1H-3a,7-methanoazulene	C15H24	204.351	-16.91	5.28	0	276.98	39	0	0	-5.29	-12.52	0.01	0	-1.29	-50.83
218		(Z)-dec-4-enal	C10H18O	154.136	-16.89	3.4	14.61	201.12	29	7	-2.82	-4.79	-19.87	0.39	7.96	4.76	-100.6
219		methyl butanoate	C5H10O2	102.068	-16.89	1.22	21.09	114.05	17	2	-3.91	-3.29	-8.1	0.32	4.42	-1.85	-6.58
220		1-methyl-ethyl 2-phenyl-ethanoate	C11H14O2	178.099	-16.88	2.49	20.08	182.66	27	3	-3.07	-5.28	-19.24	2.52	8.8	8	-127.64
221		hexan-3-one	C6H12O	100.089	-16.87	1.82	13.27	124.15	19	3	-3.76	-3.69	-10.82	0	4.47	1.18	-55.66
222		ethyl 2-phenyl-ethanoate	C10H12O2	164.084	-16.85	2.23	20.4	167.34	24	3	-3.95	-4.62	-9.57	1.57	5.12	0.26	-32.45
223		(S)-4-isopropenyl-1-methyl-cyclohex-1-ene	C10H16	136.125	-16.85	3.83	0	195.06	26	1	0	-4.77	-13.65	0	0	-0.91	-29.4
224		propane-1,3-dithiol	C3H8S2	108.007	-16.82	1.8	0	90.74	13	4	-4.35	-2.24	-8.22	0.05	3.29	-1.46	-15.78

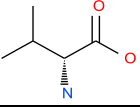
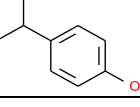
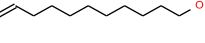
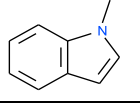
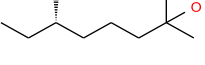
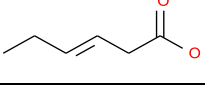
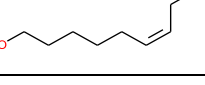
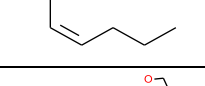
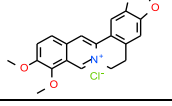
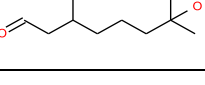
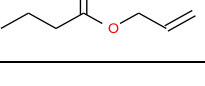
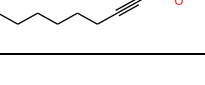
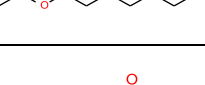
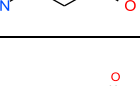
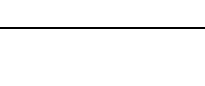
225		dec-2-enal	C10H18O	154.136	-16.8	3.87	14.61	197.83	29	6	-2.87	-4.84	-20.35	2.9	8.03	6.71	-88.69
226		4-butyl-benzaldehyde	C11H14O	162.104	-16.8	3.51	14.4	178.6	26	3	-3.49	-4.53	-15.96	2.65	7.49	5.48	-73.27
227		(S)-octan-2-ol	C8H18O	130.136	-16.79	3.03	16.99	155.57	27	6	-4.16	-4.73	-13.67	2.05	8.53	0.89	-94.04
228		4-isopropyl-benzaldehyde	C10H12O	148.089	-16.78	2.77	14.4	157.14	23	1	-2.66	-4.11	-18.01	0.23	7.95	6.28	-82.93
229		(1,5-dimethyl-1-vinyl-hex-4-enyloxy)-methanone	C11H18O2	182.131	-16.77	3.22	20.88	244.51	31	5	0	-5.16	-15.68	0	0.53	-1.57	-49.78
230		(1S,2R)-5-isopropyl-2-methyl-cyclohexanol	C10H20O	156.151	-16.77	2.95	16.05	179.36	31	2	-2.04	-4.22	-11.62	0.86	3.08	-1	-40.79
231		phenoxy-benzene	C12H10O	170.073	-16.75	3.3	6.99	165.46	23	2	0	-4.76	-15.12	0	1.22	-0.84	-51.55
232		phenyl-methyl ethanoate	C9H10O2	150.068	-16.73	1.86	21.47	150.77	21	2	-2.9	-4.32	-17.67	0	8.04	5.98	-85.62
233		4-methoxy-benzaldehyde	C8H8O2	136.052	-16.71	1.74	21.94	135.92	18	0	-2.64	-3.48	-16.92	0	9.15	3.59	-73.97
234		non-2-en-1-ol	C9H18O	142.136	-16.7	3.22	17.17	181.08	28	7	-2.29	-4.83	-14.18	2.58	3.27	-0.21	-15.68
235		(2S,3S)-ethyl 3-methyl-3-phenyl-oxirane-2-carboxylate	C12H14O3	206.094	-16.69	2.59	28.74	221.12	29	3	-3.15	-5.01	-18.18	0.82	10.71	4.5	-121.56
236		3,7-dimethyl-oct-6-enyl pentanoate	C15H28O2	240.209	-16.69	5.54	20.96	297.84	45	9	-3.6	-6.53	-17.09	4.05	9.29	2.32	-88.68
237		pentan-1-ol	C5H12O	88.089	-16.69	1.59	17.17	104.37	18	4	-3.67	-3.25	-11.32	0.67	5.52	-0.66	-53.93
238		ethyl hexanoate	C8H16O2	144.115	-16.67	2.66	20.67	166.87	26	5	-3.26	-4.86	-17.06	0	8.51	3.81	-84.94
239		1-methyl-3-nitro-benzene	C7H7NO2	137.048	-16.67	1.99	38.5	122.54	17	1	0	-3.15	-14.37	0	0	-1.19	-38.84

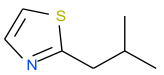
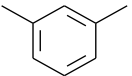
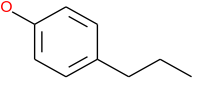
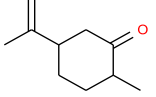
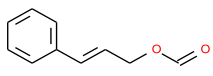
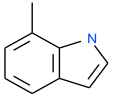

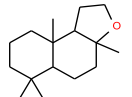
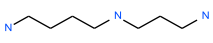
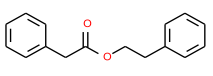
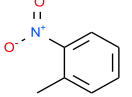
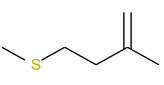
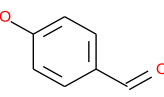
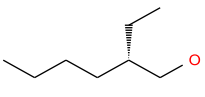
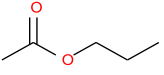
240		(S)-octan-3-ol	C8H18O	130.136	-16.66	3.12	17.13	155.4	27	6	-4.49	-4.88	-16.68	2.71	9.03	6.48	-91.98
241		(S)-2-amino-4-methyl-pentanoic acid	C6H13NO2	132.102	-16.65	-0.47	49.71	133.58	23	5	-6.72	-2.73	-16.52	0.64	13.44	8.53	-72.29
242		4-oxo-pentanoic acid	C5H8O3	117.055	-16.65	-0.08	42.23	117.6	17	4	-6.54	-2.4	-15.6	0	8.95	12.12	-61.52
243		3-methyl-but-2-en-1-ol	C5H10O	86.073	-16.65	1.33	17.17	110.67	16	2	-4.03	-3.21	-10.82	0	6.57	0.59	-52.2
244		2-methyl-pentanal	C6H12O	100.089	-16.63	1.78	14.67	117.26	19	3	-3.94	-3.25	-10.47	0.65	5.18	0.45	-56.18
245		2-pentyl-furan	C9H14O	138.104	-16.6	3.36	7.99	153.57	24	4	-2.85	-4.94	-18.22	0.97	7.45	6.28	-95.05
246		heptan-3-one	C7H14O	114.104	-16.6	2.3	13.27	142.06	22	4	-2.92	-4.08	-13.78	0.75	4.65	2.12	-58.53
247		2-phenyl-ethyl 3-methyl-butanoate	C13H18O2	206.131	-16.6	3.47	20.69	217.78	33	5	0	-5.22	-16.15	1.15	1.38	-1.5	-47.05
248		(R)-2,6-diamino-hexanoic acid	C6H14N2O2	147.113	-16.59	-2.07	70.86	144.8	25	8	-9.98	-2.44	-19.98	0.9	20.95	14.78	-81.8
249		5-methyl-2-tert-butyl-phenol	C11H16O	164.12	-16.59	3.49	16.79	193.7	28	1	-2.25	-4.89	-10.15	0.75	2.31	0.28	-41.13
250		undecan-2-one	C11H22O	170.167	-16.58	4.22	13.84	212.47	34	8	-3.8	-5.9	-18.64	5.54	7.96	7.39	-105.37
251		2-methoxy-benzaldehyde	C8H8O2	136.052	-16.58	1.62	22.03	134.6	18	0	-3.65	-3.55	-14.54	0.48	8.65	4.67	-82.43
252		4-ethyl-benzaldehyde	C9H10O	134.073	-16.58	2.55	14.4	143.16	20	1	0	-3.14	-16.53	0.18	1.77	0.2	-44.05
253		oct-3-en-2-one	C8H14O	126.104	-16.57	2.5	13.84	166.04	23	3	-2.86	-4.52	-16.49	0	6.9	4.85	-71.06
254		(R)-5-isopropenyl-2-methyl-cyclohex-2-enone	C10H14O	150.104	-16.55	2.52	13.68	206.18	25	1	0	-4.63	-13.88	0.2	0.97	-1.35	-36.08

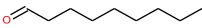
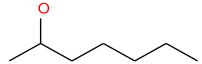
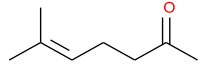
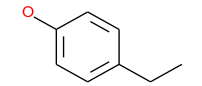
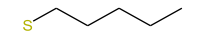
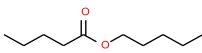
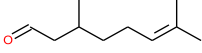
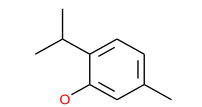
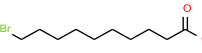
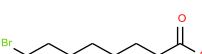
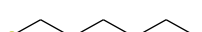
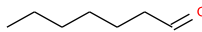
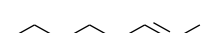
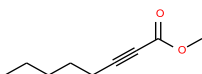
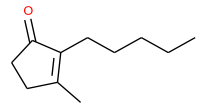
255		3-ethoxy-4-hydroxy-benzaldehyde	C9H10O3	166.063	-16.54	1.84	38.16	165.91	22	1	0	-3.51	-17.12	0.52	2.11	1.14	-45.74
256		7-methyl-bicyclo[4.3.0]nona-1,3,5,7-tetraene	C10H10	130.078	-16.53	3.48	0	157.79	20	0	0	-4.21	-12.75	0	0	-1.46	-41.64
257		phenyl-methyl 2-phenyl-ethanoate	C15H14O2	226.099	-16.52	3.37	20.5	221.9	31	4	0	-5.24	-17.64	0.21	1.22	1.98	-95.18
258		pent-2-enal	C5H8O	84.058	-16.51	1.46	14.61	107.72	14	1	-2.68	-2.67	-12.41	0.27	3.78	1.54	-54.7
259		2,6,6-trimethyl-cyclohexa-1,3-dienecarbaldehyde	C10H14O	150.104	-16.5	2.72	14.59	216.78	25	0	0	-3.97	-15.15	0.55	1.7	0.05	-36.26
260		(R)-ethyl 3-hydroxy-butanoate	C6H12O3	132.079	-16.5	0.53	37.15	135.59	21	4	-2.54	-3.39	-12.28	0	4.54	-2.01	-28.91
261		ethyl propanoate	C5H10O2	102.068	-16.48	1.22	20.67	113.59	17	2	-3.61	-3.4	-9.82	2.24	4.24	0.55	-20.03
262		2-phenyl-ethyl hexanoate	C14H20O2	220.146	-16.46	4.11	20.69	239.31	36	7	-2.95	-5.69	-19.01	6.25	8.65	4.74	-112.76
263		ethyl 3-hydroxy-butanoate	C6H12O3	132.079	-16.44	0.53	37.15	135.59	21	4	-8.68	-3.17	-9.91	5.11	7.41	14.54	-0.29
264		2,6,6-trimethyl-cyclohex-1-enecarbaldehyde	C10H16O	152.12	-16.42	3.06	14.59	210.5	27	0	-4.2	-4.3	-10.87	1.18	7.37	3.68	-98.24
265		(1-methyl-1-(4-methyl-cyclohex-4-enyl)-ethoxy)-methanone	C11H18O2	182.131	-16.4	2.93	21.02	228.59	31	2	0	-4.64	-14.77	2.44	1.27	-1.02	-44.35
266		oct-1-en-3-one	C8H14O	126.104	-16.38	2.6	13.27	163.66	23	4	-2.49	-4.76	-17.62	0.86	7.41	4.2	-84.37
267		methyl 2-phenyl-ethanoate	C9H10O2	150.068	-16.37	1.75	20.82	150.33	21	2	-3.24	-4.22	-12.4	0.55	7.06	0.85	-62.75
268		3-(4-(2-carboxy-vinyl)-phenyl)-acrylic acid	C12H10O4	218.058	-16.36	2.8	57.01	227.31	24	2	-1.91	-3.42	-14.23	0	6.16	-1.27	-42.96
269		5-isopropenyl-2-methyl-cyclohex-2-enone	C10H14O	150.104	-16.35	2.52	13.68	206.18	25	1	0	-4.61	-14.35	0	1.01	-0.42	-31.04

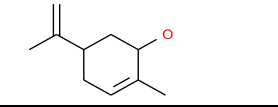
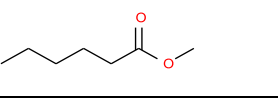
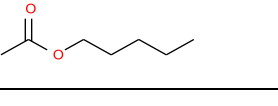
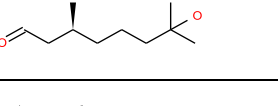
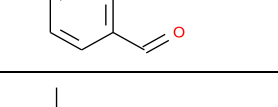
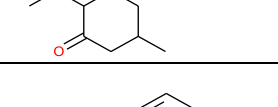
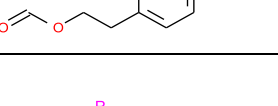
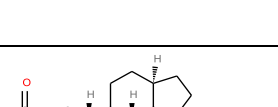
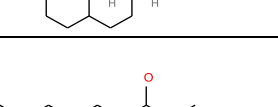
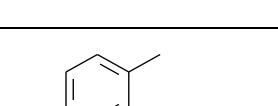
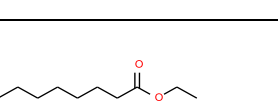
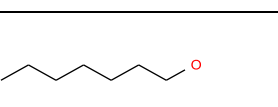
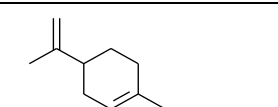
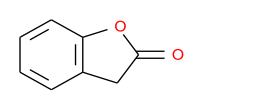

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271		nona-2,6-dienal	C9H14O	138.104	-16.34	2.92	14.61	186.2	24	4	0	-4	-17.77	0.82	1.79	0.54	-33.66
272		2-ethoxy-thiazole	C5H7NOS	129.025	-16.34	1.62	19.59	112.23	15	1	0	-3.76	-13.76	0.17	1.71	-2.94	-26.64
273		2-isopropyl-5-methyl-cyclohexanol	C10H20O	156.151	-16.31	2.95	16.05	180.11	31	2	-1.84	-4.59	-11.24	0.21	2.74	-0.91	-37.61
274		1-(pyridin-2-yl)-ethanone	C7H7NO	121.053	-16.3	0.67	23.11	117.02	16	0	-6.6	-2.94	-10.92	0.02	4.68	14.81	3.17
275		(S)-1-styryl-hexyl ethanoate	C16H22O2	246.162	-16.28	4.98	20.54	278.51	40	7	0	-6.45	-19.19	0	1.45	2.94	-108.71
276		2-methyl-pentanoic acid	C6H12O2	116.084	-16.26	1.67	28.92	124.09	19	3	-5.45	-2.86	-7.23	1.22	5.2	1.46	-16.43
277		2-methyl-propyl 2-phenyl-ethanoate	C12H16O2	192.115	-16.25	3.03	20.77	200.59	30	4	0	-5.56	-14.9	0.58	1.95	-2.26	-52.48
278		(4-isopropyl-phenyl)-methanol	C10H14O	150.104	-16.24	2.4	17.35	157.12	25	3	-3.79	-4.71	-15.33	0.53	9.38	4.56	-90.89
279		hept-2-enal	C7H12O	112.089	-16.24	2.42	14.61	144.11	20	3	-2.86	-3.7	-16.53	0	7.09	4.4	-80.91
280		2-phenyl-acetic acid	C8H8O2	137.06	-16.24	1.4	28.62	127.33	19	3	-2.36	-3.13	-14.19	0.97	3.76	2.12	-47.96
281		12-bromo-dodecanoic acid	C12H23BrO2	278.088	-16.14	5.05	28.89	253.44	37	11	-6.84	-6.26	-10.81	9.58	10.36	2.73	-105.95
282		2-methyl-pent-2-enoic acid	C6H10O2	114.068	-16.07	1.64	28.92	136.54	17	2	-6.38	-2.74	-4.46	0	5.24	1.86	-4.97
283		undecanal	C11H22O	170.167	-16.06	4.35	14.61	212.17	34	9	-2.81	-5.43	-21.14	6.29	8.02	6.69	-118.36
284		3-methyl-but-2-enyl ethanoate	C7H12O2	128.084	-16.05	1.91	21.66	158.33	21	2	0	-4.3	-13.64	0	1.32	-2.59	-30.7

285		(S)-3,7-dimethyl-oct-6-enyl pentanoate	C15H28O2	240.209	-16.04	5.54	20.96	297.84	45	9	-3.59	-6.55	-15.34	0	9.31	0.6	-76.09
286		(S)-2-methyl-pentanal	C6H12O	100.089	-16.02	1.78	14.67	117.26	19	3	-4.49	-3.39	-13.88	1.39	7.47	6.21	-73.84
287		(Z)-hept-3-en-1-ol	C7H14O	114.104	-16	2.09	17.17	147.03	22	5	-2.23	-3.74	-12.62	0.07	3.2	-0.98	-11.03
288		(R)-pyrrolidine-2-carboxylic acid	C5H9NO2	116.071	-15.98	-0.82	41.32	113.22	18	2	-4.83	-2.41	-13.12	2.07	8.53	5.09	-65.28
289		1-methoxy-2-methyl-benzene	C8H10O	122.073	-15.98	2.23	7.87	127.59	19	0	0	-3.98	-12.76	0.05	0.57	-1.48	-42.25
290		propoxy-methanone	C4H8O2	88.052	-15.97	0.88	22.76	93.44	14	2	-5.09	-2.33	-6.62	1.3	4.29	1.03	-13.94
291		biacetyl	C4H6O2	86.037	-15.95	-0.45	28.16	95.8	12	1	-7.43	-2	-10.75	0	5.23	15.78	-11.08
292		phenyl-methyl 3-methyl-butanoate	C12H16O2	192.115	-15.92	3.16	20.77	199.91	30	4	0	-5.37	-15.49	0.24	2.04	-1.14	-61.83
293		4-(4-hydroxy-4-methyl-pentyl)-cyclohex-1-enecarbaldehyde	C13H22O2	210.162	-15.9	3.69	30.78	268.82	37	5	-6.58	-5.11	-7.8	3.45	11.01	1.08	-117.04
294		1,7,7-trimethyl-bicyclo[2.2.1]heptan-2-yl propanoate	C13H22O2	210.162	-15.89	3.69	20.59	262.08	37	2	0	-4.98	-14.62	1.4	1.34	-0.2	-49.41
295		(2R,3S)-ethyl 3-phenyl-oxirane-2-carboxylate	C11H12O3	192.079	-15.88	2.15	29.44	192.59	26	3	-3.35	-4.78	-13.63	0.66	7.02	3.57	-54.11
296		(S)-2-(4-methyl-cyclohex-3-enyl)-propan-2-ol	C10H18O	154.136	-15.88	2.95	16.15	205.6	29	2	0	-4.46	-12.22	0	-0.24	-2.56	-42.74
297		(S)-5-isopropenyl-2-methyl-cyclohex-2-enone	C10H14O	150.104	-15.86	2.52	13.68	206.18	25	1	0	-4.21	-12.44	0.27	1.32	-3.31	-27.72
298		1-hydroxy-decan-3-one	C10H20O2	172.146	-15.8	2.59	29.92	203.32	32	9	-2.45	-5.17	-12.27	0	2.98	-2.26	-41.06
299		oct-2-enal	C8H14O	126.104	-15.79	2.9	14.61	162.02	23	4	-2.5	-4.13	-15.85	1.22	6.97	2.32	-77

300		(R)-2-amino-3-methylbutanoic acid	C5H11NO2	118.087	-15.78	-1.02	49.89	117.73	20	4	-7.38	-2.35	-11.46	1.45	13.66	4.97	-58.37
301		4-isopropylphenol	C9H12O	136.089	-15.76	2.72	17.86	139.51	22	1	-2.77	-3.46	-11.27	0.17	3.17	2.82	-52.99
302		undec-10-en-1-ol	C11H22O	170.167	-15.75	4.1	17.17	215.65	34	10	-2.97	-5.92	-20.92	6.29	9.55	5.29	-102.31
303		7-methyl-7-azabicyclo[4.3.0]nona-1(6),2,4,8-tetraene	C9H9N	131.073	-15.73	2.13	2.9	135.49	19	0	0	-4.03	-12.68	0.03	0	-0.54	-43.99
304		(S)-2,6-dimethyloctan-2-ol	C10H22O	158.167	-15.73	3.93	16.7	200.24	33	6	-2.67	-4.6	-10.45	0.02	2.96	-1.91	-27.46
305		hex-3-enoic acid	C6H10O2	114.068	-15.72	1.42	28.89	131.75	17	3	-5.56	-2.76	-3.2	0.7	5.25	-3.57	-19.06
306		(Z)-non-6-en-1-ol	C9H18O	142.136	-15.71	3.05	17.17	182.26	28	7	-3.4	-4.79	-18.54	0.43	9.52	4.99	-95.82
307		(Z)-hex-2-en-1-ol	C6H12O	100.089	-15.71	1.78	17.17	127.36	19	4	-2.73	-3.45	-11.63	0	3.28	0.42	-25.16
308		9,10-Dimethoxy-5,6-dihydro[1,3]dioxolo[4,5-g]isoquinolino[3,2-a]isoquinolin-7-ium chloride	C20H18ClNO4	371.814	-15.64	5.38	33.45	340.03	43	0	0	-5.97	-15.45	0	2.64	2.78	-115.84
309		7-hydroxy-3,7-dimethyloctanal	C10H20O2	172.146	-15.63	2.63	30.8	207.15	32	7	-5.23	-4.38	-13.86	3.46	10.08	4	-92.45
310		allyl butanoate	C7H12O2	128.084	-15.63	1.97	20.96	153.14	21	4	-3.08	-4.37	-18.23	0	8.75	6.58	-87.73
311		methyl non-2-ynoate	C10H16O2	168.115	-15.63	2.97	21.09	209.95	28	5	-2.15	-5.38	-20.95	2.18	8.62	7.43	-59.32
312		heptyl ethanoate	C9H18O2	158.131	-15.6	3.13	21.66	186.24	29	6	-2.94	-5.16	-19.12	2.25	8.96	6.21	-95.79
313		3-amino-propanoic acid	C3H7NO2	90.056	-15.59	-1.37	50.05	83.19	14	4	-7.14	-1.5	-10.6	0	12.25	3.77	-43.49
314		nonan-3-one	C9H18O	142.136	-15.58	3.27	13.27	177.87	28	6	-2.91	-5.02	-16.38	1.67	7.1	3.92	-85.06

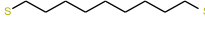
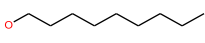
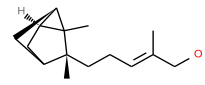
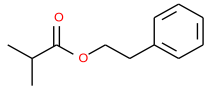
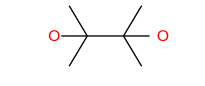
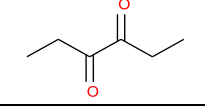
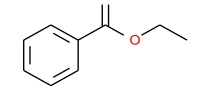
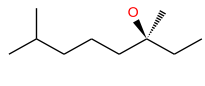
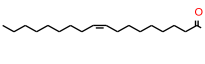
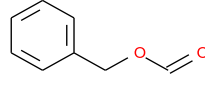
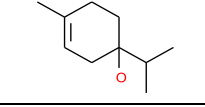
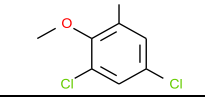
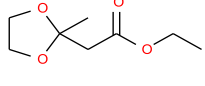
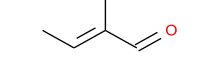
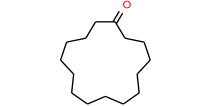
315		2-isobutyl-thiazole	C7H11NS	141.061	-15.58	2.31	11.17	135.59	20	2	0	-4.32	-12.56	0.52	0.49	-2.55	-35.48
316		m-xylene	C8H10	106.078	-15.51	2.66	0	117.85	18	0	0	-3.84	-12.07	0.05	0	-1.32	-40.32
317		4-propyl-phenol	C9H12O	136.089	-15.5	2.98	17.86	143.06	22	2	-3.08	-4.23	-16.83	0.94	8.66	6.46	-81.42
318		5-isopropenyl-2-methyl-cyclohexanone	C10H16O	152.12	-15.5	2.58	13.68	188.23	27	1	-4.11	-4.7	-10.09	0.71	7.44	2.98	-70.01
319		(3-phenyl-allyloxy)-methanone	C10H10O2	162.068	-15.49	2.38	22.48	171.61	22	3	-2.57	-4.08	-18.73	0	8.86	6.11	-80.41
320		5-methyl-7-aza-bicyclo[4.3.0]nona-1(6),2,4,8-tetraene	C9H9N	131.073	-15.49	2.48	10.79	132.9	19	0	-2.27	-3.85	-11.17	0.13	3.34	2.25	-75.44
321		thiophene-2-thiol	C4H4S2	115.975	-15.47	2.05	0	86.55	10	1	-2.08	-3.51	-12.63	0	3.67	2.18	-43.05
322		3a,6,6,9a-tetramethyl-2,4,5,5a,7,8,9,9b-octahydro-1H-benzo[e][1]benzofuran	C16H28O	236.393	-15.44	4.88	8.19	308.69	45	0	0	-5.58	-11.07	0.41	0.46	-1.47	-69.97
323		N1-(3-amino-propyl)-butane-1,4-diamine	C7H19N3	145.158	-15.44	-1.38	54.54	165.62	29	9	-6.25	-3.97	-17.87	1.63	17.55	3.55	-69.32
324		2-phenyl-ethyl 2-phenyl-ethanoate	C16H16O2	240.115	-15.43	3.68	20.42	239.78	34	5	-3.07	-6.27	-18.79	2.99	8.42	9.13	-127.33
325		1-methyl-2-nitro-benzene	C7H7NO2	137.048	-15.43	1.87	38.2	122.16	17	1	0	-3.23	-11.52	0	0	-3.56	-22.29
326		2-methyl-4-methylsulfanyl-but-1-ene	C6H12S	116.066	-15.42	2.43	0	138.56	19	3	0	-4.27	-12.96	0	0	-2.11	-34.5
327		4-hydroxy-benzaldehyde	C7H6O2	122.037	-15.41	1.39	32.01	114.63	15	0	-1.89	-2.42	-11.64	0.63	3.51	0	-35.66
328		(S)-2-ethyl-hexan-1-ol	C8H18O	130.136	-15.38	3.07	17.63	155.72	27	6	-3.08	-4.08	-11.91	2.9	3.2	1.61	-57.86
329		propyl ethanoate	C5H10O2	102.068	-15.38	1.2	21.66	114.61	17	2	-6.62	-3.07	-12.29	3.22	4.56	16.83	-4.67

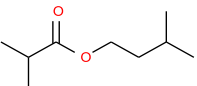
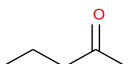
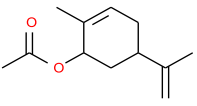
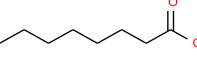
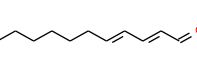
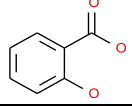
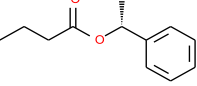
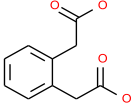
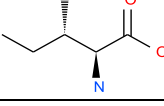
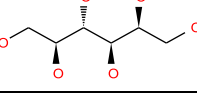
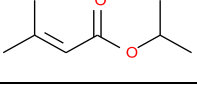
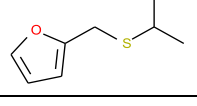
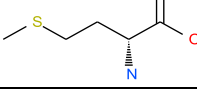
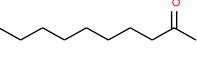
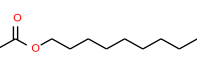
330		nonanal	C9H18O	142.136	-15.34	3.39	14.61	176.36	28	7	-3.34	-4.64	-17.07	2.01	7.08	5.71	-87.3
331		heptan-2-ol	C7H16O	116.12	-15.33	2.55	16.99	137.66	24	5	-4.31	-4.42	-14.26	3.28	8.43	5.27	-87.8
332		6-methyl-hept-5-en-2-one	C8H14O	126.104	-15.33	2.34	13.84	166.82	23	3	-2.92	-4.64	-16.55	0	7.81	6.14	-81.53
333		4-ethyl-phenol	C8H10O	122.073	-15.29	2.5	17.86	125.52	19	1	-2.97	-3.69	-14.79	0.42	8.02	4.34	-67.26
334		pentane-1-thiol	C5H12S	104.066	-15.28	2.76	0	111.47	18	4	-2.59	-3.17	-9.26	1.44	1.64	-1.46	-27.54
335		pentyl pentanoate	C10H20O2	172.146	-15.25	3.63	20.96	203.18	32	7	-2.53	-5.25	-21.84	3.22	9.09	8.3	-118.7
336		3,7-dimethyl-oct-6-enal	C10H18O	154.136	-15.25	3.37	14.61	198.02	29	5	-2.32	-4.79	-18.57	0	7.9	5.27	-97.48
337		2-isopropyl-5-methyl-phenol	C10H14O	150.104	-15.25	3	16.79	162.81	25	1	-1.03	-4.45	-12.43	0	2.99	-0.13	-39.55
338		10-bromo-decanoic acid	C10H19BrO2	250.057	-15.21	4.09	28.89	217.63	31	9	-3.17	-5.48	-19.41	5.05	9.54	5.05	-99.09
339		8-bromo-octanoic acid	C8H15BrO2	222.026	-15.19	3.12	28.89	181.81	25	7	-1.89	-3.71	-13.49	0.67	1.99	-0.2	-41.45
340		hexane-1-thiol	C6H14S	118.082	-15.18	3.24	0	129.38	21	5	-2.07	-3.69	-10.5	1.4	1.64	-1.84	-31.68
341		heptanal	C7H14O	114.104	-15.16	2.42	14.61	140.55	22	5	-2.88	-3.79	-16.43	1.39	6.98	4.33	-85.11
342		oct-2-ene	C8H16	112.125	-15.15	3.81	0	153.34	24	4	0	-4.73	-13.68	0	0	-1.05	-29.58
343		methyl oct-2-ynoate	C9H14O2	154.099	-15.14	2.49	21.09	192.05	25	4	-2.08	-4.86	-18.61	0.5	6.74	6.86	-48.81
344		3-methyl-2-pentyl-cyclopent-2-enone	C11H18O	166.136	-15.14	3.34	14.04	223.77	30	4	0	-4.89	-12.39	0.94	0.46	-3.36	-45.1

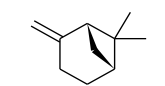
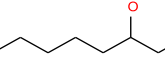
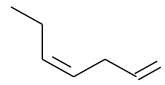
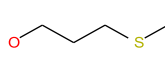
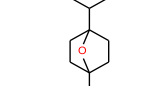
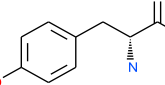
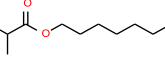
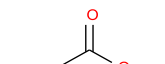
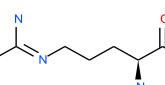
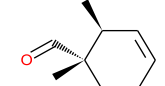
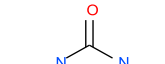
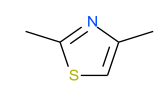
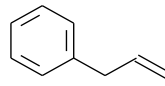
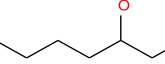
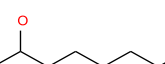
345		5-isopropenyl-2-methylcyclohex-2-enol	C10H16O	152.12	-15.12	2.81	16.05	200.94	27	2	-2.49	-4.08	-11.64	0	3.11	3.07	-53.84
346		methyl hexanoate	C7H14O2	130.099	-15.11	2.18	21.09	149.87	23	4	-2.73	-4.47	-17.05	0.05	7.7	5.57	-83.56
347		pentyl ethanoate	C7H14O2	130.099	-15.08	2.17	21.66	150.43	23	4	-4.06	-4.11	-6.6	2.28	4.25	-1.57	-2.82
348		(S)-7-hydroxy-3,7-dimethyl-octanal	C10H20O2	172.146	-15.03	2.63	30.8	207.15	32	7	-4.87	-4.46	-14.6	4.11	10.46	4.31	-104.51
349		4-methyl-benzaldehyde	C8H8O	120.058	-14.99	2.05	14.4	125.02	17	0	0	-2.77	-14.74	0	1.76	0.42	-36.08
350		2-isopropyl-5-methylcyclohexanone	C10H18O	154.136	-14.95	2.74	13.68	182.71	29	1	-3.19	-4.84	-13.28	0.44	7.87	4.77	-104.13
351		(2-phenyl-ethoxy)methane	C9H10O2	150.068	-14.95	1.85	22.48	147.48	21	3	0	-3.76	-15.09	0.79	0.82	0.38	-45.9
352		dimethylphosphane	C2H7P	62.0507	-14.93	0.71	0	49.28	10	0	-2.94	-2.36	-8.44	0.01	1.68	1.94	-17.89
353		(8S,9R,10S,13R,14S)-hexadecahydro-1H-cyclopenta[a]phenanthrene-2-carboxylic acid	C18H28O2	276.414	-14.9	4.2	28.97	297.82	47	1	0	-5.73	-11.37	0	1.31	-1.93	-69.85
354		nonan-3-ol	C9H20O	144.151	-14.87	3.6	17.13	173.31	30	7	-2.02	-4.89	-12.51	3.39	2.98	-0.61	-36.33
355		p-xylene	C8H10	106.078	-14.86	2.66	0	117.78	18	0	0	-3.77	-11.46	0.01	0	-1.33	-31.86
356		ethyl octanoate	C10H20O2	172.146	-14.82	3.63	20.67	202.69	32	7	-2.84	-5.65	-17.49	3.43	8.57	4.58	-95.93
357		heptan-1-ol	C7H16O	116.12	-14.81	2.56	17.17	140.18	24	6	-2.07	-4.06	-12.2	2.2	3.26	-1.08	-22.45
358		4-isopropenyl-1-methylcyclohex-1-ene	C10H16	136.125	-14.76	3.83	0	195.06	26	1	0	-4.06	-13.75	0.36	0.64	0.94	-25.18
359		8-oxo-7-oxa-bicyclo[4.3.0]nona-1(6),2,4-triene	C8H6O2	134.037	-14.73	1.6	21.01	131.46	16	0	0	-3.2	-12.12	0	1.39	-2.29	-43.14

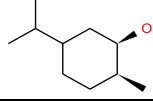
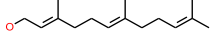
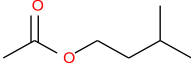
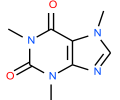
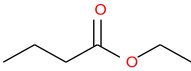
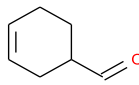
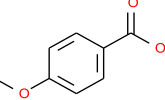
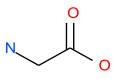

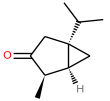
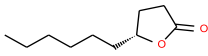
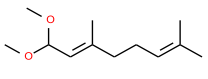
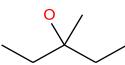
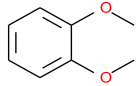
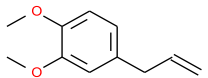
360		2,3,5,6-tetramethylpyrazine	C8H12N2	136.1	-14.69	1.05	19.78	149.71	22	0	0	-4.32	-12.26	0	2.06	-1.64	-27.31
361		o-xylene	C8H10	106.078	-14.68	2.54	0	116.1	18	0	0	-3.73	-11.63	0	0	-0.83	-40.23
362		hexan-2-one	C6H12O	100.089	-14.66	1.81	13.84	122.94	19	3	-2.87	-3.69	-11.89	0	4.96	2.19	-51.1
363		9-methyl-7-azabicyclo[4.3.0]nona-1(6),2,4,8-tetraene	C9H9N	131.073	-14.62	2.48	10.11	135.36	19	0	0	-3.88	-12.57	0.13	0.04	0.79	-47.53
364		anisole	C7H8O	108.058	-14.55	1.95	7.78	107.74	16	1	-2.07	-3.65	-12.7	0	4.56	2.75	-70.23
365		(1R,2R,4S)-2-ethyl-1,3,3-trimethylbicyclo[2.2.1]heptan-2-ol	C12H22O	182.167	-14.55	3.79	16.44	245.86	35	2	-1.82	-4.8	-9.41	0.18	2.44	-0.53	-37.63
366		pyridine	C5H5N	79.042	-14.52	0.81	9.67	71.19	11	0	-2.85	-2.73	-8.82	0	3.54	1.06	-39.75
367		decanedioic acid	C10H18O4	202.121	-14.47	2.36	57.28	211.06	30	9	-7.22	-4.18	-7.97	4.43	13.79	-1.78	-62.4
368		1-(propyldisulfanyl)propane	C6H14S2	150.305	-14.42	3.33	0	151.15	22	5	0	-4.95	-12.67	0.25	0	-2.17	-35.07
369		2-(4-(carboxymethyl)phenyl)-acetic acid	C10H10O4	194.058	-14.34	0.95	57.01	178.76	22	4	0	-3.95	-12.5	0.68	2.77	-5.57	-35.92
370		3-(4-hydroxy-3-methoxyphenyl)-acrylic acid	C10H10O4	195.066	-14.31	2.04	52.8	194.87	25	1	-3.29	-3.72	-17.59	1.61	6.94	12.57	-32.56
371		1-methyl-4-nitrobenzene	C7H7NO2	137.048	-14.31	1.99	38.5	122.47	17	1	0	-3.4	-11.75	0	0	-1.34	-30.34
372		2-methyl-pent-2-enal	C6H10O	98.073	-14.28	1.73	14.67	127.14	17	1	0	-2.93	-14.65	0	1.76	0.61	-27.02
373		non-2-enoic acid	C9H16O2	156.115	-14.24	3.42	28.89	187.56	26	6	-1.93	-4.09	-10.98	0.78	3.9	-3.27	-53.15
374		3,3-bis(4-hydroxy-2,5-dimethylphenyl)-3H-benzo[c][1,2]oxathiole 1,1-dioxide	C23H22O5S	410.483	-14.22	5.39	67.78	393.46	51	2	0	-6.42	-13.47	0	2.34	0.9	-79.85

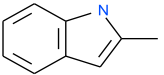
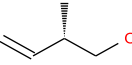
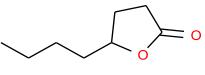
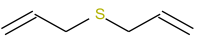

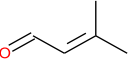
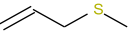
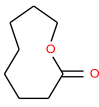
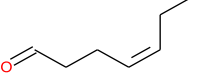
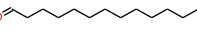

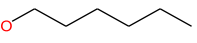
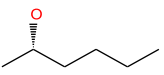
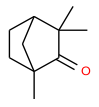
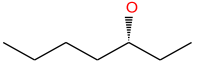
375		2-phenoxy-acetic acid	C8H8O3	153.055	-14.2	1.2	36.12	138.34	20	4	-3.13	-3.05	-15.14	2.23	5.46	6.68	-48.29
376		1,2-dimethoxy-4-(prop-1-enyl)-benzene	C11H14O2	178.099	-14.18	3.26	15.5	198.56	27	0	0	-4.72	-12.92	0	1.39	1.31	-71.4
377		cinnamic acid	C9H8O2	149.06	-14.17	2.33	28.62	151.6	20	2	-2.29	-3.67	-14.58	0.82	4.89	5.75	-25.44
378		methyl ethanoate	C3H6O2	74.037	-14.15	0.24	21.79	79.2	11	0	-6.28	-2.29	-11.08	0	4.86	16.24	-14.97
379		(R)-2-oxo-5-pentyl-tetrahydro-furan	C9H16O2	156.115	-14.12	2.27	21.43	177.62	27	4	0	-4.8	-13.4	1.95	1.48	-1.54	-43.57
380		4-methyl-phenyl ethanoate	C9H10O2	150.068	-14.07	2	20.99	156.54	21	0	-1.37	-4.38	-18.02	0	8.3	6.25	-91.34
381		2,6,6-trimethyl-bicyclo[3.1.1]hept-2-ene	C10H16	136.125	-14.06	3.89	0	200.77	26	0	0	-4.13	-10.46	0.1	0	-1.26	-35.74
382		3-phenyl-propanoic acid	C9H10O2	150.068	-14.06	1.84	28.62	145.08	20	3	-2.05	-3.02	-9.85	0.76	4.14	-2.89	-34.92
383		(R)-1-isopropyl-4-methyl-cyclohex-3-enol	C10H18O	154.136	-14.06	2.96	15.54	204.53	29	2	0	-4.6	-11.67	0.13	0.2	-0.99	-34.01
384		toluene	C7H8	92.063	-14.05	2.26	0	96.84	15	0	0	-3.38	-10.76	0.02	0	-1.57	-33.79
385		3,4a,7,7,10a-pentamethyl-1-oxo-3-vinyldodecahydro-1H-benzo[f]chromen-5-yl acetate	C22H34O7	410.501	-13.97	1.75	86.43	486.04	63	5	0	-6.22	-14.25	1.48	1.72	0.24	-77.42
386		butyl ethanoate	C6H12O2	116.084	-13.96	1.68	21.66	132.52	20	3	-6.52	-3.41	-10.22	3.64	4.52	14.92	-0.53
387		(3R,3aR,6R,7S,8aR)-3,6,8,8-tetramethyloctahydro-1H-3a,7-methanoazulen-6-ol	C15H26O	222.366	-13.93	4.19	16.33	290.46	42	1	-1.28	-4.95	-9.35	0.07	2.65	-0.96	-41.14
388		(9Z,12Z)-octadeca-9,12-dienoic acid	C18H32O2	281.248	-13.88	6.73	28.89	353.96	53	15	-2.26	-5.66	-21.71	4.03	6.01	5.8	-51.44
389		7,9-dioxabicyclo[4.3.0]nona-1,3,5-triene-3-carbaldehyde	C8H6O3	150.032	-13.85	1.8	31.51	143.91	17	0	0	-2.68	-14.6	0.07	3.06	0.36	-38.31

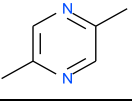
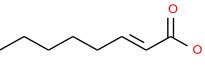

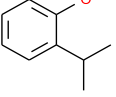
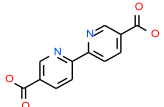

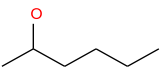
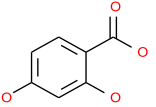
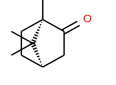
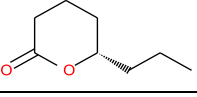
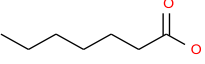

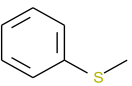

390		nonane-1,9-dithiol	C9H20S2	192.101	-13.83	4.69	0	198.18	31	10	-2.35	-4.5	-21.93	7.66	9.43	6.04	-98.24
391		nonan-1-ol	C9H20O	144.151	-13.83	3.52	17.17	175.99	30	8	-3.74	-5.11	-16.57	4.67	8.77	6.44	-86.15
392		(E)-5-((1R,3R,6S)-2,3-dimethyltricyclo[2.2.1.0 2,6]heptan-3-yl)-2-methylpent-2-en-1-ol	C15H24O	220.35	-13.82	4.6	18.45	302.43	40	5	-2.61	-4.84	-11.26	0	3.29	2.75	-57.2
393		2-phenyl-ethyl 2-methyl-propanoate	C12H16O2	192.115	-13.8	2.88	21.29	200.63	30	4	-2.38	-5.29	-16.82	1.8	8.11	6.22	-98.92
394		2,3-dimethyl-butane-2,3-diol	C6H14O2	118.099	-13.76	1.03	31.95	150.4	22	3	-2.57	-3.23	-9.02	0.3	4.46	-1.83	-24.68
395		hexane-3,4-dione	C6H10O2	114.068	-13.76	0.55	27	130.25	18	3	-7.05	-2.84	-10.62	0.52	5.13	16.62	-9.85
396		ethyl benzoate	C9H10O2	150.068	-13.74	2.39	20.99	149.49	21	2	0	-4.25	-13.83	0.5	0.66	1.87	-64.68
397		(S)-3,7-dimethyl-octan-3-ol	C10H22O	158.167	-13.74	3.87	16.84	200.41	33	6	-1.12	-5.14	-12.67	1.77	2.9	-0.83	-29.31
398		oleic acid	C18H34O2	283.264	-13.7	7.15	28.89	348.59	55	16	-2.59	-6.27	-21.2	6.44	4.78	7.66	-125.83
399		(phenyl-methoxy)-methanone	C8H8O2	136.052	-13.68	1.54	22.57	129.6	18	2	0	-3.18	-13.67	1	2.63	-1.59	-44.47
400		1-isopropyl-4-methyl-cyclohex-3-enol	C10H18O	154.136	-13.66	2.96	15.54	204.53	29	2	-3.3	-4.96	-13.57	2.92	8.73	5.83	-90.16
401		1,3,5-trichloro-2-methoxy-benzene	C7H5Cl3O	209.941	-13.54	3.85	7.96	156.49	16	0	0	-3.86	-12.64	0	1.4	0.96	-28.16
402		ethyl 2-(2-methyl-1,3-dioxolan-2-yl)-ethanoate	C8H14O4	174.089	-13.5	0.78	36.53	187.9	26	3	0	-4.56	-13.32	0.71	2.58	-1.3	-36.76
403		2-methyl-but-2-enal	C5H8O	84.058	-13.47	1.33	14.67	109.37	14	0	0	-2.89	-10.6	0	0.32	-1.78	-21.17
404		cyclopentadecanone	C15H28O	224.214	-13.46	4.46	14.11	277.17	44	0	0	-5.45	-9.5	0	0.79	-1.36	-64.86

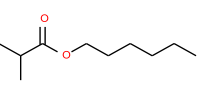
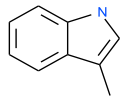
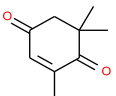
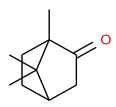
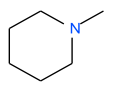
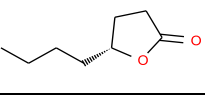
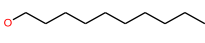
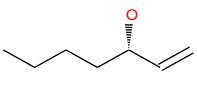
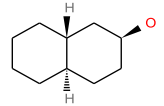
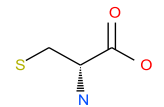
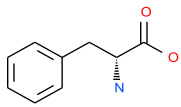
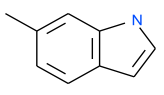
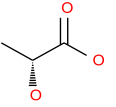
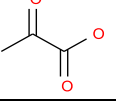

405		3-methyl-butyl 2-methylpropanoate	C9H18O2	158.131	-13.41	2.72	21.56	179.73	29	4	-2.86	-5.24	-14.97	2.79	8.6	5.24	-98.04
406		pentan-2-one	C5H10O	86.073	-13.37	1.32	13.84	105.03	16	2	-1.95	-3.22	-11.76	0	3.73	2.26	-62.85
407		5-isopropenyl-2-methylcyclohex-2-enyl ethanoate	C12H18O2	194.131	-13.32	3.23	20.64	245.9	32	2	0	-5.09	-13.44	0	1.36	1.98	-66.94
408		octanoic acid	C8H16O2	144.115	-13.3	2.8	28.89	162.68	25	6	0	-4.06	-9.8	1.8	0.46	-7.17	-34.41
409		undeca-2,4-dienal	C11H18O	166.136	-13.28	4.02	14.61	221.39	30	5	-2.67	-5.28	-15.85	4.06	8.03	5.83	-92.64
410		2-hydroxybenzoic acid	C7H6O3	139.04	-13.27	1.18	45.19	120.18	17	1	-3.56	-2.25	-13.18	0.33	6.35	7.66	-34.13
411		(R)-1-phenylethyl butanoate	C12H16O2	192.115	-13.19	3.09	20.06	203.28	30	4	0	-4.64	-16.26	1.57	1.5	4.02	-70.97
412		2-(2-(carboxymethyl)phenyl)acetic acid	C10H10O4	194.058	-13.18	0.83	57.01	178.62	22	4	0	-3.66	-12.94	0.72	3.04	-3.74	-31.16
413		(2S,3S)-2-amino-3-methylpentanoic acid	C6H13NO2	132.102	-13.12	-0.45	49.89	132.97	23	5	-6.95	-2.74	-11.66	0	12.95	7.98	-64.46
414		(2S,3R,4S,5S)-hexane-1,2,3,4,5,6-hexaol	C6H14O6	182.079	-13.12	-3.6	98.41	151.83	26	11	-6.1	-2.44	-12.23	2.6	8.85	4.46	-26.88
415		1-methyl-ethyl 3-methylbut-2-enoate	C8H14O2	142.099	-13.08	2.62	20.35	173.29	24	1	-2.6	-4.93	-13.54	0	8.64	4.95	-90.18
416		2-((1-methyl-ethylsulfanyl)-methyl)furan	C8H12OS	156.061	-13.08	2.41	7.99	148.25	22	3	-2.26	-4.86	-15.43	0	7.25	6.17	-87.53
417		(R)-2-amino-4-methylsulfanylbutanoic acid	C5H11NO2S	150.059	-13.07	-1.27	49.71	135.27	21	6	-7.53	-3.24	-17.88	2.89	16.7	15	-69.21
418		decan-2-one	C10H20O	156.151	-13.07	3.73	13.84	194.56	31	7	0	-5.55	-13.26	2.84	0.46	-0.96	-43.2
419		nonyl ethanoate	C11H22O2	186.162	-13.06	4.09	21.66	222.05	35	8	-3.75	-6.02	-15.72	4.14	9.19	6.8	-73.66

420		(1R,5R)-6,6-dimethyl-2-methylene-bicyclo[3.1.1]heptane	C10H16	136.125	-13.06	3.72	0	194.46	26	0	0	-3.73	-11.15	0	0	0.9	-29.53
421		octan-3-ol	C8H18O	130.136	-13.05	3.12	17.13	155.4	27	6	-2.16	-4	-9.93	2.23	2.99	-1.23	-27.83
422		(Z)-hex-3-enal	C6H10O	98.073	-13.03	1.52	14.61	127.43	17	3	0	-3.09	-11.81	0.32	0.37	-1.85	-22.58
423		3-methylsulfanylpropan-1-ol	C4H10OS	106.045	-12.93	0.63	17.17	104.89	16	4	-3.57	-3.31	-12.4	0	7.15	4.51	-59.77
424		4-isopropyl-1-methyl-7-oxabicyclo[2.2.1]heptane	C10H18O	154.136	-12.93	3.06	6.18	205.07	29	1	0	-4.51	-10.78	0.2	0.71	-0.39	-44.34
425		(R)-2-amino-3-(4-hydroxyphenyl)propanoic acid	C9H11NO3	182.082	-12.9	-0.57	67.05	162.95	25	5	-8.14	-3.12	-17.94	3.01	19.83	14.94	-84.33
426		octyl 2-methylpropanoate	C12H24O2	200.178	-12.87	4.33	21.56	236.13	38	8	-3.28	-6.35	-17.08	3.41	10.18	6.58	-80.25
427		acetic acid	C2H4O2	61.029	-12.87	-0.11	29.33	55.57	9	1	-5.16	-1.41	-7.04	0.03	6.36	4.22	-26.14
428		(S)-2-amino-5-((diaminomethylene)amino)pentanoic acid	C6H14N4O2	174.201	-12.86	-2.41	99.14	159.25	27	7	-9.5	-2.21	-20.9	4.53	23.89	17.34	-74.16
429		(1S,2S)-1,2-dimethylcyclohex-3-enecarbaldehyde	C9H14O	138.104	-12.85	2.12	14.59	179.66	24	1	0	-3.95	-10.09	0.5	0.31	-1.44	-30.63
430		diamino-methanone	CH4N2O	60.032	-12.82	-1.02	55.34	52.76	8	0	-4.96	-0.51	-8.13	0.02	9.46	1.69	-34.19
431		2,4-dimethylthiazole	C5H7NS	113.03	-12.8	1.39	9.86	104.79	14	0	0	-3.48	-11.89	0.04	1.51	0.43	-31.82
432		allyl-benzene	C9H10	118.078	-12.79	2.9	0	138	19	2	0	-4.55	-17.76	0.37	5.19	4.43	-78.54
433		heptan-3-ol	C7H16O	116.12	-12.79	2.64	17.13	137.5	24	5	-2.6	-3.74	-7.87	0.33	2.98	-1.63	-23.44
434		octan-2-ol	C8H18O	130.136	-12.78	3.03	16.99	155.57	27	6	-3.17	-4.82	-14.48	0.72	8.42	4.61	-76.05


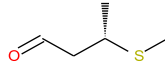
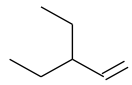
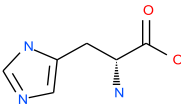
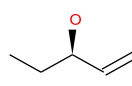
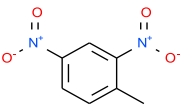

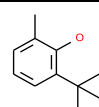
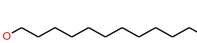
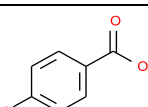

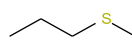
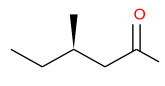
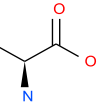
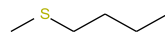
435		(1R,2S)-5-isopropyl-2-methyl-cyclohexanol	C10H20O	156.151	-12.78	2.95	16.05	179.36	31	2	0	-4.69	-9.85	0	0.09	-1.61	-40.95
436		3,7,11-trimethyl-dodeca-2,6,10-trien-1-ol	C15H26O	222.198	-12.77	5.32	17.17	309.64	42	8	-2.98	-6.68	-16.11	0	9.37	5.34	-101.5
437		3-methyl-butyl ethanoate	C7H14O2	130.099	-12.71	2	21.66	147.74	23	3	0	-3.89	-12.79	0.67	2.32	-1.3	-39.54
438		2,4,7-trimethyl-2,4,7,9-tetraaza-bicyclo[4.3.0]nona-1(6),8-diene-3,5-dione	C8H10N4O2	194.08	-12.69	-0.31	43.79	205.73	24	0	-3.92	-3.97	-14.63	0.34	11.45	8.98	-40.88
439		ethyl butanoate	C6H12O2	116.084	-12.68	1.7	20.67	131.06	20	3	0	-4	-11.14	0.97	1.36	-2.55	-25.83
440		cyclohex-3-enecarbaldehyde	C7H10O	110.073	-12.64	1.67	14.59	140.18	18	1	0	-3.26	-11.12	0	0.74	-0.76	-28.55
441		4-methoxy-benzoic acid	C8H8O3	153.055	-12.63	1.65	36.19	140.84	20	1	0	-3.4	-14.96	1.14	4.27	1.22	-33.77
442		2-amino-acetic acid	C2H5NO2	76.04	-12.61	-1.84	50.55	64.82	11	3	-6.16	-1.09	-9.53	0.11	10.95	4.9	-23
443		1,3,3-trimethyl-2-oxa-bicyclo[2.2.2]octane	C10H18O	154.136	-12.6	2.93	6.37	202.66	29	0	0	-4.35	-9.73	0.01	1.05	-1.12	-31.03
444		(1R,4R,5S)-1-isopropyl-4-methyl-bicyclo[3.1.0]hexan-3-one	C10H16O	152.12	-12.56	2.44	14.3	195.66	27	1	0	-4.66	-8.98	0.03	0.04	-1.64	-39.08
445		(R)-2-hexyl-5-oxo-tetrahydro-furan	C10H18O2	170.131	-12.52	2.75	21.43	195.53	30	5	0	-5.18	-12.39	0.89	0.72	-0.29	-27.51
446		1,1-dimethoxy-3,7-dimethyl-octa-2,6-diene	C12H22O2	198.162	-12.51	3.82	16	253.95	36	6	-3.92	-6.05	-12.24	0	8.7	5.41	-80.5
447		3-methyl-pentan-3-ol	C6H14O	102.104	-12.51	2.1	16.84	131.59	21	3	-1.97	-3.48	-9.55	1.43	2.97	0.5	-23.15
448		1,2-dimethoxy-benzene	C8H10O2	138.068	-12.47	1.92	15.5	139.09	20	0	-2.26	-4.45	-14.45	8.13	8.5	6.52	-83.58
449		4-allyl-1,2-dimethoxy-benzene	C11H14O2	178.099	-12.43	2.96	15.5	201.27	27	2	-3.3	-5.45	-10.47	0.62	8.61	3.63	-84.84

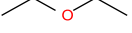
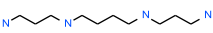
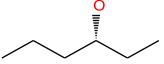
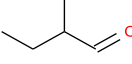
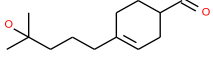

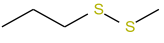

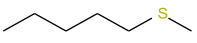
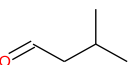
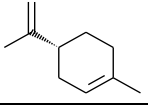
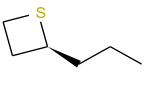


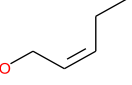
450		8-methyl-7-aza-bicyclo[4.3.0]nona-1(6),2,4,8-tetraene	C9H9N	131.073	-12.42	2.47	9.39	137.32	19	0	-2.24	-3.9	-10.58	0	4.72	4.4	-74.02
451		(S)-2-methyl-but-3-en-1-ol	C5H10O	86.073	-12.4	1.05	17.63	103.62	16	3	-1.77	-3.03	-9.76	0.46	3.15	-0.45	-22.34
452		2-butyl-5-oxo-tetrahydro-furan	C8H14O2	142.099	-12.33	1.78	21.43	159.72	24	3	0	-4.05	-10.73	1.2	0.3	-1.38	-37.89
453		3-allylsulfanyl-prop-1-ene	C6H10S	114.05	-12.27	2.51	0	139.74	17	4	0	-4.31	-13.14	0	0	2.07	-36.42
454		(R)-propane-1,2-diol	C3H8O2	76.052	-12.27	-0.54	34.1	73.97	13	3	-6.01	-1.87	-9.82	1.29	7.84	9.6	-4.51
455		3-methyl-but-2-enal	C5H8O	84.058	-12.25	1.49	14.61	110.87	14	0	0	-2.81	-10.58	0	0.55	-0.31	-32.25
456		3-methylsulfanyl-prop-1-ene	C4H8S	88.035	-12.23	1.65	0	98.85	13	2	0	-3.76	-13.69	0.16	2.01	1.93	-37.56
457		2-oxo-oxonane	C8H14O2	142.099	-12.2	1.14	22.03	163.55	24	0	0	-3.93	-8.98	0	1.18	-2.22	-33.35
458		(Z)-hept-4-enal	C7H12O	112.089	-12.14	1.95	14.61	146.82	20	4	0	-3.56	-11.65	0	0.35	-1.17	-26.52
459		tridecanal	C13H26O	198.198	-12.12	5.31	14.61	247.99	40	11	-2.61	-6.14	-19.11	4.45	9.37	6.19	-75.67
460		methanephosphine	CH5P	48.013	-12.12	0.6	0	25.95	7	1	-2.86	-1.46	-8.59	0.02	4.21	1.4	7.79
461		hexan-1-ol	C6H14O	102.104	-12.09	2.08	17.17	122.27	21	5	-2.44	-3.45	-10.05	1.64	3.18	1.62	-47.92
462		(S)-hexan-2-ol	C6H14O	102.104	-12.08	2.06	16.99	119.76	21	4	-2.13	-3.53	-8.9	2.08	3.1	-0.21	-24.69
463		1,3,3-trimethyl-bicyclo[2.2.1]heptan-2-one	C10H16O	152.12	-12.03	2.52	14.23	203.77	27	0	0	-4.08	-10.15	0.04	1.56	-0.49	-44.33
464		(R)-heptan-3-ol	C7H16O	116.12	-12.02	2.64	17.13	137.5	24	5	-1.37	-4.18	-10.64	1.45	2.8	-0.33	-22.31


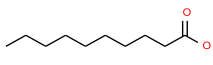

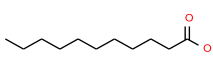

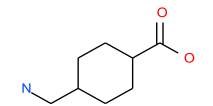
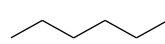
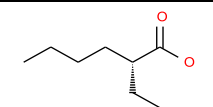
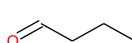
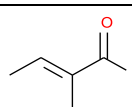
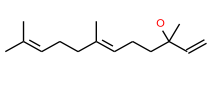



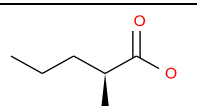
465		2,5-dimethyl-pyrazine	C6H8N2	108.069	-12	0.52	18.13	109.37	16	0	0	-3.2	-11.39	0	2.2	-0.19	-32.68
466		oct-2-enoic acid	C8H14O2	142.099	-11.98	2.94	28.89	169.65	23	5	0	-4.31	-11.56	0.16	2.14	-3.23	-28.03
467		2,3-dimethyl-pyrazine	C6H8N2	108.069	-11.95	0.4	19.49	107.45	16	0	0	-3.49	-10.59	0	1.49	-0.22	-19.01
468		2-isopropyl-phenol	C9H12O	136.089	-11.85	2.6	16.79	141.79	22	1	-2.69	-4.19	-13.43	0.49	8.45	6.43	-76.54
469		6-(5-carboxy-pyridin-2-yl)-pyridine-3-carboxylic acid	C12H8N2O4	244.048	-11.85	1.19	75.06	206.86	24	2	0	-3.82	-14.79	0.2	6.37	-0.73	-45.47
470		2,2-dimethylthietane 1,1-dioxide	C5H10O2S	134.197	-11.84	1.02	29.29	115.14	18	1	0	-2.37	-10.73	0.05	0	-0.19	-22.66
471		hexan-2-ol	C6H14O	102.104	-11.82	2.06	16.99	119.76	21	4	-1.55	-3.76	-9.72	0.48	2.93	-0.4	-18.75
472		2,4-dihydroxy-benzoic acid	C7H6O4	155.034	-11.73	0.93	62.81	130.8	18	1	-7.74	-2.18	-15.6	3.29	17.17	17.32	-83.65
473		(1R,4R)-1,7,7-trimethyl-bicyclo[2.2.1]heptan-2-one	C10H16O	152.12	-11.73	2.61	14.33	199.91	27	0	0	-4	-8.74	0.06	0.53	-1.09	-35.59
474		(S)-2-oxo-6-propyl-tetrahydro-2H-pyran	C8H14O2	142.099	-11.73	1.66	21.06	158.82	24	2	0	-4.02	-12	0.23	2.87	-0.58	-31.8
475		heptanoic acid	C7H14O2	130.099	-11.71	2.32	28.89	144.77	22	5	-6.43	-3.15	1	7.5	5.22	-1.89	-5.36
476		4-methyl-pentanoic acid	C6H12O2	117.092	-11.69	1.67	28.89	124.18	21	4	-2.91	-3.24	-10.93	0.92	4.48	4.57	-20.81
477		sulfane	H2S	34.0809	-11.61	0.48	0	11.95	3	0	-3.18	-1.89	-5.63	0	4.26	0.19	-4.52
478		methylsulfanyl-benzene	C7H8S	124.035	-11.36	2.54	0	113.65	16	1	0	-4.3	-16.07	0.17	4.65	5.3	-67.7
479		piperidine	C5H11N	85.089	-11.36	0.75	12.39	102.29	17	0	-1.61	-3.05	-7.46	0	2.66	0.34	-18.17

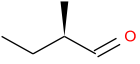
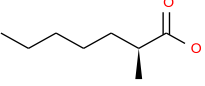

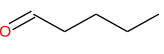
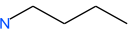
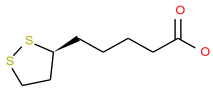
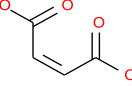

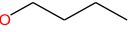
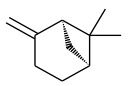
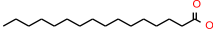




480		hexyl 2-methylpropanoate	C10H20O2	172.146	-11.3	3.37	21.56	200.32	32	6	-2.73	-5.6	-14.06	2.6	7.9	5.88	-83.24
481		9-methyl-7-azabicyclo[4.3.0]nona-1,3,5,8-tetraene	C9H9N	131.073	-11.25	2.48	10.11	135.36	19	0	-1.07	-4.11	-15.29	0	6.73	6.76	-85.68
482		2,6,6-trimethyl-cyclohex-2-ene-1,4-dione	C9H12O2	152.084	-11.22	0.95	26.93	203.88	23	0	0	-3.53	-12.56	0.06	2.01	3.33	-59.9
483		1,7,7-trimethylbicyclo[2.2.1]heptan-2-one	C10H16O	152.12	-11.22	2.61	14.33	199.91	27	0	0	-3.92	-8.36	0	0.59	-1.03	-26.62
484		1-methylpiperidine	C6H13N	99.105	-11.09	1.37	3.91	123.02	20	0	0	-3.52	-10.8	0	0.93	2.08	-40.66
485		(R)-2-butyl-5-oxotetrahydrofuran	C8H14O2	142.099	-11.06	1.78	21.43	159.72	24	3	-1.77	-3.24	-10.52	1.25	3.62	2.42	-32.2
486		decan-1-ol	C10H22O	158.167	-11.05	4	17.17	193.9	33	9	0	-5.65	-13.62	3.12	1.09	0.22	-41.29
487		(S)-hept-1-en-3-ol	C7H14O	114.104	-10.94	2.33	17.13	139.88	22	5	0	-3.89	-11.81	0.83	2.44	-2.04	-21.88
488		(2S,4aR,8aR)-decahydronaphthalen-2-ol	C10H18O	154.136	-10.92	2.4	16.07	173.04	29	1	0	-4.44	-8.53	0	0.78	-0.9	-45.86
489		(S)-2-amino-3-mercaptopropanoic acid	C3H7NO2S	122.028	-10.9	-1.75	49.71	96.43	15	5	-8.33	-1.35	-13.91	0.62	17.16	13.82	-44.86
490		(R)-2-amino-3-phenylpropanoic acid	C9H11NO2	166.087	-10.86	-0.31	49.44	152.4	24	5	-5.54	-3.51	-18.25	1.2	13.85	15.73	-85.06
491		4-methyl-7-azabicyclo[4.3.0]nona-1(6),2,4,8-tetraene	C9H9N	131.073	-10.86	2.6	10.02	133.43	19	0	-1.23	-4.21	-15.14	0.02	6.79	7.76	-75.15
492		(R)-2-hydroxypropanoic acid	C3H6O3	91.04	-10.85	-0.71	44.93	79.28	13	3	-5.9	-1.66	-7.37	0	9.14	5.91	-38.03
493		2-oxopropanoic acid	C3H4O3	89.024	-10.84	-0.49	42.74	81.86	11	2	-4.67	-1.46	-10.83	0	8.59	7.8	-26.96
494		methanethiol	CH4S	48.003	-10.82	0.89	0	32.86	6	1	-2.49	-1.41	-7.83	0.03	2.5	2.68	-3.35



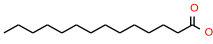
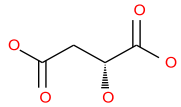
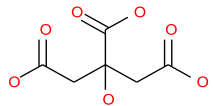
495		2-cyclohexyl-acetic acid	C8H14O2	143.107	-10.81	2.07	28.81	153.55	25	3	-2.24	-3.67	-10.97	0.54	3.96	5.3	-26.73
496		2-amino-ethanesulfonic acid	C2H7NO3S	125.015	-10.67	-2.88	64.72	88.88	14	4	-8.32	-1.18	-9.09	1.08	9.59	16.17	-5.29
497		2-dimethylamino-acetic acid	C4H9NO2	104.071	-10.6	-0.76	32.78	106.75	17	3	-4.86	-2.6	-7.02	0.43	8.19	3.79	-37.99
498		cyclohexanone	C6H10O	98.073	-10.47	1.24	13.78	116.59	17	0	0	-3.2	-9.18	0	0.4	0.83	-40.77
499		dodecanoic acid	C12H24O2	200.178	-10.45	4.73	28.89	234.3	37	10	-1.71	-5.91	-16.7	3.66	9.86	1.75	-79.91
500		2-ethyl-pyrazine	C6H8N2	108.069	-10.39	0.64	19.3	106.74	16	1	-6.77	-3.01	-8.01	0.95	4.79	19.05	5.76
501		pentan-3-one	C5H10O	86.073	-10.38	1.34	13.27	106.68	16	2	0	-3.07	-10.1	0.05	1.23	-0.52	-23.64
502		undec-10-enoic acid	C11H20O2	185.154	-10.29	3.86	28.89	220.24	34	10	-3.94	-5.35	-22.81	5.25	12.64	16.04	-117.71
503		tetrachloro-methane	CCl4	151.875	-10.26	2.65	0	88.64	5	0	0	-3.27	-8.31	0	0	0.37	-8.63
504		2-oxo-butanoic acid	C4H6O3	103.04	-10.22	0	42.17	99.08	14	3	-4.68	-1.98	-10.66	0	8.5	8.22	-28.88
505		(methyldisulfanyl)methane	C2H6S2	94.199	-10.18	1.31	0	63.33	10	1	0	-3.2	-8.02	0.12	0	-0.94	-7.32
506		3-methylsulfanylbutanal	C5H10OS	118.045	-10.15	0.8	14.61	115.45	17	3	0	-3.29	-11.03	0	1.21	0.56	-24.55
507		1-isopropyl-4-methylcyclohexa-1,4-diene	C10H16	136.125	-10.07	4.57	0	191.39	26	1	0	-5.08	-13.66	0	5.07	3.92	-84.49
508		p-cymene	C10H14	134.11	-9.99	3.38	0	149.9	24	1	0	-4.95	-13.67	2.11	4.64	4.43	-93.48
509		3-methyl-7-aza-bicyclo[4.3.0]nona-1(6),2,4,8-tetraene	C9H9N	131.073	-9.99	2.6	10.02	133.43	19	0	-0.79	-4.1	-15.36	0	6.48	7.97	-86.23

510		tetrahydro-thiophene	C4H8S	88.035	-9.91	1.74	0	89.52	13	0	0	-3.15	-8.79	0	0	1.5	-34.39
511		(S)-3-methylsulfanylbutanal	C5H10OS	118.045	-9.86	0.8	14.61	115.45	17	3	0	-3.43	-10.37	0	0.64	0.82	-35.38
512		2-ethylbutanal	C6H12O	100.089	-9.84	1.87	14.67	119.58	19	3	0	-3.44	-8.36	0.09	0.44	-1.99	-29.33
513		(R)-2-amino-3-(3H-imidazol-4-yl)propanoic acid	C6H9N3O2	156.077	-9.63	-2.32	71.23	137.25	21	5	-2.71	-2.53	-16.2	1.5	8.3	8.94	-49.08
514		(R)-pent-1-en-3-ol	C5H10O	86.073	-9.55	1.36	17.13	104.12	16	3	-5.31	-2.94	-11.74	3.24	4.86	18.4	-4.97
515		1-methyl-2,4-dinitrobenzene	C7H6N2O4	182.033	-9.5	1.59	76.46	147.87	19	2	0	-2.94	-17.34	0	5.38	6.93	-74.23
516		propan-1-ol	C3H8O	60.058	-9.5	0.63	17.17	68.56	12	2	-6.16	-2.23	-9.53	1.1	4.84	18.62	3.35
517		2-methyl-6-tert-butylphenol	C11H16O	164.12	-9.49	3.37	15.72	191.79	28	1	-2.63	-4.96	-11.93	1.31	8.69	8.04	-99
518		dodecan-1-ol	C12H26O	186.198	-9.49	4.97	17.17	229.71	39	11	-3.61	-6.34	-14.03	4.58	10.32	5.41	-70.22
519		4-hydroxybenzoic acid	C7H6O3	139.04	-9.49	1.3	46.26	119.55	17	1	-2.91	-2.27	-14.6	0.43	7.98	11.22	-38.92
520		propionaldehyde	C3H6O	58.042	-9.44	0.49	14.61	68.34	10	1	-3.71	-1.7	-12.83	0.17	3.35	16.39	-9.77
521		1-methylsulfanylpropane	C4H10S	90.05	-9.42	1.79	0	96.91	15	2	0	-3.77	-11.78	0	2.12	3.18	-53.07
522		(R)-3-methylpentanoic acid	C6H12O2	117.092	-9.4	1.77	28.89	123.04	21	4	-4.28	-3.1	-14.12	1.34	10.34	11.3	-75.97
523		(S)-2-amino-propanoic acid	C3H7NO2	90.056	-9.38	-1.85	49.27	84.13	14	3	-6.05	-1.67	-12.93	0.34	12.15	13.72	-48.86
524		1-methylsulfanylbutane	C5H12S	104.066	-9.35	2.27	0	114.81	18	3	0	-4.19	-11.78	0	2.17	2.74	-50.3

525		ethoxy-ethane	C4H10O	74.073	-9.35	1.13	8.19	87.88	15	2	0	-3.16	-8.07	0.18	1	-1.68	-17.51
526		N1,N4-di(3-amino-propyl)-butane-1,4-diamine	C10H26N4	202.216	-9.25	-1.5	66.26	232.67	40	13	-6.86	-5.43	-17.15	3.32	19.89	9.35	-51.92
527		(R)-hexan-3-ol	C6H14O	102.104	-8.99	2.16	17.13	119.59	21	4	0	-3.96	-8.27	1.84	0.61	-1.41	-32.55
528		2-methyl-butanal	C5H10O	86.073	-8.89	1.29	14.67	99.41	16	2	0	-3.08	-7.13	0.03	0.29	-1.69	-23.97
529		4-(4-hydroxy-4-methyl-pentyl)-cyclohex-3-enecarbaldehyde	C13H22O2	210.162	-8.86	3.16	30.78	265.44	37	6	-4.78	-5.35	-11.14	1.51	11.13	9.09	-47.92
530		propan-2-one	C3H6O	58.042	-8.78	0.35	14.42	68.93	10	0	-3.24	-2.13	-12.65	0	3.41	16.58	-7.64
531		1-(methyl-disulfanyl)propane	C4H10S2	122.252	-8.75	2.32	0	107.24	16	3	0	-4.38	-15.11	0.21	5.28	5.34	-54.72
532		butan-2-one	C4H8O	72.058	-8.69	0.84	13.84	87.57	13	1	-3.1	-2.61	-12.88	0	3.42	16.09	-14.89
533		1-methylsulfanyl-pentane	C6H14S	118.082	-8.6	2.76	0	132.72	21	4	0	-4.74	-15.05	0.95	6.02	4.12	-69.63
534		3-methyl-butanal	C5H10O	86.073	-8.34	1.3	14.61	100.67	16	2	0	-2.9	-7.8	0.16	0.43	-0.18	-16.71
535		(R)-4-isopropenyl-1-methyl-cyclohex-1-ene	C10H16	136.125	-8.27	3.83	0	195.06	26	1	0	-5.28	-14.84	0	6.07	7.5	-79.37
536		(S)-2-propyl-thietane	C6H12S	116.066	-7.92	3.16	0	130.89	19	2	0	-4.11	-10.85	0	3.61	2.68	-59.51
537		hexadecan-1-ol	C16H34O	242.261	-7.85	6.9	17.17	301.34	51	15	0	-6.57	-14.98	5.03	3.4	-0.03	-68.43
538		isobutyric acid	C4H8O2	89.06	-7.62	0.61	28.92	88.91	15	2	-5.54	-2.44	-10.96	0	9.89	15.73	-56.17
539		(Z)-pent-2-en-1-ol	C5H10O	86.073	-7.3	1.3	17.17	108.87	16	3	-5.31	-2.9	-6.63	0	4.96	13.93	-9.59

540		2-methyl-propan-1-ol	C4H10O	74.073	-7.28	0.95	17.63	83.72	15	2	-6.24	-2.62	-7.04	1.41	4.92	18.82	-10.99
541		decanoic acid	C10H20O2	173.154	-7.26	3.76	28.89	198.49	33	9	-2.06	-4.92	-23.57	4.71	12.43	15.3	-118.83
542		chloroform	CHCl3	117.914	-7.16	1.84	0	63.07	5	0	0	-3.11	-6.37	0	0.87	0.96	6.05
543		undecanoic acid	C11H22O2	187.17	-6.89	4.24	28.89	216.39	36	10	-3.2	-5.29	-21.16	7.49	12.57	15.91	-111.19
544		formic acid	CH2O2	47.013	-6.82	-0.34	29.25	36.86	6	1	-3.93	-0.33	-6.38	0.01	6.95	5.89	-20.27
545		4-(amino-methyl)-cyclohexanecarboxylic acid	C8H15NO2	158.118	-6.74	0.13	50.5	163.05	27	4	-7.01	-3.3	-12.3	0.86	16.91	15.79	-87.68
546		hexane	C6H14	86.11	-6.7	3.24	0	114.29	20	3	0	-4.08	-10.96	0.04	4.06	3.26	-60.93
547		(R)-2-ethyl-hexanoic acid	C8H16O2	145.123	-6.56	2.73	28.92	160.14	27	6	-5.48	-4.03	-14.05	7.08	11.91	17.44	-78.5
548		butyraldehyde	C4H8O	72.058	-6.45	0.98	14.61	86.83	13	2	-4.2	-2.1	-8.11	0.93	3.35	15.12	1.78
549		2-methyl-but-2-enoic acid	C5H8O2	101.06	-6.17	1.24	28.92	118.77	16	1	-3.69	-2.95	-13.73	0	11.85	14.21	-49.39
550		3,7,11-trimethyl-dodeca-1,6,10-trien-3-ol	C15H26O	222.198	-6.15	5.24	16.84	317.23	42	8	-2.19	-6.46	-16.29	0	11.83	9.61	-71.33
551		acetaldehyde	C2H4O	44.026	-5.26	0.09	14.15	48.44	7	0	-3.22	-1.25	-9.97	0	3.23	17.08	-6.04
552		propan-2-ol	C3H8O	60.058	-5.05	0.52	16.85	65.31	12	1	-3.98	-2.32	-8.83	0.06	4.86	16.9	-8.88
553		prop-2-ene-1-thiol	C3H6S	74.019	-5.04	1.65	0	77.56	10	2	-1.55	-2.1	-14.39	0	3.35	16.63	-16.28
554		(S)-2-methyl-pentanoic acid	C6H12O2	117.092	-4.98	1.67	28.92	124.09	21	4	-4.02	-3.42	-15.71	0.93	11.56	18.38	-72.32

555		(R)-2-methyl-butanal	C5H10O	86.073	-4.88	1.29	14.67	99.41	16	2	-3.49	-2.55	-8.68	1.25	3.42	16.03	-12.12
556		(S)-2-methyl-heptanoic acid	C8H16O2	145.123	-4.67	2.63	28.92	159.9	27	6	-3.79	-4.09	-16.92	4.38	12.23	17.89	-83.12
557		isobutyraldehyde	C4H8O	72.058	-4.54	0.72	14.67	82.56	13	1	-3.45	-2.13	-10.65	0.17	3.45	19.83	-10.99
558		pentanal	C5H10O	86.073	-4.48	1.46	14.61	104.74	16	3	-4.54	-2.5	-5.96	2.72	3.48	15.5	-4.73
559		butan-1-amine	C4H11N	73.089	-4.45	0.51	21.67	88.53	16	3	-3.98	-2.6	-8.99	1.26	6.36	14.82	-6.14
560		(S)-5-(1,2-dithiolan-3-yl)-pentanoic acid	C8H14O2S2	207.051	-3.51	2.96	29.18	187.75	27	6	-2.24	-4.67	-16.9	1.21	11.98	14.54	-98.17
561		maleic acid	C4H4O4	118.027	-3.29	0.23	57.28	110.73	14	2	-4.82	-1.54	-14.72	2.13	14.44	19.15	-43.55
562		ethanethiol	C2H6S	62.019	-2.76	1.31	0	58.66	9	1	-1.45	-1.71	-10.2	0.23	3.14	14.08	6.22
563		butan-1-ol	C4H10O	74.073	-2.2	1.11	17.17	86.46	15	3	-3.77	-2.63	-7	1.49	4.96	16.04	-12.8
564		(1S,5S)-6,6-dimethyl-2-methylene-bicyclo[3.1.1]heptane	C10H16	136.125	-2.17	3.72	0	194.46	26	0	0	-4.77	-7.01	0.42	5.73	5.65	-74.76
565		palmitic acid	C16H32O2	257.248	-1.39	6.65	28.89	305.93	51	15	-1.53	-7.58	-19.36	8.36	11.45	14.13	-97.38
566		methylsulfanyl-methane	C2H6S	62.019	-0.83	0.79	0	54.94	9	0	0	-2.79	-9.47	0.06	1.69	14.01	-2.49
567		benzene	C6H6	78.047	-0.76	1.86	0	75.9	12	0	0	-2.9	-11.06	0	1.5	16.85	5.49
568		propane-1-thiol	C3H8S	76.035	-0.68	1.8	0	75.66	12	2	-1.33	-2.12	-9.25	1.04	3.34	14.62	-10.13
569		dimethyl disulphide	C2H6S2	93.991	1.01	1.31	0	63.33	10	1	0	-3.22	-10.1	0.13	1.69	17.27	-9.43

570		N,N-dimethylmethanamine	C3H9N	59.073	1.22	0.14	3.81	76.7	13	0	0	-2.82	-9.58	0.11	2.88	15.96	-2.27
571		pyrrolidine	C4H9N	71.073	1.24	0.39	12.76	85.28	14	0	-2.64	-2.56	-4.24	0	4.61	15.77	10.62
572		tetradecanoic acid	C14H28O2	229.217	1.74	5.69	28.89	270.11	45	13	-3.37	-6.7	-14.58	6.77	13.38	17.42	-109.77
573		(R)-2-hydroxy-succinic acid	C4H6O5	136.037	2.82	-1.54	73.45	108.21	17	6	-8.7	-1.4	-15.43	0.89	20.92	33.19	-74.16
574		2-hydroxy-propane-1,2,3-tricarboxylic acid	C6H8O7	195.05	20.17	-1.97	101.69	167.15	24	9	-6.81	-1.63	-18.69	0.75	23.43	51.85	-84.66