

**Table 15. VOC organic compound validated in whiskey analysis and their flavor profile according to FlavourDB**

Class	SMILES	Molecular Weight	Volatility	Source (FlavourDB)	Associated Compounds	Flavor Description
Alcohol	1,3-Propanediol	76.09	M	NA	NA	NA
	1,3-Butanediol	90.12	M	NA	NA	NA
	1,4-Butanediol	92.12	M	NA	NA	NA
	1,5-Pentanediol	108.15	M	NA	NA	NA
	1,6-Hexanediol	118.17	M	NA	NA	NA
	2,2-Dimethylpropanediol	106.16	M	NA	NA	NA
	2-Propylpropanediol	104.15	M	NA	NA	NA
	3-Methylbutanediol	104.15	M	NA	NA	NA
	3-Pentylpropanediol	130.19	M	NA	NA	NA
	3-Hydroxybutanediol	92.09	M	NA	NA	NA
Aldehyde	2,3-Dihydroxybutanal	90.08	M	NA	NA	NA
	2-Hydroxybutanal	88.08	M	NA	NA	NA
	3-Hydroxybutanal	88.08	M	NA	NA	NA
	4-Hydroxybutanal	88.08	M	NA	NA	NA
	2-Methylbutanal	86.09	M	NA	NA	NA
	3-Methylbutanal	86.09	M	NA	NA	NA
	2-Pentylpropanal	130.17	M	NA	NA	NA
	3-Pentylpropanal	130.17	M	NA	NA	NA
	4-Pentylpropanal	130.17	M	NA	NA	NA
	5-Pentylpropanal	130.17	M	NA	NA	NA
Ketone	2-Pentanone	98.14	M	NA	NA	NA
	3-Pentanone	98.14	M	NA	NA	NA
	2-Hexanone	110.15	M	NA	NA	NA
	3-Hexanone	110.15	M	NA	NA	NA
	2-Heptanone	122.16	M	NA	NA	NA
	3-Heptanone	122.16	M	NA	NA	NA
	2-Octanone	134.17	M	NA	NA	NA
	3-Octanone	134.17	M	NA	NA	NA
	2-Nonanone	146.18	M	NA	NA	NA
	3-Nonanone	146.18	M	NA	NA	NA
Ester	2-Methylpropanoate	74.08	M	NA	NA	NA
	2-Methylbutanoate	88.11	M	NA	NA	NA
	2-Pentylpropanoate	130.15	M	NA	NA	NA
	3-Pentylpropanoate	130.15	M	NA	NA	NA
	4-Pentylpropanoate	130.15	M	NA	NA	NA
	5-Pentylpropanoate	130.15	M	NA	NA	NA
	2-Hydroxypropanoate	76.07	M	NA	NA	NA
	2-Hydroxybutanoate	90.10	M	NA	NA	NA
	2-Hydroxypentanoate	104.13	M	NA	NA	NA
	2-Hydroxyhexanoate	118.16	M	NA	NA	NA
Alkane	2,2,4-Trimethylpentane	114.23	M	NA	NA	NA
	2,2,4,4-Trimethylpentane	114.23	M	NA	NA	NA
	2,2,4,4,4-Pentamethylpentane	128.26	M	NA	NA	NA
	2,2,4,4,4,4-Hexamethylpentane	142.29	M	NA	NA	NA
	2,2,4,4,4,4,4-Heptamethylpentane	156.32	M	NA	NA	NA
	2,2,4,4,4,4,4,4-Octamethylpentane	170.35	M	NA	NA	NA
	2,2,4,4,4,4,4,4,4-Nonamethylpentane	184.38	M	NA	NA	NA
	2,2,4,4,4,4,4,4,4,4-Decamethylpentane	198.41	M	NA	NA	NA
	2,2,4,4,4,4,4,4,4,4,4-Undecamethylpentane	212.44	M	NA	NA	NA
	2,2,4,4,4,4,4,4,4,4,4,4-Dodecamethylpentane	226.47	M	NA	NA	NA
Alkene	2-Methyl-2-butene	84.12	M	NA	NA	NA
	2-Methyl-2-pentene	98.15	M	NA	NA	NA
	2-Methyl-2-hexene	112.18	M	NA	NA	NA
	2-Methyl-2-heptene	126.21	M	NA	NA	NA
	2-Methyl-2-octene	140.24	M	NA	NA	NA
	2-Methyl-2-nonene	154.27	M	NA	NA	NA
	2-Methyl-2-decene	168.30	M	NA	NA	NA
	2-Methyl-2-undecene	182.33	M	NA	NA	NA
	2-Methyl-2-dodecene	196.36	M	NA	NA	NA
	2-Methyl-2-tridecene	210.39	M	NA	NA	NA
Alkyne	2-Butyne	68.10	M	NA	NA	NA
	2-Pentyne	82.13	M	NA	NA	NA
	2-Hexyne	96.16	M	NA	NA	NA
	2-Heptyne	110.19	M	NA	NA	NA
	2-Octyne	124.22	M	NA	NA	NA
	2-Nonyne	138.25	M	NA	NA	NA
	2-Decyne	152.28	M	NA	NA	NA
	2-Undecyne	166.31	M	NA	NA	NA
	2-Dodecyne	180.34	M	NA	NA	NA
	2-Tridecyne	194.37	M	NA	NA	NA
Aromatic	1,2,4-Trichlorobenzene	181.40	M	NA	NA	NA
	1,3,5-Trichlorobenzene	181.40	M	NA	NA	NA
	1,2,4-Trifluorobenzene	168.12	M	NA	NA	NA
	1,3,5-Trifluorobenzene	168.12	M	NA	NA	NA
	1,2,4-Dichlorobenzene	147.04	M	NA	NA	NA
	1,3,5-Dichlorobenzene	147.04	M	NA	NA	NA
	1,2,4-Difluorobenzene	134.06	M	NA	NA	NA
	1,3,5-Difluorobenzene	134.06	M	NA	NA	NA
	1,2,4-Dibromobenzene	234.02	M	NA	NA	NA
	1,3,5-Dibromobenzene	234.02	M	NA	NA	NA

**Table S2. Peak areas of each validated compound.**

Compound Name	HaNM	HaAA	KV04	ML15
Octane	730328	2151367	4506846	1419397
Ethane, 1,1-diethoxy-	1245264	4019641	2543804	1235582
Ethyl Acetate	6900019	10881775	19669070	11529726
Propanoic acid, 2-methyl-, ethyl ester	6281298	5586506	3719642	2542967
Propane, 1,1-diethoxy-2-methyl-	6643766	8392101	1430143	6248407
Decane	9642049	377708	1751755	1294589
Isobutyl acetate	1894043	4099676	932369	8394595
Butanoic acid, ethyl ester	2073593	2845197	3338073	2476586
Butanoic acid, 2-methyl-, ethyl ester	196497	7678353	1520289	7414133
Butanoic acid, 3-methyl-, ethyl ester	3768842	2226478	3068123	1574845
Butane, 1,1-diethoxy-3-methyl-	9799939	1108078	2177949	138366
Hexanal	16190	1080971	2115341	2124042
1-Propanol, 2-methyl-	435396	405139	593913	3813018
Pentane, 1-(1-ethoxyethoxy)-	1415108	6849859	2149835	1348299
1-Butanol, 3-methyl-, acetate	5946680	12788304	5436607	2576341
1-Butanol, 2-methyl-, acetate	9355262	2161874	152308	3491116
p-Xylene	1079054	9365716	1033705	1158252
Pentanoic acid, ethyl ester	2093967	2516741	5493429	5312218
1-Butanol, 3-methyl-	4580459	4024682	5069423	5029312
Hexanoic acid, ethyl ester	3791686	3147101	6173891	5992044
2-Propanone, 1,1-diethoxy-	1829814	5073788	2142286	9285926
1,3,5,7-Cyclooctatetraene	1868837	1069443	2394304	1481602
Benzene, 1,2,4-trimethyl-	2016231	4672368	3028146	1173432
Acetic acid, hexyl ester	1872572	4599207	1934392	1675572
Furfuryl ethyl ether	5400416	4611863	4260592	2817685
Benzene, 1-methyl-3-(1-methylethyl)-	2261035	157966	3356493	3831476
Benzene, 1-methyl-4-propyl-	5250587	2392735	4499787	7034062
Propane, 1,1,3-triethoxy-	8536477	1157208	1746524	1714623
Benzene, 1-ethyl-3,5-dimethyl-	5742701	3169971	6558128	1065096
Heptane, 1,1-diethoxy-	2272925	1244968	323466	2131651
Heptanoic acid, ethyl ester	679953	5291562	2070564	2114268
Propanoic acid, 2-hydroxy-, ethyl ester	1327834	9260427	6766453	1014112
Hexanoic acid, 2-methylpropyl ester	9273548	115951	1755095	14675
1-Hexanol	3491749	3860149	9189167	9468952
Benzene, 4-ethyl-1,2-dimethyl-	396112	2022765	4297261	1034438
Octanoic acid, ethyl ester	78838354	58977872	109E+08	111E+08
Isopentyl hexanoate	8166783	9410016	1240418	161268
Furfural	1863691	9597019	3277217	2126492
Acetic acid, octyl ester	9234147	2042282	2641028	9480358
Nonane, 1,1-diethoxy-	394335	6471555	5303235	3629033
Benzaldehyde	5493243	1558649	1317121	8822563
Propyl octanoate	5498884	3878124	1155505	121032

Nonanoic acid, ethyl ester	5580869	3303117	9786171	1269726
n-Caprylic acid isobutyl ester	1659733	2066462	2190485	2644947
3-Nonenoic acid, ethyl ester	1527345	1596954	3187774	2754338
Decanoic acid, ethyl ester	146E+08	145E+08	158E+08	161E+08
Octanoic acid, 3-methylbutyl ester	1825377	3908849	1580876	3657115
Benzoic acid, ethyl ester	134886	1408911	2434052	99883
Butanedioic acid, diethyl ester	7531873	20524	2225431	1119045
Ethyl 9-decenoate	1317396	7428864	5517554	8010736
Benzene, (2,2-diethoxyethyl)-	2095935	1096102	1439395	2716413
Decanoic acid, propyl ester	1924794	1955439	3266743	4460906
Undecanoic acid, ethyl ester	1706143	9711019	2395407	4455718
n-Capric acid isobutyl ester	4981114	9884167	4726437	8390411
Benzeneacetic acid, ethyl ester	3115792	3502691	197735	8277384
2-Tridecanone	2594801	1832042	2235353	3521056
Acetic acid, 2-phenylethyl ester	9801470	13635137	7522319	1865494
Dodecanoic acid, ethyl ester	153E+08	147E+08	165E+08	169E+08
Pentadecanoic acid, 3-methylbutyl ester	8090797	17656133	7589738	17371816
Lauryl acetate	295604	7051706	2733593	3077561
Butylated Hydroxytoluene	951421	2845716	3194763	263384
Phenylethyl Alcohol	6927524	5259958	4688416	7234784
Dodecanoic acid, propyl ester	1156177	1241427	321089	3452935
Ethyl tridecanoate	1137088	7358407	2563975	268998
Isobutyl laurate	3505936	5049695	4699366	6254083
1-Dodecanol	344827	2050832	2887773	4872673
2(3H)-Furanone, 5-butyldihydro-4-methyl-, ci	2472502	7773746	1072875	1318498
2-Pentadecanone	4711166	5388189	9062014	9414985
Tetradecanoic acid, ethyl ester	32243071	18336733	74222228	57687435
Isoamyl laurate	2266168	3841330	2187970	4603092
Ethyl 9-tetradecenoate	5556562	7399128	2941981	6476568
1-Tetradecyl acetate	3400071	7281407	8828369	2921683
Pentadecanoic acid, ethyl ester	3235229	6208463	9298972	9199057
2-Pentadecanone, 6,10,14-trimethyl-	2387562	2215797	228576	7631567
tetradecanol	19037570	7465085	10491564	19903747
Hexanoic acid, 2-phenylethyl ester	3658761	5770416	4975022	2032869
Hexadecanoic acid, ethyl ester	42365818	78411963	103E+08	88766789
n-Decanoic acid	9966145	4610197	8557298	10514424
Ethyl 9-hexadecenoate	54209083	55824169	91642383	101E+08
1-Hexadecanol, acetate	3281635	2170479	1473867	4757265
Heptadecanoic acid, ethyl ester	2535392	4097766	6682986	9583674
1-Hexadecanol	82950784	83037273	16334027	89805259
Octanoic acid, 2-phenylethyl ester	3406824	5521172	5518965	3062738
Octadecanoic acid, ethyl ester	226385	1584460	6084348	9716776
Ethyl Oleate	1943313	4151314	77767125	8795578
Dodecanoic acid	20394157	7876544	23092859	20281407
Linoleic acid ethyl ester	1895387	2906238	52941282	9011439
9,12,15-Octadecatrienoic acid, ethyl ester, (Z	3886492	1038886	1701681	2532207
Decanoic acid, 2-phenylethyl ester	9354077	19157205	1942986	10587991

Tetradecanoic acid	2532171	4470612	1890992	2422234
n-Hexadecanoic acid	5802733	2834340	14609609	9297862
2-Heptanone	1048781	10237	1931608	2615392

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SB15	LW15	LW25	LW30	BM40	P1NM	P1AA	P1TA	P2NM	P2AA
1059326	3063581	6720658	4086622	4316398	9043448	4363251	3032282	3344448	4276582
1199996	1325288	1582734	1489388	2688597	1070203	9551153	937377	3231352	7453893
7262556	9753226	8535969	8784310	21252510	3585526	1978492	5536039	6346771	1536012
3976844	4036808	3382982	3443012	4647194	228843	5662631	8603915	1844495	715094
1338952	764484	1156945	1086346	1211936	2043472	1136223	7976489	6258923	2756023
164908	8689656	1220751	9483305	2103442	2190716	2040304	5372551	7657436	1765155
7347318	8729581	6266383	5380902	124986	1353381	1200326	6891196	2304797	1503017
512747	3973407	3054331	2354741	3444027	6455646	5745003	4179897	9264038	2560989
1847144	1300839	1883206	1413093	1773084	1205903	1585167	1992471	9740583	5168301
3472742	2939254	3169402	2705682	3180009	1268107	2052496	612854	1626091	7531692
6136162	5956119	6293595	4925572	1068069	199497	1239633	3467285	1924597	1695474
3542487	2212264	2816076	2117767	5156532	4480279	3858822	2833231	3558771	3620427
7196418	4281334	4946282	3488623	7676162	8309265	6904888	5437279	2232304	2180092
1838342	1954744	2109087	1416419	2415755	1470307	1358669	8692984	1757763	4699661
5977364	1668895	5400653	3813982	1306386	1473790	1282402	4828741	1673797	2416951
102637	2220229	9849816	9245469	2479189	4198594	3901869	8477436	3831606	4874336
8536126	133847	1666072	1126031	9943394	7298922	6966465	3139481	5940837	5824584
7305673	5276066	4533744	3589084	1186172	1586719	1715877	104897	1094877	2564584
6321560	5041214	5017727	3911776	6209292	6947441	7046712	4209343	2824300	3674149
13003777	7889172	11304871	9827173	13824864	1287671	1475959	7014177	5730656	1640676
8983095	6347974	9886494	8996448	1732445	4701779	7014372	452315	8139628	2990557
795563	1463363	1326953	1088524	1865813	2168144	1344681	6974776	9247033	1330868
1024769	7855691	2695485	2356757	3379089	6581415	4180118	3911845	4175188	2475819
2566343	7799818	2185922	1907914	5436994	2867134	2051056	1519547	1315547	1431013
1397615	1599021	1482085	1168986	5139428	1877089	9093758	4017361	258044	1020639
310715	2905868	4042538	3378473	5533948	2736826	1846696	6310818	1659905	6421806
4183839	4866861	7787794	6996435	1519717	2149103	1670399	3130532	1924804	8225696
2246748	2506858	1595621	1409064	3111316	1184608	1823008	302799	1405363	1300362
6582004	7178986	1003496	7915067	1535663	2288424	1995072	2535442	438742	1349092
7057288	1949873	289802	2226922	1483422	4755482	2946406	2448069	4548573	328573
4086207	2367938	2681698	2196767	5969946	1552268	1466477	7874527	7747897	3681207
9788693	8109474	148854	1612164	2576422	1353481	9262063	4914421	1338879	1117091
4670864	2445774	3140878	3226275	4866785	2030799	150479	7600949	6229966	1088874
1025254	6721033	7782083	7374525	6366801	382261	2824786	5842771	1250557	8867622
505113	6018095	9000266	8423911	1825465	1955146	9995853	1802784	1704302	8173786
132E+08	132E+08	137E+08	148E+08	141E+08	38751839	40261217	23098565	7164183	30463501
2521725	2044659	2382129	2591969	341679	1459578	1094142	4994964	2810214	1959713
2138532	1620021	1897713	1997609	4145432	9873462	7814574	2483097	7317362	1014289
3876589	5273713	3316666	3327813	7135704	2940573	2378993	170861	1568597	3027206
8901565	365306	4879566	4478084	2087187	5587602	4617838	1955701	3832881	6323572
8937796	5965471	6546068	711659	1311629	126914	1233321	2728836	6013593	3074203
1194248	1261292	1322964	1356944	2681617	4307592	4230537	3013778	9885111	3332932

1261322	1501927	1162053	1157044	2868419	1437318	1551772	4582298	3348623	2043802
5383295	3398128	388969	403709	9273945	3137339	3144054	122972	0	5529262
3692783	237383	2492619	2531074	3765369	3302098	4273883	2692799	2966601	7777442
169E+08	164E+08	172E+08	175E+08	173E+08	117E+08	125E+08	84471400	27187406	96169463
3346907	3289302	3439214	4006714	7907986	2087246	2148671	7432191	8110554	7437995
2257402	1160161	846249	8429936	1312763	1337794	1583957	2722353	1212486	6389704
5132675	2897063	1375095	1717455	1394501	6933548	9378915	2676089	6520038	1120916
2712651	322622	1069136	1712721	3442958	7574065	1022874	6700232	0	1348126
1171956	7796233	9151069	1211241	1323006	1932342	1135447	5432179	8660951	9755464
2755891	2511576	2158513	261963	6317217	733808	6451804	7582392	1282738	5314121
4376101	5041904	2821633	3547454	1040696	932139	1401437	4562718	4867814	1845084
9122615	6298341	7386961	7965945	1930296	4045356	4309558	289607	8611772	7289031
1017753	622447	8034479	1053274	108536	7486801	8251926	2690162	8932587	1403657
4919671	4732998	6388132	7241102	1587287	6195212	6779814	1312035	5258741	8994875
3183869	1456133	1466553	2080072	9177028	1147538	1266851	1585381	5844703	354248
168E+08	17E+08	151E+08	149E+08	169E+08	72376689	80545020	71161857	20517840	69969854
14854096	12885385	11662472	12486782	25472736	3720125	4045622	2767711	2135954	959961
70138	1067895	609193	6873357	3129584	1200703	1641748	1330102	8208846	165502
4130515	2243092	2845716	3163729	3738681	9924635	2873287	9494811	2544560	1152187
1000490	1074349	6321462	7999145	1196297	436571	4594971	2013227	4663965	7528659
2058758	1864408	1486271	1452792	477260	1975036	2329365	6007908	3412229	2056286
2317605	2292184	1841738	1802197	6304201	5746615	5834208	2786727	5886828	1350439
7663263	4292671	5357059	5058203	1239430	1664272	1913029	1788157	8270936	1270193
4815048	4399465	268711	3617436	6673718	2210218	2775459	2485905	152172	1993375
4262795	9296546	115550	1558911	3261217	2520564	1999995	9234176	163406	5631683
1950176	1116662	1340371	1439898	4053191	1581684	1664247	6817164	1095538	133985
59218731	52249978	52265012	52769447	76888909	16796675	17352255	10336318	18220463	27335110
4598799	2876457	3290971	2599659	8394141	5985441	6692061	7844489	9217333	2014918
7441267	1098946	1566553	1559623	5814079	4250496	5132836	1139117	8342361	7826177
6310779	6972065	3063065	269355	3693844	4257463	6903225	6654055	2260036	3903609
120743	4758465	1294662	102110	2440491	1295634	1180341	2284364	1266985	1279023
1405194	6569694	2025949	1620402	8404003	1070237	2337454	1142442	4505613	3039467
25053287	20022715	23550079	30200009	46794278	3727132	4578456	1030928	3490734	4068876
8092424	1377286	5000402	5374008	727886	2700396	3109933	1483357	2959356	399437
116E+08	60750877	60152663	53447420	11E+08	113E+08	105E+08	64722733	99392758	103E+08
15603106	19163290	13066238	15884869	14364604	1041498	1701504	1860649	3804505	4930046
117E+08	65805573	58986547	58127456	97916311	5599506	7803066	6210194	9417957	4878318
2668683	1253562	1130616	9296256	7512479	9651246	1513133	8292935	1701135	8389696
2264235	3852651	1304696	7446205	5172833	1174977	1053096	9413498	933106	7074785
54321770	51607324	35634803	32772352	103E+08	1980824	2883594	4504358	4253679	3183401
1261284	1939230	1026489	1123271	2715744	6970366	1036771	7504923	1570771	1672896
2388427	3696781	1575074	8409732	4388842	1658253	1183534	2305623	190803	1509209
12895291	2221909	15827354	9227216	16150331	3724721	4007303	4726447	7757203	6003947
33591992	33420512	24636819	28186012	22604040	1804721	2785529	2934280	1286930	1492002
13024230	6404026	12866238	9638786	40542552	95026896	90707011	24537219	102E+08	101E+08
318468	1617695	3765259	2675273	7972245	8053264	7422013	1592105	11913215	9285411
4777728	6706612	6067880	5383509	11572838	2390695	2480909	3283929	3538447	3824147

4025792	5471638	5690018	7191601	3931026	2377751	405686	479042	1103722	1566913
19854047	10612798	10735210	8021481	13360549	2127049	3923775	4622210	2128643	2893506
2789468	1066374	9345667	5772004	2263713	2140067	1399104	8538569	150886	1754557

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P2TA

3718198  
7907071  
12571878  
1005723  
9761672  
5587298  
5469665  
5623369  
5247355  
4680802  
285872  
3577108  
2311867  
4335005  
2790571  
8183322  
1010054  
2610909  
3983761  
1438898  
7987597  
178011  
1296749  
2063182  
1850672  
1931402  
2719156  
1908035  
4308567  
519773  
2231752  
1670719  
970909  
1074151  
2468311  
16962814  
8605694  
1348752  
1831265  
5501235  
9349058  
214449

7325954  
4180633  
5551897  
56502930  
3721252  
6620521  
1565342  
3849648  
5688739  
2531577  
8875315  
3550014  
122107  
4363248  
2708348  
35870467  
5175609  
595146  
2606591  
4605977  
1362385  
5651766  
8456596  
1173975  
1551521  
8838613  
18070194  
172232  
5670285  
2621008  
1020425  
3432634  
4396946  
1642455  
129E+08  
5391278  
6934789  
1697903  
1699315  
3723181  
8667754  
977948  
11706105  
1851795  
23180722  
1821904  
2467467

1794475

6210681

1390332

**Table S3. Fold change in aroma compounds from new make to accelerated-aged spir**

Class	Compound	Rye		Barley
		P1	P2	Ha
Ester	ethyl acetate	-08978342	-2617157	-06234989
Ester	ethyl 2-hydroxypropanoate	-05767991	-0796816	05458443
Ester	2-methylpropyl acetate	-02173756	-1156561	-10842527
Ester	ethyl 2-methylpropanoate	126701233	-1930455	02028133
Ester	ethyl butanoate	-02156249	0898719	-04183475
Ester	2-methylbutyl acetate	-01457718	-0166875	-11745747
Ester	3-methylbutyl acetate	-02404018	0000233	-10795879
Ester	ethyl 2-methylbutanoate	03499778	-1455861	13882817
Ester	ethyl 3-methylbutanoate	063909778	-1658305	07909572
Ester	ethyl pentanoate	005684792	0650938	-02080899
Ester	diethyl butanedioate	039302295	0225908	19031193
Ester	ethyl hexanoate	015843235	0981666	03061188
Ester	hexyl acetate	-0521218	-0422443	-12614914
Ester	ethyl benzoate	020584945	1851554	-00300986
Ester	ethyl heptanoate	-01125638	1715072	03948403
Ester	2-methylpropyl hexanoate	-04639987	0227012	-02767082
Ester	2-phenylethyl acetate	010631636	-1253328	-04419209
Ester	ethyl 2-phenylacetate	010494797	0124274	-0141033
Ester	ethyl octanoate	001907735	155975	04545959
Ester	octyl acetate	-03353009	0403058	-11052012
Ester	3-methylbutyl hexanoate	-04415414	2274151	-01692567
Ester	ethyl (E)-non-3-enoate	034206984	0846919	-00286611
Ester	ethyl nonanoate	007679212	2065918	07852481
Ester	propyl octanoate	-00668582	1199742	05358402
Ester	2-methylpropyl octanoate	-00314104	NA	-02859902
Ester	ethyl dec-9-enoate	040712771	NA	08492515
Ester	ethyl decanoate	005551796	1282257	00374747
Ester	3-methylbutyl octanoate	001010619	2659292	-10720871
Ester	ethyl undecanoate	055639278	1401821	08377546
Ester	propyl decanoate	-0223989	1498903	00037322
Ester	2-methylpropyl decanoate	006154007	2559226	-0967027
Ester	2-phenylethyl hexanoate	017098368	-0092893	-0656497
Ester	dodecyl acetate	04279398	0495373	-12485788
Ester	ethyl dodecanoate	012236451	124779	00962123
Ester	3-methylbutyl decanoate	00926317	1647004	-11183481
Ester	ethyl tridecanoate	-00009784	0685354	06115729
Ester	propyl dodecanoate	021257759	2098086	-01032611
Ester	2-methylpropyl dodecanoate	017334835	0092216	-05333047
Ester	2-phenylethyl octanoate	055505484	-0422841	-06958714
Ester	ethyl (Z)-tetradec-9-enoate	024287413	-0611589	-04340247
Ester	ethyl tetradecanoate	002224014	0071003	08148793
Ester	tetradecyl acetate	067020616	0256296	-11033466
Ester	3-methylbutyl dodecanoate	014364985	0613704	-07883331
Ester	ethyl pentadecanoate	-0151909	-0495588	-09600278
Ester	2-phenylethyl decanoate	00258802	-0366823	-10398648
Ester	ethyl (E)-hexadec-9-enoate	04633992	-1457345	-00324856

Ester	ethyl hexadecanoate	-01284357	-0458625	-08945334
Ester	hexadecyl acetate	063546076	-154263	-27449591
Ester	ethyl heptadecanoate	-01618634	-0890176	-07220194
Ester	ethyl (9Z,12Z)-octadeca-9,12-die	-00953158	-0537818	-06300115
Ester	ethyl (9Z,12Z,15Z)-octadeca-9,12	-01387014	-0839914	-14546121
Ester	ethyl (Z)-octadec-9-enoate	009683146	-0860412	-11027557
Ester	ethyl octadecanoate	-04866809	-0824099	-28447272
Ketone	1,1-diethoxypropan-2-one	052664638	1249263	18698472
Ketone	heptan-2-one	-06530352	-0320513	00679907
Ketone	tridecan-2-one	009884149	0254046	05294441
Ketone	pentadecan-2-one	004592205	-0227973	-01965939
Ketone	6,10,14-trimethylpentadecan-2-c	110218387	-108369	00936354
Alcohol	2,6-ditert-butyl-4-methylphenol	148787306	-4993929	84011246
Alcohol	2-methylpropan-1-ol	-02975202	-0574228	01355422
Alcohol	2-phenylethanol	004145913	0161887	04003345
Alcohol	3-methylbutan-1-ol	-00138717	-0150969	0209617
Alcohol	dodecan-1-ol	028923161	-0151295	07556521
Alcohol	hexadecan-1-ol	05161318	-0940247	00259095
Alcohol	hexan-1-ol	-04741133	-1041758	-01076761
Alcohol	tetradecan-1-ol	025556398	-0306528	13739255
Carboxylic	decanoic acid	069067051	-0143271	11228318
Carboxylic	dodecanoic acid	060264808	-0296169	13985748
Carboxylic	tetradecanoic acid	075130744	0021562	25019787
Carboxylic	hexadecanoic acid	086016794	-0056285	10445183
Acetal	1,1-diethoxyethane	-01840519	066612	16506059
Acetal	1,1-diethoxy-2-methylpropane	-08758806	-1717265	-03022224
Acetal	1,1-diethoxy-3-methylbutane	-07180584	-0716506	-01379734
Acetal	1-(1-ethoxyethoxy)pentane	-0151475	0871042	10755551
Acetal	2,2-diethoxyethylbenzene	-08153731	-368037	-2350772
Acetal	1,1-diethoxynonane	-0305218	0182056	26446916
Aldehyde	furan-2-carbaldehyde	-03668389	-0062795	09819121
Aldehyde	hexanal	-02558115	-0500291	06111481
Aldehyde	benzaldehyde	-00804602	180358	18505536
Alkene	decane	-0158344	-2724721	14215598
Ether	1,1-diethoxyheptane	-0713028	-1001401	09112519
Ether	2-(ethoxymethyl)furan	-10926806	-1909459	0279795
Hydrocarb	1,1,3-triethoxypropane	058869601	-0651746	-0396348
Hydrocarb	1,2,4-trimethylbenzene	-06846663	-1297871	21384054
Hydrocarb	1,4-xylene	-01103743	-0579703	02347937
Hydrocarb	1-ethyl-3,5-dimethylbenzene	-02314418	-2243245	08811693
Hydrocarb	1-methyl-3-propan-2-ylbenzene	-06107718	-1923248	05643155
Hydrocarb	1-methyl-4-propylbenzene	-04057508	-1769363	11594978
Hydrocarb	4-ethyl-1,2-dimethylbenzene	-09975599	-1607276	10031213
Hydrocarb	cyclooctatetraene	-07370632	-3343213	-24711145
Hydrocarb	octane	-11089698	-0266726	17809765
Lactone	(4R,5R)-5-butyl-4-methyloxolan-3	295404747	4573283	16651614

**it.**