

Parameters	RT/min	LRI	Q _{ion}		
				ID	Chemical Standard
Aldehydes					
2,4-Decadienal	67.87	1837	81	S, MS, RI	Sigma
2,4-Heptadienal (<i>E,E</i>)	49.36	1518	81	S, MS, RI	Sigma
2,4-Heptadienal (<i>Z,Z</i>)	47.49	1488	81	S, MS, RI	Sigma
2,4-Nonadienal	61.83	1728	81	S, MS, RI	Sigma
2-Heptenal	38.01	1344	41	S, MS, RI	Sigma
5-Hydroxymethylfurfural	100.53	2525	97	S, MS, RI	Sigma
5-Methyl-furfural	54.47	1601	110	S, MS, RI	Sigma
Benzeneacetaldehyde	58.90	1676	91	S, MS, RI	Sigma
Benzaldehyde	51.54	1553	106	S, MS, RI	Sigma
Decanal	49.32	1518	43	S, MS, RI	Sigma
Furfural	47.70	1492	96	S, MS, RI	Sigma
Heptanal	28.29	1201	44	S, MS, RI	Sigma
Hexanal	21.27	1097	44	S, MS, RI	Sigma
Nonanal	42.53	1412	57	S, MS, RI	Sigma
Higher alcohols					
1-Butanol	25.20	1555	56	S, MS, RI	Sigma
1-Decanol	64.67	1779	55	S, MS, RI	Sigma
1-Heptanol	46.33	1471	70	S, MS, RI	Sigma
1-Hexanol	39.61	1368	41	S, MS, RI	Sigma
1-Methoxy-2-propanol	24.03	1138	45	S, MS, RI	Sigma
1-Octadecanol	104.93	2604	83	S, MS, RI	Sigma
1-Octanol	52.77	1573	56	S, MS, RI	Sigma
1-Pentanol	32.50	1263	42	S, MS, RI	Sigma
2-Heptanol	37.20	1332	45	S, MS, RI	Sigma
<i>trans</i> -2-Hexene-1-ol	43.28	1423	57	S, MS, RI	Sigma
<i>cis</i> -2-Hexene-1-ol	41.76	1446	57	S, MS, RI	Sigma
2-Methyl-1-butanol	29.55	1220	57	S, MS, RI	Sigma
2-Pentadecanol	75.47	1983	45	S, MS, RI	Sigma
2-Pentene-1-ol	37.40	1335	57	S, MS, RI	Sigma
<i>cis</i> -3-Hexene-1-ol	41.76	1405	41	S, MS, RI	Sigma
<i>trans</i> -3-Hexene-1-ol	40.42	1380	41	S, MS, RI	Sigma
3-Octanol	42.19	1407	59	S, MS, RI	Sigma
Isoamyl alcohol	29.80	1223	55	S, MS, RI	Sigma
Isobutanol	21.66	1102	43	S, MS, RI	Sigma
Phenylethyl alcohol	71.53	1907	91	S, MS, RI	Sigma

Volatile phenols					
4-Ethylguaiaicol	79.53	2066	85	S, MS, RI	Sigma
4-Ethylphenol	86.58	2216	107	S, MS, RI	Sigma
4-Vinylguaiaicol	87.46	2236	150	S, MS, RI	Sigma
4-Vinylphenol	96.41	2439	120	S, MS, RI.	Sigma
Eugenol	86.07	2205	164	S, MS, RI	Sigma
Guaiaicol	70.93	1895	124	S, MS, RI	Sigma
Homovanillyl alcohol	116.11	2817	137	- S, MS, RI	Sigma
Vanillin	103.41	2577	151	S, MS, RI	Sigma
Tyrosol	97.96	2473	107	S, MS, RI	Sigma
Terpenes					
1,8-Terpin	82.19	2122	81	S, MS, RI	Sigma
6,7-Dihydro-7-hydroxylinalool	75.92	1992	71	S, MS, RI	Boc Science
8-Hidroxylinalool	92.01	2339	43	S, MS, RI	Aurora Fine Chemicals
α -Terpineol	61.39	1720	59	S, MS, RI	Extrasynthese
β -Farnesen	59.30	1683	69	S, MS, RI	Extrasynthese
β -Ocimene	62.74	1744	93	S, MS, RI	Extrasynthese
<i>cis</i> -Linalool oxide, furan	47.54	1489	59	S, MS, RI	Extrasynthese
Citronelol	65.03	1785	69	S, MS, RI	Extrasynthese
δ -Carene	37.71	1340	93	S, MS, RI	Extrasynthese
Dihydroactinidiolide	94.54	2398	111	S, MS, RI	Boc Science
Farnesol	93.73	2380	69	S, MS, RI	Extrasynthese
γ -Terpinene	32.29	1260	93	S, MS, RI	Extrasynthese
Geraniol	69.49	1868	69	S, MS, RI	Extrasynthese
Geranyl acetate	91.81	2334	69	S, MS, RI	Boc Science
Hotrienol	56.14	1629	71	S, MS, RI	Boc Science
Linalool	52.17	1563	71	S, MS, RI	Extrasynthese
Linalool oxide, pyran	63.76	1762	68	S, MS, RI	Boc Science
Neric acid	93.83	2381	69	S, MS, RI	Extrasynthese
Nerol	67.04	1822	69	S, MS, RI	Extrasynthese
Nerolidol	79.20	2059	69	S, MS, RI	Boc Science
Pseudoionon	83.10	2141	58	S, MS, RI	Boc Science
Terpendiol I	62.31	1736	82	MS	
Terpendiol II	74.54	1965	67	MS	
Terpinene-4-ol	55.87	1624	71	S, MS, RI	Extrasynthese
Tetrahydrolinalool	44.62	1444	73	S, MS, RI	Boc Science
<i>trans</i> -Linalool oxide, furan	45.67	1460	59	S, MS, RI	Extrasynthese

<i>trans</i> -Rose oxide	39.64	1368	139	S, MS, RI	Sigma
Linalyl formate	47.38	1487	69	S, MS, RI	Boc Science
Ethyl linalyl acetal	46.95	1480	73	S, MS, RI	Boc Science
2,6-Dimethyl-3,7-octadiene-2,6-diol	61.25	1718	82	S, MS, RI	Boc Science
2,6-Dimethyl-7-octene-2,6-diol	76.07	1995	71	S, MS, RI	Boc Science
Menthol	57.94	1660	71	S, MS, RI	Sigma
Ocimenol	58.50	1669	93	S, MS, RI	Extrasynthese

C13- norisoprenoids

α -Ionol	72.23	1920	95	S, MS, RI	Sigma
α -Ionon	70.00	1877	121	S, MS, RI	Sigma
β -Damascenone	68.46	1848	69	S, MS, RI	Sigma
TDN	64.43	1774	157	S, MS, RI	Boc Science

Lactones

<i>cis</i> -Whiskey lactone	75.95	1993	91	S, MS, RI	Sigma
δ -Nonalactone	87.43	2235	99	S, MS, RI	Sigma
γ -Butyrolactone	58.30	1666	42	S, MS, RI	Sigma
γ -Decalactone	85.06	2183	85	S, MS, RI	Sigma
γ -Hexalactone	62.40	1738	85	S, MS, RI	Sigma
γ -Nonalacton	79.55	2067	85	S, MS, RI	Sigma
γ -Octalacton	73.94	1953	85	S, MS, RI	Sigma
γ -Undecalactone	90.28	2299	85	S, MS, RI	Sigma
<i>trans</i> -Whiskey lactone	72.28	1921	99	S, MS, RI	Sigma

Esters

2-Phenylethyl acetate	68.28	1845	105	S, MS, RI	Sigma
Diethyl glutarate	65.93	1801	143	S, MS, RI	Sigma
Methyl hydroxyisovalerate	70.10	1879	131	S, MS, RI	Sigma
Diethyl hydroxysuccinate	97.00	2454	101	S, MS, RI	Boc Science
Diethyl malonate	54.35	1598	115	S, MS, RI	Boc Science
Diethyl oxalate	43.67	1429	59	S, MS, RI	Sigma
Diethyl succinate	60.09	1697	101	S, MS, RI	Sigma
Dimethyl malate	78.27	2040	103	S, MS, RI	Sigma
Ethyl benzeneacetate	66.64	1814	91	S, MS, RI	Sigma
Ethyl butanoate	18.32	1053	71	S, MS, RI	Sigma
Ethyl decanoate	57.48	1652	88	S, MS, RI	Sigma
Ethyl furoate	57.28	1648	95	S, MS, RI	Sigma
Ethyl hexadecanoate	88.91	2268	88	S, MS, RI	Sigma

Ethyl hexanoate	31.40	1247	88	S, MS, RI	Sigma
Ethyl hydrogensuccinate	96.70	2445	101	S, MS, RI	Sigma
Ethyl lactate	39.28	1363	45	S, MS, RI	Sigma
Ethyl linoleate	101.66	2645	67	S, MS, RI	Sigma
Ethyl octanoate	45.05	1447	88	S, MS, RI	Sigma
Ethyl vanillate	107.17	1425	151	S, MS, RI	Sigma
Ethyl-2-hydroxy-3-methylbutanoate	44.82	1067	73	S, MS, RI	Sigma
Ethyl-2-hydroxybutanoate	43.41	1290	59	S, MS, RI	Boc Science
Ethyl-2-methylbutanoate	19.29	1350	57	S, MS, RI	Boc Science
Ethyl-2-oxopropanoate	34.34	1541	43	S, MS, RI	Sigma
Ethyl-3-ethoxypropanoate	38.39	1350	59	S, MS, RI	Boc Science
Ethyl-3-hydroxybutanoate	50.79	1541	43	S, MS, RI	Boc Science
Ethyl-3-hydroxyhexanoate	72.00	1915	117	S, MS, RI	Boc Science
Ethyl-3-methylbutanoate	20.30	1082	88	S, MS, RI	Sigma
Ethyl-hydroxyhexanoate	52.19	1563	69	S, MS, RI	Sigma
Ethylmethyl succinate	57.80	1657	115	S, MS, RI	Mol Port
Hexyl acetate	34.16	1287	43	S, MS, RI	Sigma
Isoamyl acetate	23.81	1135	43	S, MS, RI	Sigma
Isoamyl lactate	53.70	1588	45	S, MS, RI	Sigma
Isobutyl acetate	16.97	1032	43	S, MS, RI	Sigma
Isobutyl lactate	46.90	1479	45	S, MS, RI	Sigma
Methyl hexadecanoate	87.32	2233	74	S, MS, RI	Sigma
Methyl hexanoate	28.33	1202	74	S, MS, RI	Sigma
Methyl octadecanoate	96.36	2438	74	S, MS, RI	Sigma
Methyl-2-furoate	54.67	1603	95	S, MS, RI	Sigma
Methyl-3-hydroxyoctanoate	77.70	2029	103	S, MS, RI	Boc Science
Methyl geranoate	61.25	1718	69	S, MS, RI	Boc Science
<i>o</i> -Methylbenzyl acetate	92.95	2361	104	S, MS, RI	Sigma
Phenyl acetate	57.31	1649	94	S, MS, RI	Sigma
Fatty acids					
2-Methylpropionic acid	54.73	1604	43	S, MS, RI	MolPort
Butanoic acid	58.56	1671	60	S, MS, RI	Sigma
Decanoic acid	90.90	2313	60	S, MS, RI	Sigma
Heptanoic acid	76.17	1997	60	S, MS, RI	Sigma
Hexanoic acid	70.25	1882	60	S, MS, RI	Sigma
Isovaleric acid	60.88	1711	60	S, MS, RI	Sigma
Octanoic acid	81.05	2097	60	S, MS, RI	Sigma
Propanoic acid	53.16	1579	74	S, MS, RI	Sigma

Other alcohols					
1,4-Butandiol	73.70	1949	42	S, MS, RI	Sigma
2,6-Dimethyl-4-heptanol	52.26	1565	69	S, MS, RI	Sigma
2-Butoxy-ethanol	41.34	1394	57	S, MS, RI	Sigma
2-Ethyl-1-hexanol	48.54	1505	57	S, MS, RI	Sigma
3,4-Dimethyl-2-hexanol	35.48	1306	45	S, MS, RI	Sigma
3-Ethoxy-1-propanol	41.34	1394	59	S, MS, RI	Sigma
3-Methyl-1-pentanol	37.86	1342	56	S, MS, RI	Sigma
3-Methyl-3-buten-1-ol	32.63	1265	41	S, MS, RI	Sigma
4-Ethylcyclohexanol	49.37	1518	81	S, MS, RI	Sigma
4-Methyl-1-pentanol	37.00	1329	56	S, MS, RI	Sigma
Benzylalcohol	71.50	1906	78	S, MS, RI	Sigma
Cyclohexanol	41.95	1403	43	S, MS, RI	Sigma
Furfuril alkohol	59.56	1688	98	S, MS, RI	Sigma
2,3-Butanediol	51.90	1559	45	S, MS, RI	Sigma
Sulfur compounds					
4-(Methylthio)-1-butanol	69.56	1869	61	S, MS, RI	Sigma
3-(Methylthio)-1-propanol	62.80	1745	106	S, MS, RI	Sigma
Other compounds					
2,5-Hexadione	50.09	1530	43	S, MS, RI	Sigma
2,7-Octanedione	41.95	1403	43	S, MS, RI	Aurora Fine Chemicals
2H-Pyran-2,6(3H)-dione	78.28	2040	112	S, MS, RI	MolPort
2-Pentylfuran	31.40	1247	81	S, MS, RI	Sigma
3-Penten-2-on	24.21	1141	69	S, MS, RI	Sigma
4-Hydroxy-4-methyl-2-pentanone	40.46	1381	43	S, MS, RI	Sigma
4-Methyl-2-penten-2-one	24.65	1147	55	S, MS, RI	Sigma
5-Ethyl-4-methyl-3-heptanone	26.19	1170	57	S, MS, RI	Aurora Fine Chemicals
Acetoin	35.55	1307	45	S, MS, RI	Sigma
Acetylfurane	50.27	1533	95	S, MS, RI	Sigma
Benzofurane	66.16	1805	118	S, MS, RI	Sigma
Dihydro-2-methyl-3(2H)-furanone	63.07	1750	43	S, MS, RI	Sigma
N-(2-phenylethyl)acetamide	106.27	2629	104	S, MS, RI	Sigma
N-Ethylacetamide	57.77	1657	43	S, MS, RI	Sigma

RT-retention time; LRI-linear retention indeks; Q_{ion}-ion qualifier; ID: S-retention time and mass spectrum consistant with standard, RI – retention index consistant with those fine in the literature, MS – mass spectra consistant with those find in NIST02 electronic library