表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属*2(μg/g)	確認試験*3 IR	MS	NMR	使用量順位	H12-SEQ
cis-3-hexenyl hexanoate	3	95				1.432-1.442	0.875-0.885	2			1,3	3,4	3	164	1162
trans-2-hexenyl hexanoate	3	93				1.432-1.442	0.873-0.883	1			3	4,5	3	496	1164
cis-3-hexenyl isobutyrate	3	98				1.424-1.432	0.877-0.887	1			1,3	1,4	3	522	1167
cis-3-hexenyl isovalerate	3	95				1.427-1.437	0.873-0.883	2			3	3,4	3	367	1170
cis-3-hexenyl lactate	3	95				1.441-1.451	0.981-0.991	2			1,3,6	3,4	3	227	1172
cis-3-hexenyl propionate	3	95				1.424-1.434	0.891-0.901	2			1,3	3,4	1,3	363	1181
hexyl isovalerate	1	95				1.413-1.423	0.854-0.864	1			1,3,6	4	3	510	1208
hexyl propionate	1	97				1.411-1.417	0.868-0.874	1			1,3,6	3,5	3,6	275	1216
alpha-hexylcinnamaldehyde	3	95				1.545-1.555	0.953-0.964	10			1,3	3	3	416	1223
3-hydroxy-4,5-dimethyl-2(5H)-furanone	12,20	97		MP	25-29					10	1	4	-	184	1250
hydroxycitronellal diethyl acetal	3	95				1.435-1.445	0.903-0.913	1			1	-	-	280	1268
2-hydroxyethanethiol	2	98				1.499-1.505	1.114-1.120				3,6	3,4,5	3,6	144	1541
indole	10,18	97		MP	51-54					10	2,3,5,6	3,4,5	1,3,6	340	1278
isoamyl cinnamate	3	96				1.531-1.541	0.992-1.002	1			1,2,3	3,4,5	3	299	1294
isoamyl octanoate	1	98				1.423-1.429	0.857-0.863	1			1,5	5	-	411	1309
isoamyl salicylate	1	98				1.504-1.509	1.051-1.057	1			1,2,3,5	3,4,5	3,6	383	1315
isoamyl valerate	1	98				1.413-1.419	0.860-0.866	1			-	4,5	-	334	1320
isobutanal diethyl acetal	1	97				1.391-1.397	0.822-0.828	1			3	3,5	3	278	1327
isobutyl 2-methylbutyrate	1	98				1.403-1.409	0.856-0.862	1			-	5	-	255	1329
isobutyl benzoate	1	98				1.490-1.496	0.997-1.003	1			1,3,5	3,4,5	3	360	1338
isobutyl butyrate	1	98				1.400-1.406	0.861-0.867	1			1,2,3,5	3,5	3,6	250	1340
isobutyl hexanoate	1	98				1.412-1.418	0.857-0.863	1			1,2,3,5	3,4,5	3	317	1347
isobutyl isovalerate	1	98				1.403-1.409	0.852-0.858	1			1,3,5	3,5	3	288	1350
isobutyl lactate	1	98				1.415-1.421	0.974-0.980	1			3	-	3	521	1351
isophorone	4	97				1.475-1.481	0.920-0.926				3,6	4,5	1,6	489	1397
isopropyl 2-methylbutyrate	1	98				1.395-1.401	0.851-0.857	1			1,6	-	-	267	1400
isopropyl butyrate	1	98				1.391-1.397	0.858-0.864	1			1,3,5	3,5	3,6	291	1404
isopropyl cinnamate	3	98				1.542-1.548	1.017-1.023	1			1,3,5,6	3,5	3,6	442	1405
isopropyl hexanoate	1	98				1.405-1.409	0.854-0.860	1			3	1,3,4	3	471	1410
isopropyl isobutyrate	1	95				1.384-1.394	0.844-0.854	1			1,3	4,5	3	515	1411
isopropyl propionate	1	98				1.384-1.390	0.863-0.869	1			2,3	3,4,5	3	361	1425
isovaleraldehyde diethyl acetal	1	95				1.395-1.403	0.825-0.832	1			-	4,5	-	279	1446
cis-jasmone	4	98				1.496-1.502	0.940-0.947				3,6	3,4,5	1,3,6	161	1453
lauric acid	10,18		98	SP	42-47					20	1,3,5,6	3,5	3,6	55	1457
levulinic acid	2		97			1.439-1.445	1.136-1.147				1,2,3,6	3,4,5	3,6	126	1462
linalyl butyrate	3	95				1.447-1.457	0.892-0.902	1			1	4	6	487	1478
d-8-p-menthene-1,2-epoxide	8	97				1.464-1.474	0.926-0.936		+65 to +80		-	4,5	-	439	1468
3-(l-menthoxy)-1,2-propanediol	2	98				1.471-1.477	0.992-1.004		-86 to -80		-	-	1	68	1515
2-mercaptopropionic acid	2	95				1.477-1.487	1.194-1.204				2,3,5,6	3,4,5	3,6	408	1546
2-methoxy-3(5)-methylpyrazine	2	98				1.504-1.510	1.079-1.086				2	-	-	389	1557
1-methoxy-4-propylbenzene	2	98				1.503-1.506	0.941-0.947				1,2,5	5	-	253	2215
methyl 2-furoate	1	98				1.485-1.491	1.179-1.185	1			1,2,3,5,6	3,4,5	3,6	313	1588
methyl 3-hydroxyhexanoate	1	95				1.426-1.436	1.000-1.010	1			1	-	6	258	1605
methyl 3-nonenoate	3	95				1.432-1.442	0.890-0.900	1			1,6	4	6	520	1608
methyl beta-naphthyl ether	10,18	98		MP	70-75					10	-	5	-	473	1570/1916
methyl butanethioate	1	97				1.457-1.467	0.960-0.975	1			3,6	3,4,5	6	206	1634
methyl decanoate	1	98				1.423-1.429	0.872-0.878	1			3,6	3,4,5	3,6	477	1642
methyl ethyl ketone	1	98				1.376-1.382	0.803-0.810				2,3,6	3,4,5	3,6	117	1648

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属*2(μg/g)	確認試験*3 IR	MS	NMR	使用量順位	H12-SEQ
methyl jasmonate	3	95				1.470-1.477	1.022-1.033	2			6	-	1,6	281	1669
methyl N-acetylanthranilate	9,17	95		MP	96-103					10	-	-	1	405	1682
alpha-methyl naphthyl ketone	2	95				1.623-1.633	1.114-1.124				3,5	3,4,5	3,6	460	1684
methyl palmitate	10,18	96		SP	26-29			1		10	3,5,6	3,5	3	402	1698
methyl trans-2-hexenoate	3	98				1.430-1.439	0.914-0.921	1			-	4,5	-	277	1587
methyl valerate	1	98				1.395-1.401	0.888-0.894	1			1,2,3,6	3,4,5	3,6	478	1726
2-methyl-1-phenyl-2-propanol	2	98				1.512-1.518	0.974-0.980				2,3,5	3,5	3	282	612
2-methyl-1-phenyl-2-propyl acetate	9,17	98		SP	28-36			1		10	-	4,5	-	151	660
3-methyl-2-butenyl acetate	3	98				1.428-1.434	0.916-0.922	1			3,6	3	6	398	2193
2-methyl-2-pentenoic acid	12,20	95		MP	24-28					10	1,2,3	3,4	3	202	1749
5-methyl-2-phenyl-2-hexenal	3	92				1.526-1.536	0.970-0.978	10			2,6	4	1,6	319	1750
4-methyl-5-thiazoleethanol decanoate	1	98				1.486-1.492	1.012-1.018	1			-	4,5	-	204	2308
4-methyl-5-thiazoleethanol isobutyrate	1	98				1.494-1.500	1.102-1.108	1			2	-	1	197	2312
2-methylpentanoic acid	2	95				1.411-1.417	0.921-0.931				6	4,5	6	425	1898
4-methylpentanoic acid	2	95				1.410-1.420	0.920-0.930				1,2,5,6	4,5	6	427	1899
2-methylundecanal	1	94				1.428-1.438	0.823-0.833	10			2,5,6	4,5	6	541	1895
myristic acid	12,20		98	SP	51-60					10	1,3,5,6	3,5	3,6	63	1907
myrtenol	4	93				1.490-1.500	0.976-0.986				1,3	3,4,5	1,3	465	1909
nonanal	1	95				1.418-1.428	0.819-0.831	10			1,2,3,6	3,4,5	3,6	131	1954
nonanal diethyl acetal	1	98				1.418-1.424	0.835-0.841	1			3,5	4,5	3	482	1955
nonanoic acid	2	97				1.428-1.435	0.903-0.910				1,3,5,6	3,4,5	3,6	304	1960
6-nonenol	4	94				1.444-1.454	0.844-0.854				1,2,3,5,6	4,5	3	488	1975
cis-6-nonenol	4	94				1.444-1.454	0.844-0.854				1,2,3,5,6	4,5	3	347	1975
nonyl acetate	1	97				1.421-1.427	0.866-0.872	1			1,2,3,5	4,5	3	540	1983
octahydro-2H-1-benzopyran-2-one	2	98				1.487-1.495	1.089-1.099				-	-	1	93	2009
octanal diethyl acetal	1	98				1.414-1.420	0.834-0.840	1			-	4	-	302	2013
octanal dimethyl acetal	1	95				1.412-1.422	0.845-0.855	3			1,3	3,4	3	366	2014
octanal propyleneglycol acetal	1	97				1.427-1.434	0.886-0.893	1			-	4	-	545	2016
2-octanone	2	95				1.410-1.420	0.815-0.825				1,3,5,6	3,4,5	3,6	352	1659
palmitic acid	10,18		98	SP	58-65					10	1,3,5,6	3,5	3,6	76	2073
2-pentadecanone	10,18	97		MP	32-42					10	1,3	3,4,5	3	241	2078
2,3-pentanedione	2	93				1.398-1.408	0.957-0.967				1,2,3,6	3,4,5	3,6	110	58
3-pentanone	2	98				1.389-1.395	0.814-0.820				3	3,4,5	3,6	426	2082
4-pentenoic acid	4	97				1.424-1.432	0.974-0.986				1,3	3,4,5	3,6	188	2085
phenethyl 2-methylbutyrate	1	95				1.481-1.489	0.976-0.986	2			6	4	1,6	503	2101
phenethyl butyrate	1	97				1.487-1.493	0.994-1.000	1			2,3,5,6	3,5	1,3,6	269	2106
phenethyl isovalerate	1	97				1.482-1.487	0.975-0.981	1			1,2	4	6	535	2115
phenethyl phenylacetate	9,17	98		SP	26-31			1		10	1,2,3	3,4,5	3	238	2120
4-phenyl-3-buten-2-one	12,20	96		MP	36-42					10	1,6	4	6	511	244
phenylacetic acid	10,18		98	MP	74-78					10	1,2	4,5	3,6	150	2152
3-phenylpropanol	2	98				1.523-1.529	1.000-1.006				1,2,3,5,6	3,4,5	3,6	369	579
3-phenylpropyl acetate	1	98				1.493-1.499	1.014-1.020	1			3	3	1,3	450	2160
3-phenylpropyl isobutyrate	1	98				1.483-1.489	0.978-0.983	1			-	-	1	453	2168
piperitone	4	95				1.480-1.490	0.925-0.935				1	4,5	-	113	2183
piperonal propyleneglycol acetal	1	95				1.528-1.538	1.231-1.241	1			-	5	-	256	1022
piperonyl acetate	1	97				1.523-1.529	1.237-1.243	1			1	4	-	315	2186
propanal diethyl acetal	1	95				1.385-1.395	0.824-0.834	1			3,6	3,4,5	6	342	2200
propyl hexanoate	1	95				1.408-1.418	0.864-0.874	1			1,5	4,5	-	309	2227
propyl isobutyrate	1	98				1.393-1.399	0.863-0.869	1			3	3,4,5	3	385	2228

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属*2(μg/g)	確認試験*3 IR	MS	NMR	使用量順位	H12-SEQ
propyleneglycol diacetate	1	96				1.412-1.416	1.055-1.060	1			5	4,5	-	354	2245
pyruvic acid	2	96				1.424-1.434	1.260-1.290				1,3,5,6	3,4,5	3	263	2267
raspberry ketone	12,20	98		MP	80-85					10	1,2,5,6	5	6	54	2268
stearic acid	10,18		98	MP	65-73					10	1,3	3,4,5	3	134	2296
styralyl butyrate	1	98				1.484-1.490	0.989-0.995	1			1	-	6	406	2299
styralyl isobutyrate	1	98				1.480-1.486	0.981-0.987	1			1	4	-	301	2302
styralyl propionate	1	98				1.487-1.494	1.007-1.013	1			6	4	6	359	2304
alpha-terpineol	4	96				1.478-1.488	0.930-0.941				1,3,5	3,5	3,6	259	2321
thymol	10,18	98		MP	48-52					10	2,3,5	3,4,5	3	219	2390
tiglic acid	11,19	98		MP	61-65					10	3,6	1,3,5	3,6	289	2392
2-tridecanone	10,18	97		MP	25-31					10	1,3,5,6	3,4,5	3,6	138	1724
triethyl citrate	1	98				1.439-1.445	1.138-1.145	1.0			1,3,6	3,4,5	3	9	2415
triethyleneglycol diacetate	1	98				1.435-1.441	1.115-1.121	1			3	3,4,5	3	458	5000
valeraldehyde diethyl acetal	1	98				1.401-1.407	0.829-0.835	1			-	4,5	-	290	2479
valeraldehyde propyleneglycol acetal	1	98				1.415-1.420	0.900-0.906	1			-	4	-	537	2482
gamma-valerolactone	1	95				1.429-1.439	1.051-1.061	3			1,2,3,6	3,4	3,6	327	2486
vanillin acetate	9,17	98		MP	75-80			1		10	1,5,6	5	-	60	59
vanillin propyleneglycol acetal	1	94				1.536-1.546	1.205-1.215	特例除外			-	4	-	146	2492

＊1 融点区分

MP ・・・ Melting point　融点
SP ・・・ Solidification point　凝固点

＊2 重金属規格設定基準

固体化合物において、最終精製法が蒸留法など重金属混入の懸念がない場合を除き、重金属の項目を規格項目として採用することとした。
重金属規格設定を必要とする化合物については公定書の設定値である10μg／gを原則とする。

＊3 参照スペクトルデータベース番号

1) FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)
2) 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)
3) 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)
4) Wiley's Registry of Mass spectral Database
5) NIST/EPA/NIH Mass Spectral Library
6) Sigma-Aldrich カタログ

資料－４－３

日本香料工業会　自主規格　一覧
(平成１９年度)

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
acetaldehyde bis(2-methylbutyl) acetal	1	97				1.412-1.418	0.833-0.839	1				4,5		694	12
acetaldehyde diamyl acetal	1	97				1.414-1.420	0.833-0.840	1			3	3	3	570	13
acetaldehyde dibutyl acetal	1	98				1.405-1.411	0.830-0.836	1			1,2			683	15
acetaldehyde ethyl hexyl acetal	1	93				1.405-1.415	0.828-0.838	1				4		639	27
acetaldehyde hexyl isoamyl acetal	1	97	sum of acetaldehyde hexyl isoamyl acetal(ca.52%), acetaldehyde dihexyl acetal(ca.27%) and acetaldehyde diisoamyl acetal(ca.18%)			1.418-1.423	0.833-0.838	1				1		500	34
acetaldehyde phenethyl propyl acetal	1	98				1.475-1.481	0.948-0.954	1			6		1	992	36
acetaldehyde propyleneglycol acetal	1	95				1.391-1.401	0.927-0.937	1					1	87	37
acetone	2	99				1.356-1.362	0.790-0.795				1,3,6	3,4,5	3,6	999	45
acetone propyleneglycol acetal	1	98				1.384-1.402	0.888-0.906	1				4,5	1	1005	47
2-acetyl-3,5(3,6)-dimethylpyrazine	2	98				1.510-1.520	1.070-1.080				1		6	1151	67
2-acetyl-3-ethylpyrazine	2	97				1.509-1.518	1.070-1.080				1,5,6	4,5	6	655	69
2-acetylthiazole	2	98				1.542-1.552	1.220-1.230				2,6	3,4,5	1	353	83
allyl 2-ethylbutyrate	3	98				1.419-1.425	0.883-0.889	1			1	4,5		1018	91
allyl acetate	3	98				1.401-1.407	0.926-0.932	2			3,6	3,4,5	3,6	1053	95
allyl butyrate	3	95				1.409-1.419	0.897-0.907	1			1,3	3,5	3	662	98
allyl isovalerate	3	98				1.414-1.420	0.882-0.888	1			1,2,3,5	3	3	965	112
allyl levulinate	3	98				1.438-1.444	1.024-1.030	1				5		1004	113
allyl propionate	3	98				1.407-1.413	0.913-0.921	1			1,2,5	4,5		1085	123
allyl valerate	3	98				1.417-1.423	0.891-0.897	1			3	3,5	3	600	131
alpha-methylionone	4	90				1.495-1.505	0.927-0.937				1	4,5		1021	1794
amyl heptanoate	1	98				1.422-1.428	0.861-0.867	1			1			962	151
amyl octanoate	1	98				1.424-1.431	0.860-0.866	1			1,2,3	3,5	3	949	161
amyl phenylacetate	1	98				1.484-1.490	0.979-0.985	1			5	4,5		705	162
amyl salicylate	1	98				1.505-1.511	1.052-1.058	1			2	4,5		1013	164
4-tert-amylcyclohexanone	2	92				1.464-1.474	0.920-0.930				3,5	5	3	933	2342
anisole	2	98				1.514-1.520	0.993-0.999				1,2,3,5,6	3,4,5	3(C,H),6	1086	186
anisyl formate	1	95				1.517-1.527	1.139-1.149	1			1,2,6	4,5	6	1069	192
anisyl propionate	1	95				1.503-1.513	1.080-1.090	1			1,6	4,5	1,6	1024	198
anisylacetone	2	95				1.515-1.525	1.043-1.053				1,2,3	3	3	675	188
benzaldehyde diethyl acetal	1	95				1.474-1.484	0.963-0.973	1			3	3,4,5	3(C,H)	338	202
benzaldehyde glyceryl acetal	1	95	異性体合算			1.532-1.542	1.184-1.197	2			1,2	4		617	205
benzothiazole	2	96				1.637-1.647	1.241-1.251				3	3,4,5	1,3,6	1045	210
benzyl 2-methylbutyrate	1	98				1.485-1.491	0.990-0.999	1			5	4,5		654	212
benzyl acetoacetate	1		93			1.498-1.516	1.111-1.121	3			1	4,5		720	214
benzyl crotonate	3	96				1.515-1.525	1.035-1.045	1			3	3	3	485	220
benzyl hexanoate	1	98				1.486-1.492	0.979-0.985	1				4		606	225
benzyl nonanoate	1	97				1.481-1.487	0.953-0.959	1				4		964	237
benzyl salicylate	1	95				1.577-1.587	1.177-1.187	1			1,2,3	3,4,5	3	1006	241
dl-borneol	12,20	95		MP	200-208					10	1,2,3,5,6	4,5		125	251

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
borneol	12,20	95		MP	200-210					10	1,2,3,5,6	4,5		1138	251
butanal propyleneglycol acetal	1	95				1.406-1.416	0.905-0.915	1				4		564	1754
2-buten-4-olide	3	98				1.465-1.475	1.197-1.212	3				4,5	6	1137	3070
butyl decanoate	1	98				1.427-1.433	0.859-0.865	1			3	3,4	3	590	284
2-butyl ethyl ether	2	97				1.372-1.382	0.740-0.750					4,5	1	274	285
2-butyl isothiocyanate	2	96				1.488-1.498	0.937-0.947					4		384	291
butyl methacrylate	3	99				1.422-1.426	0.893-0.899	1			3,6	3,4,5	3(C,H),6	1106	296
butyl nonanoate	1	97				1.425-1.431	0.860-0.867	1				4,5		650	301
butyl oleate	3		98-104			1.449-1.454	0.865-0.870	1			3,5	3,5	3	193	303
butyl palmitate	1	98				1.439-1.445	0.856-0.863	1			3	3,4,5	3	1055	304
2-tert-butylcyclohexyl acetate	9,17	98		MP	25-29	1.448-1.456	0.938-0.948	1		10	3	3		295	3123
dl-camphor	12,20	90		MP	170-180					10	1,2			143	338
camphor	12,20	90		MP	170-180					10	1,2,3	3,4,5	3	218	339
carvacrol	2	95				1.518-1.528	0.974-0.984				1,2,6	4,5	6	629	341
l-carvone	8	97				1.495-1.501	0.959-0.965		-57 to -62		1,2,3,6	3	3,6	3	345
d-carvone	8	96				1.494-1.503	0.953-0.963		47 to 61		1,2,3,6	3,4,5	3,6	556	344
carvone oxide	4	94				1.477-1.487	1.035-1.045					1,4,5	1	722	347
cinnamaldehyde propyleneglycol acetal	3	95				1.542-1.552	1.059-1.069	1				4		580	376
cinnamyl cinnamate	3		95-100.5	MP	40-46	1.612-1.622	1.099-1.109	1			1,2	4,5		724	383
cinnamyl propionate	3	97				1.531-1.537	1.032-1.039	1			1,2	4		686	389
citral diethyl acetal	3	95				1.446-1.459	0.864-0.882	2			1,6	4,5		574	393
citral propyleneglycol acetal	3	95	異性体合算			1.466-1.476	0.925-0.935	1				4		306	396
citronellyl isobutyrate	3		98			1.438-1.445	0.873-0.883	1			1,2	4		316	411
citronellyl isovalerate	3		98(ただしtetrahydrogeranyl isovalerateを含む)			1.440-1.446	0.871-0.877	1			3	3	3	536	412
citronellyl tiglate	3		98			1.460-1.468	0.901-0.909	1			6		6	1076	416
creosol	2	95				1.531-1.541	1.089-1.099				1,3	3,4	3,6	569	419
crotonic acid	12,20		98	MP	70-74					10	3,5	3,4,5	1,3	1139	430
cyclamen aldehyde	1	95	異性体合算			1.501-1.511	0.945-0.958	5			1,2,5	5		926	434
cyclohexyl isovalerate	1	98				1.439-1.445	0.925-0.931	1			3	3	1,3,6	649	454
cyclohexyl propionate	1	98				1.439-1.445	0.953-0.962	1			3,5	3,4,5	1,3(C,H)	1115	457
cyclopentanone	2	98				1.434-1.440	0.948-0.958				1,3,5,6	1,4,5	1,3,6	1152	472
cyclotene isobutyrate	3	97				1.472-1.479	1.053-1.061	2				4		641	477
trans,trans-2,4-decadienal	3	89				1.510-1.520	0.866-0.876(25℃)	10			1,2	4,5		1033	487
decanal propyleneglycol acetal	1	98	異性体合算			1.433-1.439	0.881-0.887	1			1	1	1	303	494
trans-4-decenoic acid	4		98			1.445-1.452	0.913-0.920				1	1,4	1	160	510
decyl butyrate	1	97				1.427-1.433	0.859-0.865	1			1	5	6	986	520
delta-damascone	4	95	異性体合算			1.485-1.495	0.927-0.937				1	4		974	485
delta-tridecalactone	1	98				1.458-1.464	0.939-0.946	5			3,5	3,5	3	665	2406
diallyl disulfide	4	95	sum of diallyl disulfide(80%), diallyl sulfide(10%), diallyl trisulfide (5%)			1.537-1.550	0.998-1.015				1,3,5	3,4,5	3	305	534
dibutyl sebacate	1	98				1.439-1.445	0.935-0.941	1			1,3	3,4	3	596	541

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
dibutyl succinate	1	98				1.428-1.434	0.975-0.981	1			3	3,4,5	3	1046	542
diethyl carbonate	1	98				1.380-1.390	0.970-0.980	1			3,6	3,4,5	3,6	636	546
diethyl diethylmalonate	1	98				1.418-1.428	0983-0.993(20/4)	1			3,5,6	3,4,5	3,6	945	-
diethyl maleate	3	98				1.437-1.443	1.066-1.072	1			2,3,5	3,5		674	551
diethyl oxalate	1	96				1.405-1.415	1.075-1.085	1			3,5,6	3,4,5	3,6	630	553
dihydroactinidiolide	3	95				1.495-1.501	1.052-1.062	10					1	634	564
dihydrocarvone	4	95				1.467-1.477	0.922-0.932				1,2,3	3,4,5	3	190	569
dihydrocoumarin	1	97				1.550-1.560	1.188-1.198	1			1,2,3,6	3,4,5	3(C,H),6	1082	580
2,5-dihydroxy-2,5-dimethyl-1,4-dithiane	10,18	95		MP	79-85					10	3	3	3	555	591
1,3-dimethoxybenzene	2	97				1.521-1.527	1.060-1.074				3	3,5	1,3	672	605
1,4-dimethoxybenzene	10,18	97		MP	53-57					10	1,3	3,5	3	966	605
dimethyl malonate	1	98				1.411-1.417	1.153-1.159	1			3,6	3,4	3,6	560	618
3,4-dimethyl-1,2-cyclopentanedione	10,18	95		MP	65-71					10	1			311	630
3,5-dimethyl-1,2-cyclopentanedione	10,18	95		MP	87-93					10	3	3	3	401	631
3,7-dimethyl-1,6-nonadien-3-ol	4	97	異性体合算			1.458-1.468	0.861-0.867					5		706	3372
2,2-dimethyl-5-(1-methyl-1-propenyl)tetrahydrofuran	4	95				1.442-1.452	0.862-0.872					4,5	1	1034	650
2,6-dimethyl-5-heptenal propyleneglycol acetal	3	97	異性体合算			1.447-1.453	0.910-0.916	1				1		932	651
3,7-dimethyl-6-octen-3-ol	4	97				1.449-1.459	0.850-0.860					4		568	584
2,5-dimethylfuran	2	98				1.438-1.448	0.895-0.904				1,3,5,6	1,3,4,5	1,3,6	637	663
3,7-dimethyloctanol	2	97				1.431-1.441	0.826-0.836				1,2,3,5,6	3,4,5	3,6	378	2359
3,4-dimethylphenol	10,18	97		MP	62-69					10	1,3,6	3,4	3,6	554	2511
2,5-dimethylphenol	10,18	98		MP	74-78					10	1	4,5	6	1038	2510
dioctyl adipate	1	98				1.444-1.450	0.924-0.930	1			3,6	3,4,5	3,6	1047	3553
dipropyl disulfide	2	97				1.493-1.501	0.956-0.962				1,3,6	3,4	3,6	592	2222
dodecanal	1	90				1.430-1.440	0.826-0.836	10			1,2,5,6	5		266	694
2-dodecanone	10,18	98		MP	18-24					10	6	1		666	525
cis-6-dodecen-4-olide	3	95				1.463-1.471	0.955-0.965	5				4		1070	706
2-dodecenal	3		95			1.452-1.462	0.843-0.853	10			1,2	4,5		1009	701
dodecyl propionate	1	98				1.432-1.436	0.860-0.866	1			3	3	3	287	713
5-ethenyl-4-methylthiazole	4	97				1.560-1.570	1.091-1.100				3,6	3,4,5	1,3,6	1003	1786
2-ethoxy-3(5)(6)-methylpyrazine	2	99				1.494-1.497	1.033-1.037				1,5	5	6	1108	725
ethyl (methylthio)acetate	1	95				1.454-1.465	1.051-1.071	1			1,3	3,4,5	3	690	736
ethyl 10-undecenoate	3	97				1.435-1.442	0.876-0.882	1			1,6	4,5	6	695	734
ethyl 2,4-decadienoate	3	98				1.481-1.490	0.898-0.906(25℃)	1			5			1099	737
ethyl 2-ethylhexanoate	1	98				1.411-1.417	0.860-0.866	1				4,5		1036	750
ethyl 2-hexenoate	3	96				1.430-1.440	0.895-0.905	1				4,5(trans)		1042	755
ethyl 2-methyl-3(4)-pentenoate	3	95	異性体合算			1.415-1.425	0.883-0.893	1			3	3	3	502	762
ethyl 3-(furfurylthio)propionate	1	98				1.500-1.509	1.125-1.133	1			1		1	594	779
ethyl 3-hexenoate	3	96	異性体合算			1.415-1.430	0.880-0.910	1			1	5		682	780
ethyl 5-acetoxyoctanoate	9,17	98		MP	32-36	1.427-1.433	0.976-0.982	1		10		4		955	796
ethyl acetoacetate ethyleneglycol acetal	1	98				1.429-1.435	1.083-1.091	1				4,5		577	807
ethyl acetoacetate propyleneglycol acetal	1	95	異性体合算			1.422-1.432	1.042-1.052	2			1			182	808
ethyl alpha-acetylcinnamate	3	98				1.555-1.561	1.098-1.104	1				4		920	738
ethyl alpha-ethyl-beta-methyl-beta-phenylglycidate	9,17	95		SP	37-42			2		10		4		386	746
ethyl benzoylacetate	1	92				1.524-1.534	1.107-1.120	1			1,3,6	3	3	614	818

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
ethyl butyryllactate	1	98				1.413-1.419	1.001-1.007	1			3	3	3	526	823
ethyl ethanethioate	1	95				1.440-1.461	0.970-0.985	1			3,6	3,4,5	1,6	1136	878
ethyl linoleate	3		98-104			1.451-1.461	0.872-0.882	1			3,6	3,4	6	260	848
ethyl maltol butyrate	1	98				1.494-1.500	1.125-1.131	1			3	3	3	499	928
ethyl methyl sulfide	2	96				1.435-1.445	0.840-0.850				1,3,5	3,4,5	3	212	1649
ethyl oleate	3		98-104			1.447-1.455	0.867-0.875	1			1,3,5,6	3,5	3,6	85	861
ethyl pivalate	1	98				1.388-1.394	0.853-0.859	1			3,6	3,4,5	3,6	620	866
ethyl tiglate	3	98				1.432-1.438	0.923-0.929	1			3,6	3,4,5	3,6	698	879
ethyl trans,cis-2,4-decadienoate	3	90	異性体合算			1.476-1.491	0.890-0.911	2				4	1	715	880
ethyl vanillyl ether	2	98				1.527-1.533	1.110-1.117					4	1	652	2496
3-ethyl-2-hydroxy-2-cyclopenten-1-one	12,20	97		MP	37-43					10	6	4	6	371	828
5-ethyl-3-hydroxy-4-methyl-2(5H)-furanone	2	90				1.485-1.495	1.137-1.147				1,2,6	4	6	702	897
2-ethylbutanal	1	95				1.398-1.408	0.811-0.821	5			1,3,5,6	3,5	3,6	273	905
2-ethylhexanol	2	98				1.428-1.435	0.832-0.839				1,3,6	3,4,5	3(C,H),6	339	922
4-ethylphenol	10,18	97		MP	40-46					10	1,3,6	3,4,5	3,6	1002	933
furfural propyleneglycol acetal	1	98				1.472-1.478	1.130-1.136	1			3	3	3	387	965
furfuryl ethanethioate	1	95				1.519-1.530	1.152-1.165	1			6	4,5	1,6	627	982
furfuryl hexanoate	1	95				1.455-1.465	1.011-1.021	1				4	6	621	973
furfuryl methyl disulfide	2	95				1.564-1.574	1.178-1.188						1	963	1651
furfuryl methyl sulfide	2	95				1.517-1.527	1.080-1.090				3	3,4,5	1,3,6	1031	979
furfuryl propionate	1	98				1.458-1.464	1.083-1.089	1			1,6	4,5	6	1000	981
4-(2-furyl)-3-buten-2-one	12,20	98		MP	36-40					10	3,5	4,5	1	1155	985
geranic acid	4	90	異性体合算			1.479-1.489	0.952-0.962				5			989	993
geranyl butyrate	3		97			1.453-1.463	0.894-0.904	1			1,2,3,5	4,5	3	296	1002
geranyl hexanoate	3		97			1.458-1.464	0.891-0.897	1			1	4		1074	1005
geranyl phenylacetate	3		97			1.507-1.513	0.978-0.984	1			1,2	4		601	1009
geranyl propionate	3		96			1.456-1.466	0.901-0.911	1			1,2,3	4	3	248	1010
heptanal	1	90				1.410-1.420	0.816-0.826	10			1,2,3,6	3,4	3,6	565	1030
heptanal diethyl acetal	1	95				1.410-1.420	0.831-0.841	1				4,5		710	1033
heptanal propyleneglycol acetal	1	98	異性体合算			1.425-1.430	0.889-0.895	1				1		1028	1031
2,3-heptanedione	2	96				1.410-1.420	0.917-0.927				1,3	3,4	3	589	1036
2-heptanol	2	97				1.416-1.426	0.813-0.825				1,3,6	3,4,5	3,6	700	1038
4-heptanone	2	97				1.402-1.412	0.810-0.820				1,3,5,6	3,5	3,6	929	682
heptyl butyrate	1	98				1.419-1.424	0.861-0.867	1			1,6	4,5	6	716	1057
heptyl octanoate	1	98				1.430-1.436	0.858-0.864	1			1	5		957	1070
delta-hexadecalactone	1	90				1.456-1.466(25C)	0.918-0.928(25C)	7				4		659	1077
hexanal dibutyl acetal	1	95				1.419-1.429	0.833-0.843	1			3	3	3	656	1089
hexanal hexyl isoamyl acetal	1	97	sum of hexanal hexyl isoamyl acetal(ca.51%), hexanal dihexyl acetal(ca.26%) and hexanal diisoamyl acetal(ca.21%)			1.427-1.432	0.835-0.840	1			1	1	1	440	1096
3,4-hexanedione	2	90				1.407-1.417	0.940-0.950				1,3,5	3,4,5	3,6	1073	1082
trans-2-hexenal diethyl acetal	3	93				1.418-1.426	0.843-0.853	1			1,6	4,5	6	92	1114

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
cis-3-hexenal diethyl acetal	3	99				1.420-1.426	0.850-0.856	1				4		643	1113
trans-2-hexenal propyleneglycol acetal	3	90				1.438-1.444	0.919-0.926	1				4,5		96	1118
cis-2-hexenyl acetate	3	97	異性体合算			1.425-1.431	0.900-0.907	1				4,5		607	1140
5-hexenyl isothiocyanate	4	96				1.506-1.516	0.955-0.965				3	3	3	178	1168
cis-3-hexenyl octanoate	3	97	異性体合算			1.438-1.444	0.873-0.879	1			3	3	3	618	1177
cis-3-hexenyl phenylacetate	3	97				1.497-1.507	0.991-0.997	1			3	3,4,5	1,3	713	1179
cis-3-hexenyl pyruvate	3	90				1.437-1.447	0.987-0.997	1				4,5		183	1183
cis-3-hexenyl salicylate	3	96				1.517-1.527	1.060-1.070	2			3	3	3(C,H)	1098	1184
cis-3-hexenyl tiglate	3	97				1.456-1.462	0.915-0.921	1			1,3,6	1,4	3	1029	1186
cis-3-hexenyl trans-2-hexenoate	3	94				1.452-1.462	0.898-0.908	1			1	1	1	1020	1132
cis-3-hexenyl valerate	3	98	異性体合算			1.431-1.439	0.881-0.889	1			1		1	923	1187
2-hexyl acetate	1	98				1.402-1.408	0.863-0.869	1			1,2	4,5		610	1194
hexyl benzoate	1	98				1.490-1.496	0.978-0.984	1			1,3	3,4	3	612	1196
hexyl decanoate	1	98				1.432-1.438	0.857-0.863	1				5		1043	1201
hexyl isobutyrate	1	98				1.410-1.416	0.857-0.863	1			1	4		572	1205
hexyl lactate	1	95				1.424-1.434	0.952-0.962	1			3	3	3	470	1209
hexyl nonanoate	1	96				1.431-1.436	0.858-0.863	1			3	3	3	343	1212
hexyl phenylacetate	1	98				1.483-1.489	0.968-0.974	1			3,5	1,3,5	3	671	1214
2-hydroxy-2-cyclohexen-1-one	12,20	97		MP	34-41					10	1			928	1243
5-hydroxy-4-octanone	2	95				1.427-1.437	0.917-0.927				3,5	3,4,5		341	1255
4-hydroxybenzaldehyde	9,17	98		MP	114-119			10		10	1,3,6	3,4,5	3,6	605	1259
3-hydroxybutane-2-thiol	2	95				1.476-1.486	1.006-1.022				1	4	1	633	1535
3-hydroxyhexanoic acid	2		95			1.440-1.450	1.070-1.080				3	3		696	1274
2-hydroxyphenol	10,18	99		MP	102-106					10	3,5,6	3,5	6	940	363
3-hydroxyphenol	10,18	98		MP	105-115					10	1,3,5,6	3,4,5	3,6	1095	2269
l-limonene	8	90				1.468-1.478	0.840-0.850		-90 to -80		6	4,5	6	53	1466
alpha-irone	4	94				1.497-1.507	0.930-0.940				1	4		1156	1283
isoamyl benzoate	1	98				1.490-1.496	0.986-0.992	1			1,2,3	3	3	557	1292
isoamyl heptanoate	1	98				1.420-1.426	0.859-0.865	1				4,5		1052	1298
isoamyl laurate	1	97				1.433-1.439	0.855-0.861	1			1,3,6	3,4,5	3,6	1056	1304
isoborneol	12,20	90		MP	208-214					10	1,2,3,5,6	4,5	3,6	1135	1321
isobornyl acetate	3	90				1.460-1.470	0.980-0.990	1			1,2,3	3,4,5	3	231	1322
isobutanal propyleneglycol acetal	1	96	異性体合算			1.407-1.412	0.903-0.909	1			1	1	1	534	1328
isobutyl beta-naphthyl ether	10,18	97		MP	30-34					10			1	587	1339
isobutyl cinnamate	3	98				1.538-1.544	1.003-1.009	1			1,2,5,6	5	6	959	1341
isobutyl crotonate	3	98				1.426-1.432	0.889-0.895	1			1,2,6	4,5	6	1041	1342
isobutyl isothiocyanate	2	95				1.491-1.501	0.935-0.951				3	3,4,5	3	575	1349
isobutyl salicylate	1	98				1.505-1.511	1.064-1.070	1			1,2,3	3,4,5	3	1025	1364
isobutyl valerate	1	98				1.406-1.412	0.859-0.865	1				4,5		1103	1369
2-isobutyl-3(5)(6)-methoxypyrazine	2	99				1.488-1.494	0.990-0.998				1	4	6	1010	1370
isoeugenyl acetate	11,19	98		MP	78-82			1		10	1,2	3,5		943	1383
isomenthone	2	98	異性体合算			1.449-1.456	0.895-0.905				1			381	1393
isopropyl isothiocyanate	2	95				1.487-1.497	0.945-0.955				5	4,5		693	1412
isopropyl octanoate	1	98				1.414-1.420	0.853-0.859	1			3	4	3,6	1133	1422
isopropyl phenylacetate	1	98				1.485-1.491	0.998-1.004	1			5	4,5	1	1144	1424
2-isopropyl-4-methylthiazole	2	95				1.494-1.504	0.997-1.007				1,3	1,3,4	1,3	328	1434
l-isopulegol	8	90				1.467-1.477	0.905-0.915		-20.6 to -19.6		1,2,3,6	3,4,5	3,6	47	1442
isopulegol	4	90	異性体合算			1.467-1.477	0.908-0.918				1,2,5	4,5		214	1442

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分[*1]	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験[*2] IR	MS	NMR	使用量順位	H12-SEQ
isovaleraldehyde propyleneglycol acetal	1	95	異性体合算			1.412-1.420	0.895-0.902	1			1,6	1	1	336	1450
limonen-10-ol	4	95				1.495-1.505	0.958-0.976					4		958	1503
d-limonene	8	90				1.468-1.478	0.840-0.850		95 to 104		1,2,3,6	3,4,5	3,6	1	1465
linalool oxide (furanoid)	4	95	異性体合算			1.447-1.457	0.940-0.950				2			254	1472
linalool oxide (pyranoid)	12,20	90		MP	37-43[*3]	1.465-1.485	0.975-1.000			10	3	3		285	3417
linalyl benzoate	3	92				1.505-1.520	0.979-0.989	2			1,2			689	1477
linalyl formate	3	90				1.450-1.463	0.910-0.922	3			1,2	4,5	6	599	1480
linalyl hexanoate	3	95				1.448-1.458	0.884-0.894	1			1	4,5		1067	1481
linalyl isobutyrate	3	95				1.445-1.455	0.883-0.895	1			1,2	4		581	1482
linalyl propionate	3	93				1.445-1.455	0.893-0.903	1			1,2,6	4		622	1486
linoleic acid	4		98-102			1.462-1.470	0.898-0.905				1,3,5,6	3,4,5	3,6	141	1487
menthalactone	3	96				1.494-1.504	1.060-1.070	1			1		1	939	1900
menthyl 3-hydroxybutyrate	1	95				1.453-1.463 (25)	0.970-0.980 (25)	1			3	3	3	175	1517
menthyl acetate	1	98				1.443-1.449	0.923-0.929	1			1,3,5	3,4,5		1062	1520
menthyl butyrate	1	99				1.445-1.451	0.908-0.918	1			3	3	3	583	1521
menthyl hexanoate	1	99				1.447-1.453	0.900-0.910	1			3	3	3	691	1525
menthyl isovalerate	1	95				1.442-1.452	0.900-0.910	1			1,6	4		632	1527
menthyl lactate	9,17	90		MP	42-47			1		10	1			333	1528
menthyl octanoate	1	99				1.449-1.455	0.894-0.904	1			3	3	3	692	3426
menthyl valerate	1	98				1.445-1.451	0.905-0.911	1				4		586	1533
3-[(2-mercapto-1-methylpropyl)thio]-2-butanol	2	94				1.515-1.525	1.042-1.062				1	4	1	582	1802
3-mercaptopropionic acid	2	98				1.490-1.496	1.220-1.226				3,5,6	3,4,5	3,6	645	1547
methional	1	90				1.479-1.493	1.037-1.060	10			1,6	3,4,5	3,6	272	1550
methionol	2	98				1.485-1.495	1.024-1.034				1,3,6	3,4,5	3,6	362	1554
4-methoxy-2,5-dimethylfuran-3(2H)-one	4	97				1.475-1.481	1.091-1.101				6	4	1,6	318	619
4-methoxycinnamaldehyde	11,19	96		MP	56-63			10		10	1	4,5		708	1567
2-methoxycinnamaldehyde	11,19	96		MP	45-49			5		10	1	5		937	1566
methoxypyrazine	2	99				1.507-1.512	1.110-1.150				1,2,3,5,6	4,5	3,6	1134	1576
methyl 2-(methylthio)butyrate	1	98				1.454-1.461	1.025-1.034	1				1,4		1140	1581
methyl 2-methyl-3-furyl disulfide	2	97				1.554-1.566	1.159-1.180				1	4	1	1130	1590
methyl 2-nonynoate	3	97				1.445-1.451	0.914-0.920	1			3,5,6	3,4,5	1,3,6	984	1693
methyl 3-acetoxyhexanoate	1	97				1.419-1.425	1.018-1.024	1				4		310	1601
methyl beta-methyl-beta-phenylglycidate	1		98			1.509-1.517	1.122-1.130	1			3	3	3	517	1607
methyl crotonate	3	95				1.418-1.428	0.942-0.952	1			3,6	3,5	3,6	975	1640
methyl ethanethioate	1	98				1.460-1.468	1.020-1.028	1				1,4,5	1	625	1549
methyl formate	1	95				1.341-1.346	0.970-0.976	特例除外			3,6	3,4,5	3(C,H),6	1116	1650
methyl lactate	1	97				1.410-1.420	1.090-1.100	1			3,5	3,4	3(C)	1087	1670
methyl laurate	1	95				1.427-1.437	0.865-0.875	1			1,3,6	3,4,5	6	335	1671
methyl myristate	1	98				1.434-1.440	0.865-0.872	1			1,3,6	3,4	3,6	372	1680
methyl N,N-dimethylanthranilate	1		98			1.552-1.562	1.093-1.103	1			3	3,4,5	1,3	613	1681
methyl N-formylanthranilate	9,17	98		MP	51-55			1		10		4	1	987	1686
methyl nonanoate	1	97				1.419-1.425	0.873-0.879	1			1,3,6	3,4,5	3,6	611	1688
methyl octanoate	1	98				1.414-1.420	0.876-0.886	1			1,3,5,6	3,5	3,6	436	1692
methyl octyl sulfide	2	95				1.450-1.460	0.842-0.852	1			1			676	1695
methyl oleate	3		98.0-104.0			1.446-1.456	0.871-0.881	1			3,6	3,4,5	3,6	226	1696
methyl phenethyl ether	2	98				1.494-1.508	0.949-0.960				3	3,4	1,3	609	1700
methyl stearate	9,17	95		MP	36-42			1		10	3,5,6	3,5	3	968	1715
4-methyl-1-phenyl-2-pentanol	2	96				1.490-1.510	0.938-0.948				1	5		717	1374

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比 重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
5-methyl-2,3-hexanedione	2	94				1.406-1.419	0.908-0.919				1			591	57
3-(5-methyl-2-furyl)butanal	1	99				1.470-1.476	1.008-1.018	10					1	1089	1734
5-methyl-2-hepten-4-one	4	95				1.436-1.446	0.846-0.856						1	1072	1738
5-methyl-2-hexanone	2	98				1.404-1.410	0.811-0.817				3,5	3,5	3	960	1662
4-methyl-2-pentanone	2	98				1.390-1.400	0.797-0.807				1,3,6	3,4,5	3,6	640	1663
5-methyl-2-thiophenecarboxaldehyde	1	98				1.579-1.585	1.156-1.167	10			3,5	3,5	1,3,6	988	1756
6-methyl-3-heptanone	2	95				1.410-1.420	0.816-0.826				5	4,5		638	1296
2-methyl-4-phenyl-2-butyl isobutyrate	1	97				1.475-1.485	0.950-0.959	1					1	1094	621
2-methyl-4-propyl-1,3-oxathiane	2	98	異性体合算			1.475-1.485	0.973-0.983					1,4		646	1781
4-methyl-5-thiazoleethanol butyrate	1	98				1.496-1.510	1.106-1.112	1			3	3	1,3	111	2307
4-methyl-5-thiazoleethanol formate	1	95				1.518-1.524	1.215-1.221	2			3	1,3	1,3	608	2309
4-methyl-5-thiazoleethanol hexanoate	1	98				1.491-1.497	1.065-1.071	1			3	3	1,3	501	2311
4-methyl-5-thiazoleethanol octanoate	1	98				1.488-1.494	1.036-1.042	1			3	3	1,3	78	2314
4-methyl-5-thiazoleethanol propionate	1	98				1.502-1.506	1.136-1.140	1			3	3	1,3	349	2315
4-methylbenzaldehyde	1	95				1.541-1.551	1.013-1.023	10			1			251	2395
2-methylbutyl 2-methylbutyrate	1	95				1.408-1.418	0.856-0.867	1			1,3,6	4	6	348	1807
2-methylbutyl butyrate	1	95				1.407-1.417	0.864-0.874	1				4		597	1810
2-methylbutyl hexanoate	1	98				1.418-1.424	0.862-0.868	1				4,5		1022	1814
2-methylbutyl isovalerate	1	98				1.410-1.419	0.856-0.864	1			1,2	4	6	653	1816
2-methylbutyric acid	2	98				1.403-1.409	0.935-0.941				1,2,3,6	3,4,5	3,6	19	1822
alpha-methylcinnamaldehyde	3	95				1.597-1.607	1.034-1.044	5			1,2,3,6	3,4,5	3(C,H),6	1117	1823
4-methyldecan-4-olide	1	95				1.441-1.455	0.940-0.950	3			1,3	3	6	677	1652
2-methylfuran	2	95				1.430-1.440	0.912-0.922				1,3,5,6	1,3,4,5	1,3,6	283	1833
2-methylheptanoic acid	2	97				1.422-1.428	0.900-0.910				6		1,6	982	1840
2-methylhexanoic acid	2	98				1.416-1.423	0.912-0.918				1,3	3,5	3,6	919	1843
methylionone	4		90			1.494-1.504	0.924-0.938				3,5	3,4	3	308	1661
3-methylnonane-2,4-dione	2	97				1.442-1.452	0.917-0.927					4		1051	1849
4-methylphenol	10,18	97		MP	31-37					10	1,3,6	3,4,5	3	709	422
2-methylphenol	10,18	98		MP	29-33					10	1,3,6	3,4,5	3,6	1017	421
4-methylphenyl acetate	1	98				1.498-1.506	1.046-1.054	1			1,2,3,6	3,4,5	3,6	711	2400
4-methylphenyl isobutyrate	1	98				1.484-1.490	0.993-0.999	1			1,2,3,5,6	4,5	3,6	1131	427
2-methyltetrahydrofuran-3-one	2	97				1.426-1.432	1.040-1.050				1,3	3,4,5	3(C,H)	323	1865
3-(methylthio)hexanol	2	98				1.476-1.489	0.964-0.974				1,6		1,6	954	1880
6-(methylthio)hexyl isothiocyanate	2	98				1.534-1.540	1.035-1.041				3	3	3	578	1882
3-(methylthio)propyl acetate	1	98				1.461-1.467	1.036-1.044	1				4		571	1889
3-(methylthio)propylamine	2	98				1.489-1.495	0.958-0.964				3	3,4	3	628	1892
nerol	4	90				1.470-1.480	0.874-0.884				1,2,3	3,4,5	3,6	185	1923
nerolidol	4	97				1.470-1.488	0.871-0.881				2,3,6	3,4,5	1,6	106	1927
neryl acetate	3	90				1.456-1.466	0.908-0.918	1			1,2,3	3,4,5	3,6	148	1930
neryl butyrate	3	98				1.457-1.463	0.898-0.904	1			1	4		616	1931
neryl crotonate	3	98				1.475-1.481	0.918-0.924	1			3	3	3	518	1932
neryl isobutyrate	3	95				1.453-1.463	0.894-0.904	1			1	4		579	1934
2,6-nonadienal	3	95	異性体合算			1.468-1.478	0.860-0.875	5			2,6	5	6	946	1942
2,4-nonadienal	3	90				1.516-1.526	0.869-0.879	5				4,5		1113	1941
3,6-nonadienol	4	95				1.462-1.473	0.865-0.875					3	3	365	1948
cis,cis-3,6-nonadienol	4	95				1.463-1.473	0.866-0.876				3	3	3	429	1948
2,6-nonadienol	4	95				1.461-1.471	0.863-0.883				1,2			918	1950
nonanal dimethyl acetal	1	98				1.418-1.424	0.847-0.853	1				1,4,5		593	1956
2-nonanol	2	97				1.425-1.435	0.821-0.831				1,3,6	3,4,5	3,6	635	1962

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
cis-3-nonenol	4	93				1.443-1.453	0.840-0.850				6	4,5		1030	1974
2-nonenol	4	97				1.441-1.451	0.840-0.850				5	4,5		1142	1977
cis-6-nonenyl acetate	3	93				1.432-1.442	0.885-0.895	1			3	3	3(C)	1120	1979
cis-9-octadecenyl acetate	3	92				1.448-1.453	0.868-0.874	1			1,3	1,3	1	396	2067
4,5-octanedione	2	95				1.414-1.424	0.908-0.918				3	3	3	664	3174
2-octanol	2	95				1.421-1.431	0.815-0.825				1,3	3,4,5	3,6	1054	2020
1-octen-3-yl acetate	3	95				1.418-1.428	0.873-0.883	1			2	4		1126	2026
2-octen-4-one	4	90				1.439-1.449	0.844-0.864				1	4,5	1	998	2030
trans-2-octenol	4	97				1.441-1.449	0.839-0.846				2	1,4	1	1128	2037
octyl butyrate	1	98				1.421-1.427	0.861-0.867	1			1,3	3,4,5	3,6	1011	2048
octyl isovalerate	1	95				1.420-1.430	0.850-0.860	1			1,3,5	3,5	3	678	2057
oleic acid	4		97-104			1.455-1.465	0.889-0.899				1,3,6	3,4,5	3,6	18	2065
4-oxoisophorone	4	98		MP	22-26	1.487-1.497	1.030-1.040					4,5		719	2071
4-pentenyl isothiocyanate	4	95				1.513-1.519	0.970-0.976				3	3	3	83	2086
perillyl acetate	3	90				1.474-1.487	0.981-0.991	1				4	1	661	2097
phenethyl formate	1	95				1.503-1.513	1.060-1.070	2			3	3,4	1,3	648	2110
phenethyl hexanoate	1	97				1.483-1.489	0.970-0.976	1			6	4,5	1,6	1066	2112
phenethyl isothiocyanate	2	97				1.585-1.595	1.090-1.100				1,3,6	1,3,4	1,3	379	2114
phenethyl octanoate	1	98				1.480-1.486	0.953-0.959	1				4	1,6	644	2119
phenethyl propionate	1	98				1.490-1.500	1.011-1.019	1			5	4,5	1	619	2122
phenethyl salicylate	9,17	98		MP	41-46			1		10	1,2,5	4,5		660	2123
phenethyl tiglate	3	98				1.511-1.517	1.017-1.023	1				4	1	576	2125
1-phenyl-1,2-propanedione	2	96				1.527-1.537	1.095-1.107				1,3,5,6	3,4,5	3,6	1146	2141
2-phenyl-2-butenal	3	95				1.553-1.566	1.024-1.039	10				4	1	1105	2142
phenylacetaldehyde	1		95			1.522-1.532	1.028-1.038	5			2,3,5,6	3,4,5	1	257	2146
phenylacetaldehyde diisobutyl acetal	1	97				1.468-1.474	0.916-0.922	1			1	4		373	2148
phenylacetaldehyde glyceryl acetal	1	95				1.527-1.537	1.155-1.165	1					1	1158	2150
2-phenylpropanal	1	95				1.513-1.523	1.000-1.013	3			1,2,3,5	4,5	6	1154	1229
3-phenylpropionic acid	10,18	98		MP	46-50					10	1,3,5,6	3,5	3,6	985	2159
3-phenylpropyl butyrate	1	98				1.487-1.493	0.983-0.989	1			1,6	5	6	680	2162
phytol	4	95				1.460-1.470	0.850-0.863				3	4	3	651	2173
beta-pinene	4	95				1.473-1.483	0.867-0.877				6	4,5	1,6	79	2177
pinocarvyl isobutyrate	3	90				1.466-1.476	0.959-0.969	1			3	3	3	326	3567
propyl 4-methylpentanoate	1	98				1.410-1.416	0.866-0.872	1			1,2			688	2229
propyl formate	1	96				1.372-1.382	0.902-0.912	1			1,2,3	3,4,5	3,6	294	2224
propyl isovalerate	1	98				1.401-1.409	0.861-0.867	1			1,3,5,6	3,5	3,6	673	2230
propyl lactate	1	98				1.414-1.420	1.003-1.009	1			3	4	3	1153	2231
propyl octanoate	1	98				1.418-1.425	0.862-0.868	1				4		598	2235
propyl sorbate	3	98				1.488-1.494	0.922-0.928	1			3	3	3	264	2241
propyl valerate	1	98				1.404-1.410	0.868-0.874	1			3,5	3,4,5	3	679	2244
propyleneglycol dioctanoate	1	98				1.436-1.442	0.923-0.929	1			3	3	3	707	2248
propyleneglycol dipropionate	1	98				1.415-1.421	1.009-1.015	1				4		1016	2249
rose oxide	4	95	異性体合算			1.450-1.460	0.867-0.883					4	1	388	2278
santalyl acetate	3		96 (異性体合算)			1.482-1.492(25C)	0.982-0.992(25C)	1			1,2			979	2286
sclareolide	9,17	98		MP	121-125			1		10	1,2,6	2	1,6	1088	2289
4-terpineol	4	90				1.475-1.485	0.932-0.942				1,3	3,4,5	3	114	2320
terpinolene	4	88				1.480-1.500	0.855-0.872				5	4,5		220	2325
terpinyl propionate	3	98	異性体合算			1.462-1.468	0.948-0.957	1			1,2	4		953	2335

表示名	判断樹番号	含量(%)(GC)	含量(%)(GC以外・成分情報)	融点区分*1	融点又は凝固点(℃)	屈折率(20℃)	比 重(20℃)	酸価	旋光度又は比旋光度(°)	重金属(μg/g)	確認試験*2 IR	MS	NMR	使用量順位	H12-SEQ
2-tetrahydrofurfuryl acetate	1	96				1.430-1.440	1.053-1.067	1			3	3,4	1,3	667	2353
2-tetrahydrofurfuryl alcohol	2	97				1.446-1.456	1.051-1.059				1,2,3,5,6	3,4,5	3,6	647	2354
2-thienylmethanethiol	2	98				1.601-1.606	1.203-1.213					4		983	2371
thiophene	2	98				1.524-1.530	1.062-1.068				3,6	3,4,5	3,6	996	2384
trans-2-tridecenal	3	94				1.455-1.465	0.844-0.854	5			1,2,6			995	2413
3,5,5-trimethylhexanol	2	90				1.428-1.442	0.821-0.835				1,3	3,4	3,6	604	2437
2,4-undecadienal	3	95	異性体合算			1.507-1.517	0.863-0.873	10					1	976	2448
10-undecen-2-one	4	90				1.437-1.442	0.840-0.850					4		1026	3016
10-undecenal	3	90				1.439-1.450	0.840-0.856	10			1,2,3,6	3,4	3,6	595	2464
trans-2-undecenal	3	95				1.451-1.461	0.842-0.852	5				4,5	1	1060	2466
10-undecenoic acid	12,20	97		MP	22-28					10	1,3,5	3,4,5	3	670	2470
valeraldehyde dibutyl acetal	1	97				1.417-1.423	0.833-0.839	1			3	1,3	3	615	2478
zingerone	10,18	95		MP	38-44	1.537-1.547	1.136-1.146			10	1,5	4,5		704	2512

*1 融点区分

MP ・・・ Melting point　融点
SP ・・・ Solidification point　凝固点

*2 参照スペクトルデータベース番号

1) FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)
2) 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)
3) 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)
4) Wiley's Registry of Mass spectral Database
5) NIST/EPA/NIH Mass Spectral Library
6) Sigma-Aldrich カタログ

*3 融点設定基準

固体化合物において、最終精製時は液体の為比重・屈折率の規格が存在するが、通常流通時には固体の為調査時に流通規格が得られなかったものについて、実測し規格設定した。

資料－５

平成１８年度作成
日本香料工業会
食品香料化合物参考規格集

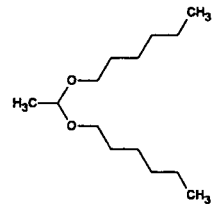
Acetaldehyde dihexyl acetal

ｱｾﾄｱﾙﾃﾞﾋﾄﾞ ｼﾞﾍｷｼﾙ ｱｾﾀｰﾙ

化学式　C14H30O2

分子量　230.39

CAS　No. 5405-58-3



SEQ　No. 19　エーテル類

FEMA　No.

JECFA No.

規格項目	JFFMA参考規格	参考1:JECFA規格	参考2:FCC規格
名称	Acetaldehyde dihexyl acetal		
含量	95.0 % 以上(GC法)		
比重	0.834-0.844 (d20/20)		
屈折率	1.418-1.428 (n20D)		
酸価	1.0 以下		
融点･凝固点	-		
旋光度(°)	-		
重金属	-		
溶状			
確認試験*	IR　:- MS　:4,5 NMR　:-		

*確認試験の参照文献番号

1). FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)

2). 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)

3). 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)

4). Wiley's Registry of Mass spectral Database

5). NIST/EPA/NIH Mass Spectral Library

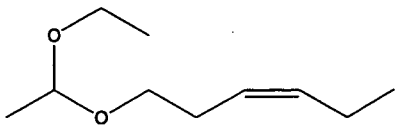
6). Sigma-Aldrich

Acetaldehyde ethyl cis-3-hexenyl acetal

ｱｾﾄｱﾙﾃﾞﾋﾄﾞ ｴﾁﾙ cis-3-ﾍｷｾﾆﾙ ｱｾﾀｰﾙ

化学式　C10H20O2

分子量　172.26



CAS No. 28069-74-1

SEQ No. 25　エーテル類

FEMA No. 3775

JECFA No. 943

規格項目	JFFMA参考規格	参考1:JECFA規格	参考2:FCC規格
名称	Acetaldehyde ethyl cis-3-hexenyl acetal	acetaldehyde ethyl cis-3-hexenyl acetal	
含量	98.0 % 以上(GC法)	min. 97 %	
比重	0.848-0.856 (d20/20)	0.846-0.856 (d25/25)	
屈折率	1.419-1.430 (n20D)	1.430-1.435 (n20D)	
酸価	2.0 以下	max. 2.0	
融点･凝固点	-	-	
旋光度(°)	-	-	
重金属	-	-	
溶状		Solubility in ethanol : miscible at room temperature	
確認試験*	IR :1,3 MS :3,4,5 NMR :	ID Test : IR	

*確認試験の参照文献番号

1). FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)

2). 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)

3). 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)

4). Wiley's Registry of Mass spectral Database

5). NIST/EPA/NIH Mass Spectral Library

6). Sigma-Aldrich

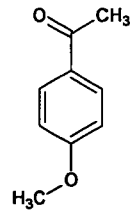
Acetanisole

アセトアニソール

化学式　C9H10O2

分子量　150.17

CAS　No. 100-06-1



SEQ　No. 38　ケトン類

FEMA　No. 2005

JECFA No. 810

規格項目	JFFMA参考規格	参考1:JECFA規格	参考2:FCC規格
名称	Acetanisole	Acetanisole	Acetanisole
含量	97.0 % 以上(GC法)	min. 97 % sum of o,m,p- isomers	min. 98.0 % GC(M-1b)
比重	-	-	-
屈折率	-	-	-
酸価	-	-	-
融点・凝固点	MP : 36.0 to 42.0℃	MP : 36 to 38℃	-
旋光度(°)	-	-	-
重金属	10.0 mg/ kg 以下		Lead max : 10.0mg/kg
溶状		Solubility in ethanol : very soluble	Solubility in alcohol : 1 g in 5mL 50% alc
備考			Chlorinated Cmpds. - passes test
確認試験*	IR　:1,2,3,5,6 MS　:3,4,5 NMR　:3,6	ID Test : IR	ID Test: IR

*確認試験の参照文献番号

1). FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)

2). 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)

3). 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)

4). Wiley's Registry of Mass spectral Database

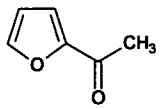
5). NIST/EPA/NIH Mass Spectral Library

6). Sigma-Aldrich

2-Acetylfuran

2-アセチルフラン

化学式　C6H6O2



分子量　110.11

CAS　No. 1192-62-7

SEQ　No. 77　ケトン類

FEMA　No. 3163

JECFA No. 1503

規格項目	JFFMA参考規格	参考1:JECFA規格	参考2:FCC規格
名称	2-Acetylfuran	2-Furyl methyl ketone	2-Furyl Methyl Ketone
含量	95.0 % 以上(GC法)	min. 97 %	min. 97.0 % GC(M-1b)
比重	-	1.102-1.107 (d25/25)	1.102-1.107 (d25/25)
屈折率	-	1.505-1.510 (n20D)	1.505-1.510 (n20D)
酸価	-	max. 1.0	-
融点・凝固点	SP : 27.0 to 34.0℃	-	-
旋光度(°)	-	-	-
重金属	10.0 mg/ kg 以下		-
溶状		Solubility in ethanol : Soluble	Solubility in alcohol : 1mL in 2mL 95% ethanol
確認試験*	IR　:1,2,3,5,6 MS　:3,4,5 NMR　:3,6	ID Test : IR	ID Test: IR

*確認試験の参照文献番号

1). FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)

2). 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)

3). 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)

4). Wiley's Registry of Mass spectral Database

5). NIST/EPA/NIH Mass Spectral Library

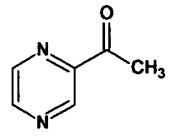
6). Sigma-Aldrich

Acetylpyrazine

アセチルピラジン

化学式　C6H6N2O

分子量　122.12



CAS　No. 22047-25-2

SEQ　No. 78　ケトン類

FEMA　No. 3126

JECFA No. 784

規格項目	JFFMA参考規格	参考1:JECFA規格	参考2:FCC規格
名称	Acetylpyrazine	Acetylpyrazine	2-Acetylpyrazin
含量	99.0 % 以上(GC法)	min. 99 %	min. 99.0 % GC(M-1a)
比重	-	-	-
屈折率	-	-	-
酸価	-	-	-
融点・凝固点	MP : 75.0 to 80.0℃	MP : 74 to 80℃	MP : 75 to 78℃
旋光度(°)	-	-	-
重金属	10.0 mg/ kg 以下		-
溶状		Solubility in ethanol : moderately soluble	Solubility in alcohol : 1 g in 20 mL 95% alc
確認試験*	IR　:1,2,3,5,6 MS　:3,4,5 NMR　:3,6	ID Test : IR	ID Test: IR

*確認試験の参照文献番号

1). FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)

2). 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)

3). 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)

4). Wiley's Registry of Mass spectral Database

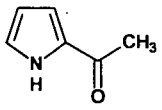
5). NIST/EPA/NIH Mass Spectral Library

6). Sigma-Aldrich

2-Acetylpyrrole

2-アセチルピロール

化学式　C6H7NO



分子量　109.13

CAS　No. 1072-83-9

SEQ　No. 82　ケトン類

FEMA　No. 3202

JECFA No. 1307

規格項目	JFFMA参考規格	参考1:JECFA規格	参考2:FCC規格
名称	2-Acetylpyrrole	Methyl 2-pyrrolyl ketone	2-Acetylpyrrole
含量	97.0 % 以上(GC法)	min. 97 %	min. 98.0 % GC(M-1a)
比重	-	-	-
屈折率	-	-	-
酸価	-	-	-
融点・凝固点	MP : 87.0 to 93.0℃	MP : 87 to 93℃	MP : 88 to 92℃
旋光度(°)	-	-	-
重金属	10.0 mg/ kg 以下		-
溶状		Solubility in ethanol : Soluble	Solubility in alcohol : 1 g in 6 mL ethanol
備考			Residue on Ignit.:0.3%
確認試験*	IR　:3,6 MS　:3,4,5 NMR　:1,3,6	ID Test : NMR	

*確認試験の参照文献番号

1). FAO/WHO合同食品添加物専門家委員会(Joint FAO/WHO Expert Committee on Food Additive;JECFA)

2). 米国食品化学物質規格集(Food Chemicals Codex 5th Edition; FCC)

3). 有機化合物のスペクトルデータベース SDBS(独立行政法人産業技術総合研究所)

4). Wiley's Registry of Mass spectral Database

5). NIST/EPA/NIH Mass Spectral Library

6). Sigma-Aldrich