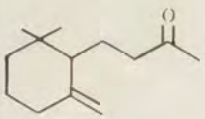
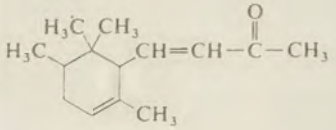
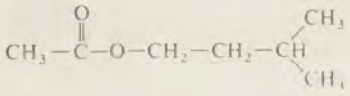
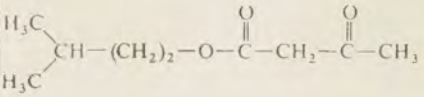
	γ-Ionone	α-Irone
Other names	4-(2,2-Dimethyl-6-methylenecyclohexyl)-3-buten-2-one	*cis*-(2,6)-*cis*-(2¹,2²)-α-Irone 6-Methyl-α-ionone 4-(2,5,6,6-Tetramethyl-2-cyclohexen-1-yl)-3-buten-2-one
Empirical formula	$C_{13}H_{20}O$	$C_{14}H_{22}O$
Structure		
Physical/chemical characteristics[5]		The physical constants refer to those usually encountered for a commercial product.
Appearance	Liquid	Yellowish liquid
Assay		98% min
Molecular weight	192.30	206.33
Boiling point		110-112°C at 3.2 mm Hg (synthetic)
Specific gravity	0.932 at 20°C	0.932–0.936 at 25°C; 0.9349 at 20°C from orris root; 0.9355 at 20°C synthetic
Refractive index	1.4999 at 25°C	1.5020-1.5030 at 20°C; 1.5003 at 30°C from orris root; 1.4970 at 20°C synthetic
Optical rotation		−226°0′ at 20°C (from orris root)
Solubility		1:4 in 70% alcohol
Organoleptic characteristics		Characteristic orris and violet-like odor
Synthesis	By condensation of cyclogeranic aldehyde with acetone, followed by separation from the β-ionone-rich reaction mixture[6]	See references 8, 9, and 10. The commercial product corresponds generally to the α-isomer
Natural occurrence	Not reported found in nature; dihydro-γ-ionone has been reported as a constituent in ambergris oil[7]	For structure and isomers see References 11, 12, and 13. Occurs in orris root, raspberry, and some flowers of *Pittosporum* sp.
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Candy 10.0 ppm Gelatins and puddings 10.0 ppm	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 2.3 ppm Candy 4.1 ppm Baked goods 5.4 ppm Chewing gum 1.4 ppm
Regulatory status:	FEMA No. 3175	FDA 121.1164; FEMA No. 2597

REFERENCES

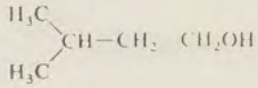
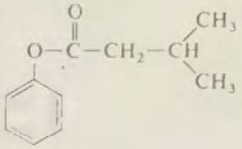
For References 1–5, see end of Part III.

6. Willhalm, Steiner and Schinz, *Helv. Chim. Acta*, 41, 1359, 1958.
7. Ruzička, Seidel and Pfeiffer, *Helv. Chim. Acta*, 31, 827, 1948.
8. Schinz et al., *Helv. Chim. Acta*, 30, 1810, 1947.
9. Barton and Mousseron-Canet, *J. Chem. Soc.* (London), p. 271, 1960.
10. Eschinazi, *J. Am. Chem. Soc.*, 81, 2905, 1959.
11. Ruzicka et al., *Helv. Chim. Acta*, 30, 2168, 1947.
12. Naves and Bachmann, *Helv. Chim. Acta*, 30, 2222, 1957.
13. Gildemeister and Hoffmann, *Die Aetherischen Oele*, Vol. 3c, Akademie Verlag, 1963, 305.

	Isoamyl acetate	Isoamyl acetoacetate
Other names	Common amyl acetate β-Methylbutyl acetate (In commercial practice *amyl* invariably means *isoamyl*, unless it is prefaced by the *n*- for normal.)	Isoamyl β-ketobutyrate Isoamyl 3-oxobutanoate
Empirical formula	$C_7H_{14}O_2$	$C_9H_{16}O_3$
Structure		
Physical chemical characteristics[1]		
Appearance	Colorless liquid	Colorless liquid
Assay	95% min[2]	
Molecular weight	130.18	172.23
Melting point	−78.5°C	
Boiling point	142.5°C; 30°C at 2 mm Hg	222–224°C
Specific gravity	0.868–0.878[2] at 25°/25°C	0.954 at 10°C
Refractive index	1.4000–1.4040 at 20°C;[2] 1.4017 at 18°C	
Acid value	Not more than 1[2]	
Solubility	1:3 and more in 60% alcohol; almost insoluble in water; soluble in ether and most common organic solvents	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Powerful, fruity odor with a bittersweet taste reminiscent of pear; if impure, the odor is strong, penetrating, and almost shocking	Ethereal, sweet, winey odor; green-apple flavor
Synthesis	Usually prepared by esterification of commercial isoamyl alcohol with acetic acid	By transesterification of ethyl acetylacetate with isoamyl alcohol in the presence of sodium
Natural occurrence	Reported found in the volatile portion of banana fruit and cocoa bean	
Reported uses[3]	Non-alcoholic beverages 28 ppm Ice cream, ices, etc. 56 ppm Candy 190 ppm Baked goods 120 ppm Gelatins and puddings 100 ppm Chewing gum 2700 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2055	FDA 121.1164

REFERENCES

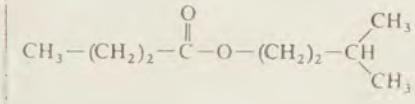
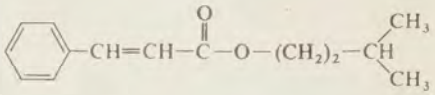
For References 1–5, see end of Part III.

	Isoamyl alcohol	Isoamyl benzoate
Other names	Isobutyl carbinol Isopentyl alcohol 3-Methyl-1-butanol	Isopentyl benzoate
Empirical formula	$C_5H_{12}O$	$C_{12}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily, clear liquid	Colorless liquid
Assay		99% min
Molecular weight	88.15	192.26
Melting point	117.2 C	
Boiling point	132 C	261–262°C
Flash point		100°C
Specific gravity	0.812 at 20°C	0.986–0.990 at 25°/25°C; 0.9910 at 17.4 C
Refractive index	1.4084 at 17.8°C	1.492–1.495 at 20°C; 1.4950 at 17.4°C
Acid value		1 max
Solubility	Soluble in water; soluble in most organic solvents	Insoluble in water; soluble 1:3 in 80% alcohol
Organoleptic characteristics	Characteristic pungent odor and repulsive taste	Fruity, slightly pungent odor
Synthesis	Industrially prepared by rectification of fusel oil	By transesterification of methyl benzoate and isoamyl alcohol in the presence of potassium isoamylate;[9] also by heating benzoyl chloride and isoamyl acetate[10]
Natural occurrence	Constitutes the major portion of fusel oil; also known as fermentation amyl alcohol. It has been identified as an ester among the constituents of Roman camomile oil,[6] and in several essential oils: French peppermint, Java citronella, Reunion geranium, tea, *Teucrium chamaedrys*,[7] *Eucalyptus amigdalina*, *Achillea ageratum*, *Artemisia camphorata*, and others; also in the aromas of strawberry and raspberry; identified in rum.[8]	In vinegar; in cocoa
Reported uses[3]	Non-alcoholic beverages 17 ppm Alcoholic beverages 100 ppm Ice cream, ices, etc. 7.6 ppm Candy 52 ppm Baked goods 24 ppm Gelatins and puddings 46 ppm Chewing gum 300 ppm	Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 2.5 ppm Candy 3.5 ppm Baked goods 7.4 ppm Gelatins and puddings 4.6 ppm Chewing gum 200 ppm
Regulatory status	FDA 121.1164; FEMA No. 2057	FDA 121.1164; FEMA No. 2058

REFERENCES

For References 1–5, see end of Part III.

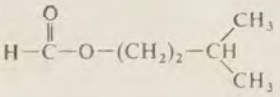
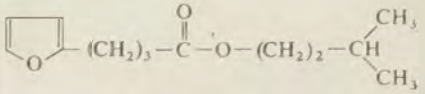
6. Kobig, *Justus Liebigs Ann. Chem.*, 195, 92, 1879.
7. Rovesti, *Ind. Parfum.*, 12, 334, 1957.
8. Fenaroli et al., *Riv Ital. EPPOS*, 9, 484, 1965; 2, 75, 1966.
9. Reimer and Downes, *J. Am. Chem. Soc.*, 43, 949, 1921.
10. Zetsche, *Helv. Chim. Acta*, 9, 181, 1926.

	Isoamyl butyrate	Isoamyl cinnamate
Other names	Isopentyl butyrate	Isoamyl β-phenylacrylate Isoamyl 3-phenylpropenoate Isopentyl cinnamate
Empirical formula	$C_9H_{18}O_2$	$C_{14}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to pale-yellow liquid
Assay	98% min[2]	98% min[2]
Molecular weight	158.24	218.29
Boiling point	177–178°C	
Flash point	65°C	
Specific gravity	0.860–0.864 at 25°/25°C;[2] 0.8642 at 20°C	0.992–0.997 at 25°/25°C;[2] 0.9995–1.0015 at 15°C
Refractive index	1.4090–1.4140 at 20°C;[2] 1.4110 at 20°C	1.5350–1.5390[2] (1.5360–1.5375) at 20°C
Acid value	Not more than 1[2]	Not more than 1.0[2] (0.2)
Solubility	1:4 and more in 70% alcohol[2]	1:7 in 80% alcohol[2]
Organoleptic characteristics	Strong, characteristic, fruity (pear-like) odor; sweet, corresponding taste	Balsamic odor reminiscent of cocoa
Synthesis	Usually prepared by esterification of commercial isoamyl alcohols with butyric acid by heating in the presence of Twitchell reagent;[6] or by fermentation from butyric acid and isoamyl alcohol[7,8]	By esterification of cinnamic acid with commercial isoamyl alcohols, which vary in isomer distribution according to source
Natural occurrence	Reported found in the oil of *Eucalyptus macarthuri* and in coconut oil; also identified in cocoa bean and in cider	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 13 ppm Ice cream, ices, etc. 34 ppm Candy 79 ppm Baked goods 51 ppm Gelatins and puddings 60 ppm Chewing gum 570 ppm	Non-alcoholic beverages 3.1 ppm Ice cream, ices, etc. 4.2 ppm Candy 13 ppm Baked goods 13 ppm
Regulatory status	FDA 121.1164; FEMA No. 2060	FDA 121.1164; FEMA No. 2063

REFERENCES

For References 1–5, see end of Part III.

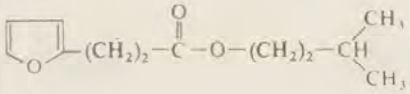
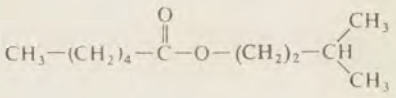
6. **Zaganiaris and Varvoglis,** *Ber. Dtsch. Chem. Ges.*, 69, 2280, 1936.
7. **Rona and Ammon,** *Werner Biochem.* 221, 385, 1930; **Rona and Muhlbock,** *Werner Biochem.*, 223, 139, 1930.
8. **Mardaschew,** *Arh. Biol. Nauka*, 37, 399, 1935.

	Isoamyl formate	Isoamyl-2-furanbutyrate
Other names	Isopentyl formate	2-Furanbutyric acid, isoamylester Isoamyl furfurylpropionate α-Isoamyl furfurylpropionate Isopentyl-2-furanbutyrate
Empirical formula	$C_6H_{12}O_2$	$C_{13}H_{20}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Pale-yellow liquid
Assay	92% min (97% min)	
Molecular weight	116.16	224.30
Boiling point	123–124°C	
Flash point	53°C	
Specific gravity	0.878–0.885 at 25°C; 0.8870–0.8900 at 15°C	
Refractive index	1.3960–1.4000 (1.3970–1.3990) at 20°C	
Acid value	2 max (0.9)	
Solubility	Soluble in alcohol; slightly soluble in water; miscible with ether	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Fruity, characteristic odor suggestive of black currant and plum with a corresponding sweet taste	Sweet, buttery, fruity odor; caramel-like flavor
Synthesis	By reacting concentrated H_2SO_4 over a mixture of isoamyl alcohols and sodium formate[6]	From furfural
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 8.4 ppm Ice cream, ices, etc. 14 ppm Candy 22 ppm Baked goods 16 ppm Gelatins and puddings 2.0–28 ppm Chewing gum 250 ppm	Non-alcoholic beverages 0.03–5.0 ppm Ice cream, ices, etc. 2.8 ppm Candy 6.0 ppm Baked goods 0.50–8.0 ppm Gelatins and puddings 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2069	FDA 121.1164; FEMA No. 2070

REFERENCES

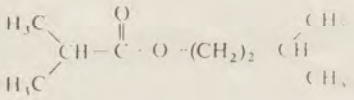
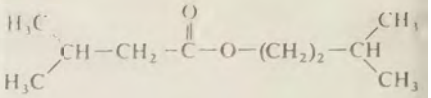
For References 1–5, see end of Part III.

6. Wagner, German Patent 529,135, 1929.

	Isoamyl-2-furanpropionate	Isoamyl hexanoate
Other names	2-Furanpropionic acid, isoamylester Isoamyl furfurhydracrylate α-Isoamyl furfurylacetate Isopentyl-2-furanpropionate	Isoamyl caproate Isoamyl capronate Isoamyl hexylate Isopentyl hexanoate
Empirical formula	$C_{12}H_{18}O_3$	$C_{11}H_{22}O_2$
Structure		
Physical/chemical characteristics[4]		
Appearance	Pale-yellow liquid (colorless when freshly made)	Colorless liquid
Assay		98% min[2]
Molecular weight	210.27	186.30
Boiling point		94–96 C at 10 mm Hg
Flash point		88 C
Specific gravity		0.858–0.863 at 25/25 C;[2] 0.8650–0.8670 at 15 C
Refractive index		1.4180–1.4220[2] (1.4195–1.4205) at 20 C
Acid value		Not more than 1.0[2] (0.2)
Solubility	Insoluble in water; soluble in alcohol	1:3 in 80% alcohol;[2] insoluble in water
Organoleptic characteristics	Sweet, green, slightly floral odor with a distinct fruital note; similar flavor	Fruity odor
Synthesis	From furfurhydracrylic acid with isoamyl alcohol	By esterification of caproic acid with the isomeric amyl alcohols obtained from fusel oil and other sources
Natural occurrence	Not reported found in nature	Reported found in fermentation products (wine) and the rind of California orange
Reported uses[3]	Non-alcoholic beverages 0.02–0.33 ppm Ice cream, ices, etc. 0.33–0.65 ppm Candy 1.6–3.6 ppm Baked goods 1.6–3.6 ppm	Non-alcoholic beverages 7.8 ppm Ice cream, ices, etc. 14 ppm Candy 17 ppm Baked goods 15 ppm Gelatins and puddings 3.7 ppm
Regulatory status	FDA 121.1164; FEMA No. 2071	FDA 121.1164; FEMA No. 2075

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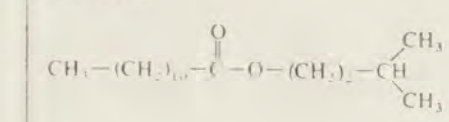
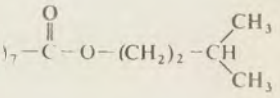
For References 1–5, see end of Part III.

	Isoamyl isobutyrate	Isoamyl isovalerate
Other names		Isopentyl isovalerate
Empirical formula	$C_9H_{18}O_2$	$C_{10}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid
Assay	98% min	97.5% min
Molecular weight	158.24	172.27
Boiling point	170°C	193°C
Flash point		72°C
Specific gravity	0.8620–0.8690 at 15°C; 0.8627 at 20°C	0.8600–0.8625 at 15°C; 0.8583 at 18.7°C
Refractive index	1.4070–1.4110 at 20°C	1.4125–1.4135 at 20°C; 1.4100 at 25°C
Acid value	0.09 max	0.09 max
Solubility		1:6.5–8 in 70% alcohol; insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Fruity odor with an undertone reminiscent of apricot and pineapple	Characteristic fruity odor and sweet apple-like flavor
Synthesis	By passing vapors of isobutyl alcohol and isoamyl alcohol over an Ag-activated Cu-MnO catalyst[6]	By passing vapors of isoamyl alcohol and isovaleric aldehyde over a copper uranium based catalyst at 240–280°C in the presence of hydrogen[7]
Natural occurrence	Not reported found in nature	Reported found in banana fruits,[8] in the ether oil from leaves of *Eucalyptus microcorys*,[9] in wine, oil of hop, and olive oil
Reported uses[3]		Non-alcoholic beverages 8.5 ppm Ice cream, ices, etc. 14 ppm Candy 33 ppm Baked goods 41 ppm Gelatins and puddings 1.0–61 ppm Chewing gum 390 ppm Jellies 10 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2085

REFERENCES

For References 1–5, see end of Part III.

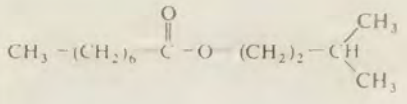
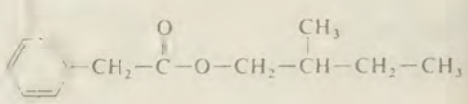
6. Wasskewitch and Bulanova, *Zh. Obshch. Khim.*, 8, 1096, 1938.
7. Abramow and Dolgow, *Chem. Abstr.*, 34, 7847, 1940; 42, 1561, 1948.
8. Kothenbach and Eberlein, *Chem. Zentralbl.*, 1, 1105, 1905.
9. Jones and Lahey, *Proc. R. Soc. Queensl.*, 50, 44, 1939.

	Isoamyl laurate	Isoamyl nonanoate
Other names	Isoamyl dodecanoate Isoamyl dodecylate Isopentyl laurate	Isoamyl nonylate Isoamyl pelargonate Isopentyl nonanoate Nonate
Empirical formula	$C_{17}H_{34}O_2$	$C_{14}H_{28}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless, oily liquid
Molecular weight	270.46	228.37
Boiling point		260–265°C
Specific gravity		0.86
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Very faint, oily, fatty odor; fatty flavor	Nutty, oily, apricot-like odor; fruity, winey, cognac-rum flavor
Synthesis		From isoamyl alcohol and pelargonic acid
Natural occurrence	Reported found at the 3% level in fusel oil from raisins[6,7]	In banana and strawberry
Reported uses[3]	Non-alcoholic beverages 0.04–3.0 ppm Ice cream, ices, etc. 0.16–6.0 ppm Candy 0.50–6.0 ppm Baked goods 0.50–6.0 ppm Also used as a solvent for various flavors and fragrances	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 3.3 ppm Candy 3.0 ppm Baked goods 4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2077	FDA 121.1164; FEMA No. 2078

REFERENCES

For References 1–5, see end of Part III.

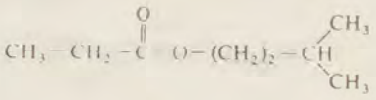
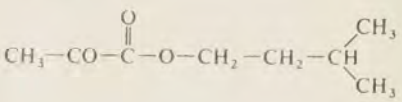
6. **Kepner and Webb**, *Am. J. Enol. Vitic.*, 12, 159, 1961.
7. **Kepner and Webb**, *Chem. Abstr.*, 56, 7798b, 1962.

	Isoamyl octanoate	Isoamyl phenylacetate
Other names	Isoamyl caprylate Isoamyl octylate Isopentyl octanoate	Isoamyl α-toluate Isopentyl phenylacetate
Empirical formula	$C_{13}H_{26}O_2$	$C_{13}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid
Assay	98% min[2]	98% min
Molecular weight	214.35	206.28
Boiling point		265–266 C at 723 mm Hg
Flash point	104 C	>100 C
Specific gravity	0.855–0.861 at 25°/25°C;[2] 0.8620–0.8660 at 15°C	0.975–0.977 at 25°/25°C; 0.982 at 20°C
Refractive index	1.4250–1.4290 at 20°C[2]	1.4850–1.4870 at 20°C; 1.4872 at 21°C
Acid value	Not more than 1.0[2] (0.2)	1 max
Solubility	1:7–10 in 80% alcohol[2]	1:3 in 80% alcohol
Organoleptic characteristics	Fruity odor	Sweet, pleasant odor reminiscent of cocoa with a slight birch-tar undertone
Synthesis	By esterification of octanoic acid with commercial isoamyl alcohols, which vary in isomer distribution according to source	By esterification of phenylacetic acid with isoamyl alcohol in the presence of concentrated sulfuric acid;[6] by heating benzyl nitrile and isoamyl alcohol in the presence of excess concentrated H_2SO_4
Natural occurrence	Reported found in wine, banana, strawberry, and apple	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 6.6 ppm Ice cream, ices, etc. 5.1 ppm Candy 7.4 ppm Baked goods 3.5 ppm Gelatins and puddings 2.1 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 16 ppm Candy 12 ppm Baked goods 14 ppm Gelatins and puddings 0.15–3.4 ppm Toppings 0.25–0.80 ppm
Regulatory status	FDA 121.1164; FEMA No. 2080	FDA 121.1164; FEMA No. 2081

REFERENCES

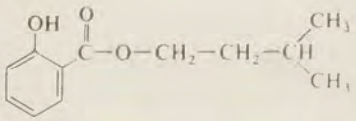
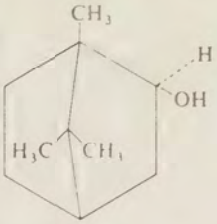
For References 1–5, see end of Part III.

6. Guye and Chavanne, *Bull. Soc. Chim. Fr.*, 3(15), 292, 1896.

	Isoamyl propionate	Isoamyl pyruvate
Other names	Isopentyl propionate	Isoamyl α-ketopropionate Isoamyl 2-oxopropanoate Isopentyl pyruvate
Empirical formula	$C_8H_{16}O_2$	$C_8H_{14}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Assay	98% min[2]	
Molecular weight	144.21	158.20
Boiling point	160 C	185 C; 86 C at 14 mm Hg
Flash point	41 C	
Specific gravity	0.866–0.871 at 25°/25°C;[2] 0.8720–0.8760 at 15°C	0.978 at 17 C
Refractive index	1.4050–1.4090 at 20°C[2]	
Acid value	Not more than 1.0[2] (0.2)	
Solubility	1:3 in 70% alcohol;[2] insoluble in water; soluble in most organic solvents	
Organoleptic characteristics	Apricot-pineapple odor. The taste is somewhat harsh when freshly distilled but subsequently yields a pleasant apricot-plum bittersweet flavor.	
Synthesis	By esterification of propionic acid with the isomeric amyl alcohols obtained from fusel oil and other sources	By air oxidation of boiling isoamyl lactate; also by reacting methyl magnesium iodide over isoamyl α-hydroxy isobutyrate
Natural occurrence	Reported found in cocoa bean and Bulgarian peppermint	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.8 ppm Ice cream, ices, etc. 13 ppm Candy 38 ppm Baked goods 6.1 ppm Gelatins and puddings 0.80–3.7 ppm Chewing gum 750 ppm	Non-alcoholic beverages 4.7 ppm Ice cream, ices, etc. 8.1 ppm Candy 9.2 ppm Baked goods 12 ppm
Regulatory status	FDA 121.1164; FEMA No. 2082	FDA 121.1164; FEMA No. 2083

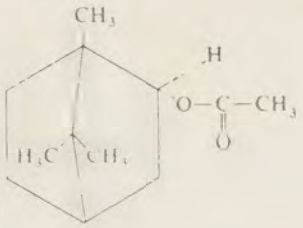
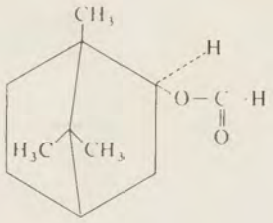
REFERENCES

For References 1–5, see end of Part III.

	Isoamyl salicylate	Isoborneol
Other names	Isoamyl 2-hydroxybenzoate Isoamyl *o*-hydroxybenzoate Isopentyl salicylate (Known commercially as amyl salicylate)	Isobornyl alcohol Isocamphol
Empirical formula	$C_{12}H_{16}O_3$	$C_{10}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	White, crystalline solid
Assay	98% min[2] (99% min)	92% min[2]
Molecular weight	208.26	154.24
Melting point		212–213°C (*d*-214–217°C; *l*-212–214°C)
Boiling point	273°C; 151–152°C at 15 mm Hg	
Flash point	133°C	
Specific gravity	1.047–1.053 at 25/25°C;[2] 1.065 at 15°C	
Refractive index	1.5050–1.5085 at 20°C;[2] 1.505 at 20°C	
Acid value	Not more than 1[2]	
Optical rotation		−30.6° at 19°C (*l*-form from alcohol); +33.89°C (*d*-form from alcohol); −19.6° at 15°C (*l*-form from toluene)
Solubility	1:2 to 1:3 in 90% alcohol;[2] very slightly soluble in water	1 gm in 2 ml of 70% alcohol[2]
Organoleptic characteristics	Characteristic aromatic, strong, herbaceous, persistent odor; bittersweet taste reminiscent of strawberry	Piney, camphoraceous odor
Synthesis	By esterification of salicylic acid with the isomeric amyl alcohols obtained from fusel oil and other sources	By the hydrolysis of isobornyl acetate,[2] or by catalytic reduction of camphor (both *d*- and *l*-isomers). The optically inactive compound can be prepared by treating camphene with a 1:1 mixture of sulfuric acid and glacial acetic acid[6] and then hydrolyzing the isobornyl acetate.
Natural occurrence	Not reported found in nature	Rarely found in nature (in the oil of *Abies sibirica* and a few other essences); probably present in the essential oil from roots of *Chamaeciparis formosensis*[7]
Reported uses[3]	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 2.9 ppm Candy 3.0 ppm Baked goods 3.0 ppm	Non-alcoholic beverages 6.2 ppm Ice cream, ices, etc. 23 ppm Candy 11 ppm Baked goods 8.3 ppm Chewing gum 0.80 ppm
Regulatory status	FDA 121.1164; FEMA No. 2084	FDA 121.1164; FEMA No. 2158

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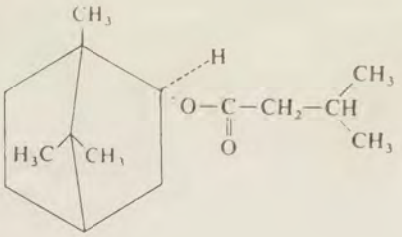
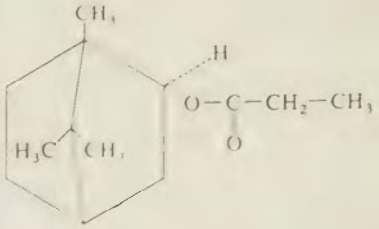
For References 1–5, see end of Part III.

	Isobornyl acetate	Isobornyl formate
Other names	2-Camphanyl acetate	
Empirical formula	$C_{12}H_{20}O_2$	$C_{11}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Clear, colorless liquid; tends to yellow slightly on aging	Liquid
Assay	97% min[2]	
Molecular weight	196.29	182.26
Boiling point	102–103°C at 12–13 mm Hg	110°C at 20 mm Hg
Specific gravity	0.980–0.984 at 25/25°C;[2] 0.9905 at 15°C	1.000 at 18°C
Refractive index	1.4620–1.4650 at 20°C;[2] 1.46589 at 14.4°C	1.4717 at 18°C
Optical rotation	[illegible] to [illegible][2]	
Acid value	Not more than 1[2]	
Solubility	1:3 in 70% alcohol;[2] 1:1 in 90% alcohol; readily soluble in most organic solvents	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Pleasant, camphor-like odor reminiscent of some varieties of pine needles and hemlock; fresh, burning taste	Characteristic aromatic, pine-needles odor
Synthesis	By treatment of camphene with acetic acid, usually in the presence of a catalyst; also by acetylation of isoborneol. Depending on the starting material (*d*-camphene or *l*-camphene), the resulting acetate may exhibit a slight optical activity. The commercial product is considered to be optically inactive	By reaction of formic acid with camphene in the presence of a catalyst;[6,7] also in the absence of a catalyst. The resulting products do not exhibit well defined optical characteristics[8] The corresponding optically active esters have been prepared from *d*- or *l*-camphene and formic acid in the presence of phthalic anhydride.
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 9.6 ppm Ice cream, ices, etc. 12 ppm Candy 3.9 ppm Baked goods 9.5 ppm Gelatins and puddings 70 ppm	Non-alcoholic beverages 0.06–1.0 ppm Ice cream, ices, etc. 0.03–1.0 ppm Candy 0.74 ppm Baked goods 0.80 ppm
Regulatory status	FDA 121.1164. FEMA No. 2160	FDA 121.1164; FEMA No. 2162

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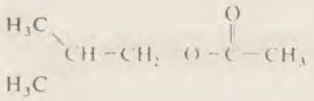
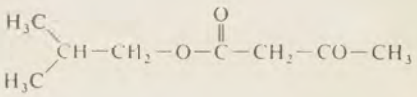
For References 1–5, see end of Part III.

6. **Brus and Vebra,** *Compt. Rend.*, 191, 267, 1930.
7. **Schering and Kahlbaum,** German Patent 573,979, 1925.
8. **Pariselle,** *Compt. Rend.*, 180, 1833, 1925.

	Isobornyl isovalerate	Isobornyl propionate
Other names		
Empirical formula	$C_{15}H_{26}O_2$	$C_{13}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Molecular weight	238.37	210.31
Boiling point		245°C
Specific gravity		0.978 at 15.5°C
Refractive index		1.4640
Solubility	Insoluble in water; soluble in alcohol; very slightly soluble in glycerin and propylene glycol	Almost insoluble in water; poorly soluble in propylene glycol and glycerin; soluble in alcohol
Organoleptic characteristics	Warm, herbaceous, camphoraceous odor; slightly green and woody	Characteristic, definite turpentine odor but less pungent than the corresponding acetate
Synthesis		From isoborneol and propionic acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.60–1.0 ppm Ice cream, ices, etc. 0.30–1.0 ppm Candy 0.90 ppm Baked goods 0.80–2.0 ppm	Non-alcoholic beverages 0.01–1.0 ppm Ice cream, ices, etc. 0.80–1.0 ppm Candy 1.2 ppm Baked goods 1.8 ppm
Regulatory status	FDA 121.1164; FEMA No. 2166	FDA 121.1164; FEMA No. 2163

REFERENCES

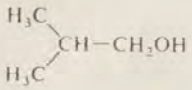
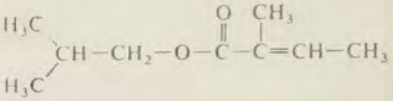
For References 1–5, see end of Part III.

	Isobutyl acetate	Isobutyl acetoacetate
Other names		Isobutyl-β-ketobutyrate Isobutyl-3-oxobutanoate
Empirical formula	$C_6H_{12}O_2$	$C_8H_{14}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	95% min	
Molecular weight	116.16	158.20
Boiling point	116.5 C	84.5°C at 11 mm Hg
Flash point	30 C (19 C)	
Specific gravity	0.8710 0.8785 (0.8921) at 15°C	0.9697 at 25°C
Refractive index	1.3890 1.3910 at 20°C	1.4219 at 25°C
Acid value	0.2 max	
Solubility	Soluble in most organic solvents	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Fruity (currant-pear), floral (hyacinth-rose) odor; characteristic ether-like, slightly bitter flavor	Sweet, winey, brandy-like odor; sweet and slightly fruity flavor
Synthesis	By direct esterification of isobutyl alcohol with acetic acid	From isobutyl acetate by heating in the presence of sodium isobutylate
Natural occurrence	Occurring in a few natural products, such as *Endoconidiophora coerulescens*,[6] raspberry, pear, and pineapple	
Reported uses[3]	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 16 ppm Candy 36 ppm Baked goods 35 ppm Gelatins and puddings 170 ppm Chewing gum 860 ppm Icings 5.5 ppm	Non-alcoholic beverages 4.0 ppm Ice cream, ices, etc. 7.0 ppm Candy 25 ppm Baked goods 25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2175	FDA 121.1164; FEMA No. 2177

REFERENCES

For References 1–5, see end of Part III.

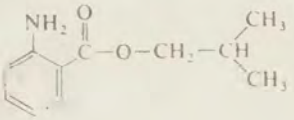
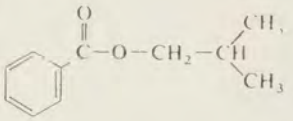
6. Birkinshaw and Morgan, *Biochem. J.*, 47, 55, 1950.

	Isobutyl alcohol	Isobutyl angelate
Other names	Isobutanol 2-Methylpropanol	Isobutyl *cis*-α,β-dimethylacrylate Isobutyl *cis*-2-methyl-2-butenoate Isobutyl *cis*-α-methylcrotonate
Empirical formula	$C_4H_{10}O$	$C_9H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless liquid
Molecular weight	74.42	156.23
Melting point	−108°C	
Boiling point	108.4°C	177°C
Specific gravity	0.803 at 20°C	
Refractive index	1.396 at 20°C	
Solubility	Soluble in water (forming azeotropes); miscible with most common organic solvents	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Disagreeable odor	Faint, pleasant, camomile-like odor and flavor
Synthesis	From isobutylene; by reduction of isobutyraldehyde with sodium amalgam or in the presence of a catalyst; by fermentation of isobutyraldehyde; isolated during fermentation of carbohydrates	By esterification of isobutyl alcohol with angelic acid
Natural occurrence	Reported found (free or esterified) in the essential oils of: Java citronella, tea, *Eucalyptus amygdalina*, and a few others; also present in apple and currant aromas; identified among the volatile constituents in rum;[6] present in fusel oil from beets and potatoes	Reported found in the essential oil of Roman camomile[7]
Reported uses[3]	Non-alcoholic beverages 12 ppm Alcoholic beverages 1.0 ppm Ice cream, ices, etc. 7.0 ppm Candy 34 ppm Baked goods 32 ppm Cream 4.0 ppm	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 1.5 ppm Candy 5.0 ppm Icings 3.0–100 ppm
Regulatory status	FDA 121.1164; FEMA No. 2179	FDA 121.1164; FEMA No. 2180

REFERENCES

For References 1–5, see end of Part III.

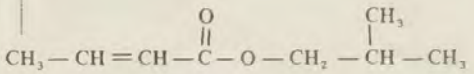
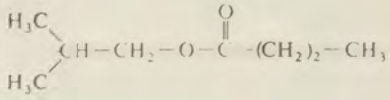
6. Fenaroli et al., *Riv. Ital. EPPOS*, 9, 484, 1956; 2, 75, 1966.
7. Fittig et al., *Justus Liebigs Ann. Chem.*, 195, 79, 1879.

	Isobutyl anthranilate	Isobutyl benzoate
Other names	Isobutyl 2-aminobenzoate Isobutyl *o*-aminobenzoate	
Empirical formula	$C_{11}H_{15}O_2N$	$C_{11}H_{14}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay		98% min
Molecular weight	193.25	178.23
Boiling point	169–170°C at 13.5 mm Hg	241–242°C
Flash point		96°C
Specific gravity		0.994–0.997 at 25°/25°C; 0.9896 at 30°C
Refractive index		1.493–1.496 at 20°C
Acid value		1 max
Solubility		1:2 in 80% alcohol; insoluble in water; miscible with alcohol and ether
Organoleptic characteristics	Faint, orange-flowers odor	Floral-leafy odor reminiscent of rose and geranium
Synthesis	By heating the anhydride of *N*-carboxyl anthranilic acid with sodium isobutoxide and subsequently hydrolyzing the reaction product	From benzoic acid and isobutyl alcohol in the presence of HCl catalyst;[6] or by ester exchange between methylbenzoate and isobutyl alcohol in the presence of potassium isobutylate[7]
Natural occurrence	Not reported found in nature	In cocoa; in banana
Reported uses[5]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 4.0 ppm Candy 12 ppm Baked goods 12 ppm Chewing gum 5.0–1,700 ppm	Non-alcoholic beverages 2.0–9.0 ppm Ice cream, ices, etc. 7.9 ppm Candy 12 ppm Baked goods 10–23 ppm
Regulatory status	FDA 121.1164; FEMA No. 2182	FDA 121.1164; FEMA No. 2185

REFERENCES

For References 1–5, see end of Part III.

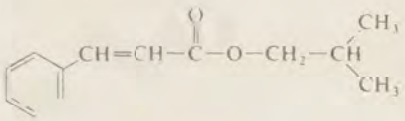
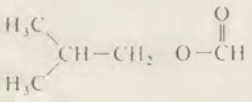
6. **Stohmann, Rodatz and Herzberg,** *J. Prakt. Chem.*, 2(36), 4, 1887.
7. **Reimer and Downes,** *J. Am. Chem. Soc.*, 43, 949, 1921.

	Isobutyl-2-butenoate	Isobutyl butyrate
Other names	Isobutyl crotonoate	2-Methyl propanyl butyrate
Empirical formula	$C_8H_{14}O_2$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Assay		98% min[2]
Molecular weight	142.19	144.21
Boiling point	171°C	157–158°C; 51–52°C at 12 mm Hg
Specific gravity	0.8910 at 20°C	0.858–0.863 at 25°/25°C;[2] 0.8619 at 20°C
Refractive index	1.4291 at 20°C	1.4020–1.4050 at 20°C[2]
Acid value		Not more than 1.0[2]
Solubility		1:8 in 60% alcohol;[2] slightly soluble in water
Organoleptic characteristics		Fruity odor reminiscent of apple or pineapple; sweet flavor reminiscent of rum
Synthesis	By heating the corresponding acid and alcohol with sulfuric acid[6]	By esterification of butyric acid with isobutyl alcohol in the presence of concentrated H_2SO_4;[8] or by enzymatic action of hog pancreas on a mixture of isobutyl alcohol and butyric acid in the absence of water[9]
Natural occurrence	In grapes[7]	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 3.0 ppm Chewing gum 25.0 ppm Jellies, preserves, spreads 3.0 ppm Milk, dairy products 3.0 ppm	Non-alcoholic beverages 8.3 ppm Alcoholic beverages 2.0 ppm Ice cream, ices, etc. 16 ppm Candy 25 ppm Baked goods 24 ppm Gelatins and puddings 14 ppm Chewing gum 2,000 ppm
Regulatory status	FEMA No. 3432	FDA 121.1164; FEMA No. 2187

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For References 1–5, see end of Part III.

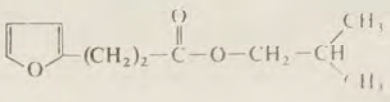
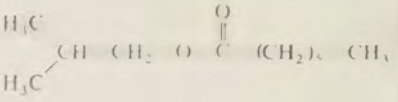
6. Schgámberg, *Z. Physik Chem.*, 174, 466, 1935.
7. Stern et al., *J. Agric. Food Chem.*, 15, 1100, 1967.
8. Grünzweig, *Chem. Ann.*, 162, 207, 1872.
9. Rona and Ammon, *Biochem. Z.*, 221, 386, 1930.

	Isobutyl cinnamate	Isobutyl formate
Other names	Isobutyl-3-phenylpropenoate Isobutyl-β-phenylacrylate	Tetryl formate
Empirical formula	$C_{13}H_{16}O_2$	$C_5H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	98% min	
Molecular weight	204.27	102.13
Melting point		−95.3°C
Boiling point	145 C at 13 mm Hg	97–98.2°C
Flash point	> 100 C	
Specific gravity	1.001–1.004 at 25°C	0.8798 (0.875) at 20°C
Refractive index	1.539–1.541 at 20 C	1.3855 at 20°C
Acid value	1 max	
Solubility	1:3 in 80% alcohol	Slightly soluble in water; completely miscible with alcohol and ether; soluble in most organic solvents
Organoleptic characteristics	Sweet, fruity, balsamic odor; sweet taste reminiscent of currant	Fruity, ether-like odor; sweet taste reminiscent of rum
Synthesis	By heating cinnamyl chloride and isobutyl alcohol[6]	From isobutyl alcohol and carbon monoxide in the presence of sodium isobutylate at 110°C and 400 atm[7]
Natural occurrence	Not reported found in nature	In pineapple and apple; in vinegar
Reported uses[3]	Non-alcoholic beverages 1.3 ppm Alcoholic beverages 2.0 ppm Ice cream, ices, etc. 3.4 ppm Candy 5.4 ppm Baked goods 5.4 ppm	Non-alcoholic beverages 2.2 ppm Ice cream, ices, etc. 7.1 ppm Candy 19 ppm Baked goods 8.2 ppm Gelatins and puddings 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2193	FDA 121.1164; FEMA No. 2197

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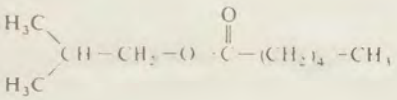
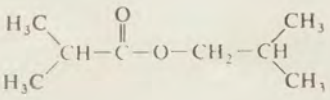
For References 1–5, see end of Part III.

6. Sudborough and Thompson, *J. Chem. Soc.*, 83, 676, 1903.
7. E. I. du Pont de Nemours & Co., U.S. Patent 2,117,600, 1935.

	Isobutyl-2-furanpropionate	Isobutyl heptanoate
Other names	Isobutyl furfurylacetate Isobutyl-3-(2-furyl)-propanoate Isobutyl furylpropionate	Isobutyl heptoate Isobutyl heptylate
Empirical formula	$C_{11}H_{16}O_3$	$C_{11}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to pale, straw-yellow liquid	Colorless liquid
Molecular weight	196.25	186.30
Boiling point		209 C (95–97 C at 12 mm Hg)
Specific gravity		0.8593 at 20 C
Solubility	Almost insoluble in water; soluble in alcohol	Soluble in most organic solvents
Organoleptic characteristics	Fruity, winey, brandy-like odor; pungent taste above 50 ppm; sweet, dry, brandy flavor at low levels	Characteristic green odor and corresponding taste when freshly prepared
Synthesis	By esterification of 2-furanpropionic acid with isobutanol	By direct esterification of heptanoic acid with isobutyl alcohol or by treating heptanoic acid and isobutyl alcohol in the presence of defatted *Chelidonium majus* seeds at 20 C for 3 days[6]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 8.1 ppm Ice cream, ices, etc. 14 ppm Candy 17 ppm Baked goods 21 ppm Gelatins and puddings 4.0–30 ppm Chewing gum 12 ppm Icings 20 ppm	Non-alcoholic beverages 0.50–1.5 ppm Ice cream, ices, etc. 2.4–10 ppm Candy 7.0–25 ppm Baked goods 7.0–25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2198	FDA 121.1164; FEMA No. 2200

REFERENCES

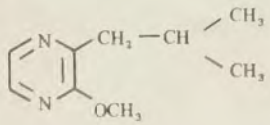
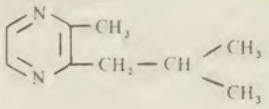
For References 1–5, see end of Part III.
6. Bournot, *Biochem. Z.*, 65, 156, 1914.

	Isobutyl hexanoate	Isobutyl isobutyrate
Other names	Isobutyl caproate Isobutyl capronate Isobutyl hexylate	
Empirical formula	$C_{10}H_{20}O_2$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	98% min	98% min
Molecular weight	172.27	144.21
Melting point		−80 to −81°C
Boiling point		144–151°C; 148–149°C
Flash point	76°C	49°C
Specific gravity	0.854–0.858 at 25°C	0.875 at 0°C
Refractive index	1.412–1.416 at 20°C	1.3999 at 20°C
Acid value	1 max	
Solubility	1:2 in 80% alcohol; 1:1 in 90% alcohol	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Fruity odor with cocoa-like undertone	Odor and taste reminiscent of pineapple
Synthesis	By direct esterification	By catalytic reaction passing vapors of isobutyl alcohol over $CuO + Al_2O_3$, $ZnO + Al_2O_3$, or $CuO + ZnO + Al_2O_3$ at 350–400°C under pressure[6]
Natural occurrence	In banana, grapes, and wine	Reported found in the essential oil of hops[7] and in *Vitis vinifera*
Reported uses[3]	Non-alcoholic beverages 5.4 ppm Ice cream, ices, etc. 3.9 ppm Candy 8.1 ppm Baked goods 8.3 ppm Chewing gum 2.0 ppm	Non-alcoholic beverages 7.5 ppm Alcoholic beverages 2.0 ppm Ice cream, ices, etc. 7.4 ppm Candy 16 ppm Baked goods 17 ppm Gelatins and puddings 3.3–10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2202	FDA 121.1164; FEMA No. 2189

REFERENCES

For References 1–5, see end of Part III.

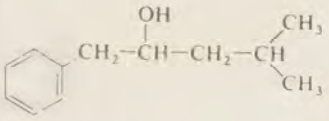
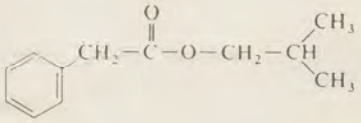
6. Ipatieff and Haensel, *J. Org. Chem.*, 7, 194, 1942.
7. Buttery et al., *Nature*, 200, 435, 1936.

	2-Isobutyl-3-methoxypyrazine	2-Isobutyl-3-methylpyrazine
Other names	2-Methoxy-3-(2-methylpropyl)pyrazine	2-Methyl-3-isobutyl pyrazine 2-Methyl-3-(2-methylpropyl)-pyrazine
Empirical formula	$C_9H_{14}ON_2$	$C_9H_{14}N_2$
Structure		
Physical/chemical characteristics		
Assay	C: 65.03%; H: 8.49%; O: 9.63%; N: 16.85%	C: 71.96%; H: 9.39%; N: 18.65%
Molecular weight	166.22	150.22
Boiling point		74°C at 10 mm Hg
Mass spectra	40(3), 41(2), 53(3), 66(1), 68(3), 80(2), 81(6), 94(15), 95(9), 106(2), 109(3), 124(100), 125(8), 151(22), 152(2), 165(4), 166(9)[11]	41(17), 42(13), 53(5), 60(1), 67(12), 82(1), 93(4), 108(100), 135(10), 150(5)[14]
IR spectra[7]	S (3.39, 3.43, 3.50, 6.49, 6.85, 6.9, 7.2, 7.7, 8.6, 9.9) M (3.28, 3.46, 7.4, 8.4, 9.4, 11.8) W (3.33, 6.34, 7.9, 8.1, 9.2, 10.5, 10.8, 11.2, 13.3)	
Organoleptic characteristics	The extremely powerful odor has a reported threshold value of 2 parts per trillion in water; diluted water solutions exhibit a characteristic odor of green bell peppers[7]	
Synthesis	By condensation of leucine amide with glyoxal, followed by methylation with CH_2N_2[6]	By condensation of ethylenediamine with 5-methyl-2,3-hexanedione[12]
Natural occurrences	Reported present as a flavor constituent in green bell pepper, coffee, galbanum oil, potato products, peas[8-10]	Reported present in coffee and potato products[13,15]
Reported uses[3]	Non-alcoholic beverages 0.05 ppm Ice cream, ices, etc. 0.05 ppm Candy 0.05 ppm Baked goods 0.05 ppm Gelatins and puddings 0.05 ppm Chewing gum 0.05 ppm Condiments 0.05 ppm Meat, meat sauces, soups 0.05 ppm Milk, dairy products 0.05 ppm Cereals 0.05 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 5.0 ppm
Regulatory status	FEMA No. 3132	FEMA No. 3133

REFERENCES

For References 1–5, see end of Part III.

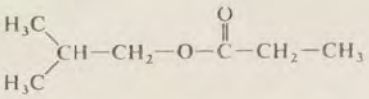
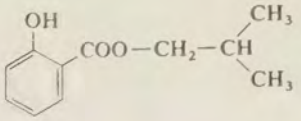
6. Buttery, Seifert, Lundin, Guadagni and Ling., *Chem. Ind.* (London), 15, 490, 1969.
7. Buttery et al., *J. Agric. Food Chem.*, 17(6), 1322, 1969.
8. Gianturco et al., *J. Agric. Food Chem.*, 19(3), 530, 1971.
9. Murray et al., *Chem. Ind.* (London), 27, 897, 1970.
10. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
11. Friedel et al., *J. Agric. Food Chem.*, 19, 530, 1971.
12. Flament and Stoll, *Helv. Chim. Acta*, 50, 1754, 1967.
13. Stoll et al., *Helv. Chim. Acta*, 50, 1754, 1967.
14. Buttery et al., *J. Agric. Food Chem.*, 19, 1045, 1971.
15. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.

	α-Isobutylphenethyl alcohol	Isobutyl phenylacetate
Other names	Benzyl isoamyl alcohol Isobutyl benzylcarbinol α-Isobutyl phenylethyl alcohol 4-Methyl-1-phenyl-2-pentanol	Isobutyl α-toluate
Empirical formula	$C_{12}H_{18}O$	$C_{12}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Assay		98% min[2] (99%)
Molecular weight	178.27	192.26
Boiling point	250 C	253°C
Flash point		116 C
Specific gravity	0.96	0.984–0.988 at 25 /25°C[2]
Refractive index		1.4860–1.4880 at 20 C[2]
Acid value		Not more than 1[2] (0.02%)
Solubility	Insoluble in water; soluble in alcohol	1:2 and more in 80% alcohol[2]
Organoleptic characteristics	Green, floral, somewhat herbaceous odor; buttery, oily, caramellic flavor	Sweet, musk-like fragrance; sweet, honey-like flavor
Synthesis	By reacting isobutyl aldehyde with benzyl magnesium chloride[6]	By esterification of phenylacetic acid with isobutyl alcohol
Natural occurrence		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0–10 ppm Alcoholic beverages 50 ppm Ice cream, ices, etc. 38 ppm Candy 54 ppm Baked goods 15–50 ppm	Non-alcoholic beverages 2.8 ppm Ice cream, ices, etc. 2.8 ppm Candy 5.5 ppm Baked goods 5.0 ppm Gelatins and puddings 5.0 ppm Maraschino cherries 3.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2208	FDA 121.1164; FEMA No. 2210

REFERENCES

For References 1–5, see end of Part III.

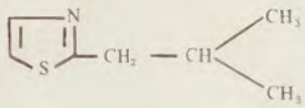
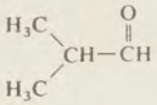
6. Petyunin, *Chem. Abstr.*, 38, 950, 1944.

	Isobutyl propionate	Isobutyl salicylate
Other names		Isobutyl *o*-hydroxybenzoate
Empirical formula	$C_7H_{14}O_2$	$C_{11}H_{14}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay		98% min[2] (98.5%)
Molecular weight	130.18	194.23
Melting point		−5.9°C
Boiling point	137–138°C; 66.5°C at 60 mm Hg	259 C
Flash point		121 C
Specific gravity	0.8600–0.8635 at 20°/20°C	1.062–1.066 at 25°/25°C;[2] 1.0700–1.0720 at 15°C
Refractive index	1.3975 at 20°C	1.5070–1.5100 at 20°C[2]
Acid value		Not more than 1[2] (0.2)
Solubility	Insoluble in water; soluble in most organic solvents	1:9 in 80% alcohol;[2] 1:1–2 in 90% alcohol
Organoleptic characteristics	Odor similar to the corresponding ethyl ester but more refined and fresher; bitter flavor	Orchid, wintergreen-like odor similar to amyl salicylate; bitter taste
Synthesis	By direct esterification or by reacting propionyl chloride with isobutyl alcohol in the presence of Mg dust in ether solution[6]	By esterification of isobutyl alcohol and salicylic acid
Natural occurrence	Probably occurring in grape (var. white Sauvignon)[7], apple, pear, and rum	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 5.4 ppm Ice cream, ices, etc. 4.2 ppm Candy 25 ppm Baked goods 35 ppm	Non-alcoholic beverages 3.5 ppm Ice cream, ices, etc. 1.8 ppm Candy 2.6 ppm Baked goods 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2212	FDA 121.1164; FEMA No. 2213

REFERENCES

For References 1–5, see end of Part III.

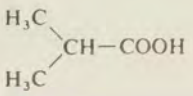
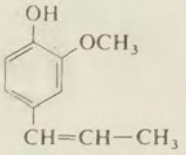
6. Spassow, *Ber. Dtsch. Chem. Ges.*, 70, 1928, 1937.
7. Chaundhary et al., *Am. J. Enol. Vitic.*, 15, 190, 1964.

	2-Isobutyl thiazole	Isobutyraldehyde
Other names		Isobutyl aldehyde Isobutyric aldehyde 2-Methyl propanal
Empirical formula	$C_7H_{11}NS$	C_4H_8O
Structure		
Physical/chemical characteristics		
Appearance		Colorless liquid
Molecular weight	141.23	72.10
Boiling point	172–180°C	63.5°C at 754 mm Hg
Specific gravity	0.9953 at 25°C	0.7904 at 20°C
Refractive index	1.4939 at 25°C	1.3738 at 20°C
Solubility		Forms azeotropic mixtures with water
Organoleptic characteristics		Characteristic odor
Synthesis	Via cyclization of aliphatic amides with α,β-dibromo ether[6]	By oxidation of isobutyl alcohol with potassium dichromate and concentrated sulfuric acid[6]
Natural occurrence	Reportedly identified as the odorous component in tomatoes[7,8] and in processed tomatoes;[9] a flavor constituent of tomatoes	Reported found in apple and currant aromas and in the essential oils from tobacco leaves[7] and tea leaves;[8] also in the essential oils of: *Pinus jeffreyi* Murr. leaves,[9] *Citrus aurantium* leaves,[10] and *Datura stramonium*[11]
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm Gelatins and puddings 1.0 ppm Meat, meat sauces, soups 1.0 ppm Sauces 1.0 ppm Vegetables 1.0 ppm	Non-alcoholic beverages 0.30 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 0.25–0.50 ppm Candy 0.67 ppm Baked goods 0.50–1.0 ppm
Regulatory status	FEMA No. 3134	FDA 121.1164; FEMA No. 2220

REFERENCES

For References 1–5, see end of Part III.

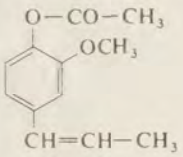
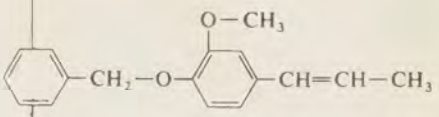
6. **Cottet, Gallo and Metzger,** *Bull. Soc. Chim. Fr.*, 12, 4499, 1967.
7. **Viani et al.,** *Helv. Chim. Acta.* 52(4), 887, 1969.
8. **Stevens,** *J. Am. Soc. Hort. Sci.*, 95(1), 9, 1970; *Chem. Abstr.*, 72, 131227p, 1970.
9. **Neipawer et al.,** *Flavour Ind.*, 2, 465, 1971.
10. **Pfeiffer,** *Ber. Dtsch. Chem. Ges.*, 5, 699, 1872.
11. **Onishi and Yamasaki,** *Bull. Agric. Chem. Soc. Jap.*, 19, 137, 1955.
12. **Yamamoto and Kato,** *J. Agric. Chem. Soc. Jap.*, 10, 661, 1934.
13. **Sondern,** *J. Am. Pharm. Assoc.*, 22, 114, 1933.
14. **Peyron,** *Soap Perfum. Cosmet.*, 33, 373, 1960.
15. **Ssivolobow,** *Chem. Zentralbl.*, 2, 227, 1916.

	Isobutyric acid	Isoeugenol
Other names	Isopropylformic acid 2-Methylpropanoic acid	1-Hydroxy-2-methoxy-4-propenylbenzene 2-Methoxy-4-propenylphenol 4-Propenyl guaiacol
Empirical formula	$C_4H_8O_2$	$C_{10}H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Pale-yellow, rather viscous liquid
Assay		99.5% min[2]
Molecular weight	88.10	164.21
Melting point	−46.1°C	14–18°C
Boiling point	154.7°C	12°C[2]
Congealing point		
Flash point	76°C	>100°C
Specific gravity	0.95296 at 15°C; 0.948 at 15.5°C	1.079–1.085 at 25°/25°C[2]
Refractive index	1.39525 at 15°C	1.5720–1.5770 at 20°C[2]
Solubility	1:5 in water; soluble in alcohol and ether	1:5 in 50% alcohol;[2] 1:1 in 70% alcohol
Organoleptic characteristics	Odor and flavor similar to *n*-butyric acid	Floral odor reminiscent of carnation
Synthesis	By oxidation of isobutyl alcohol	By the alkaline isomerization of eugenol obtained from essential oils high in eugenol[6]
Natural occurrence	Reported found in several essential oils: *Arnica montana*, Roman camomile, *Laurus nobilis*, imperatoria, and in carob fruits (*Siliqua dulcis*); also identified in the essence of *Seseli tortuosum*,[11] *Artemisia transiliensis*,[12] and in strawberry aroma[13]	The commercial product is a mixture of *cis*- and *trans*-isomers. Reported found in the essential oils of ylang-ylang[7] and nutmeg;[8] also in the oil from flowers of *Michelia champaca*[9] and in the oil from seeds of *Nectandra puchury*[10]
Reported uses[3]	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 12 ppm Candy 41 ppm Baked goods 38 ppm Chewing gum 470 ppm Margarine 30 ppm	Non-alcoholic beverages 3.7 ppm Ice cream, ices, etc. 3.8 ppm Candy 5.0 ppm Baked goods 11 ppm Chewing gum 0.30–1,000 ppm Condiments 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2222	FDA 121.1164; FEMA No. 2468

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For References 1–5, see end of Part III.

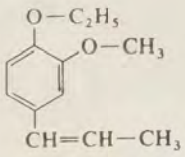
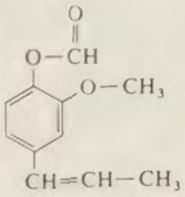
6. Tiemann, *Ber. Dtsch. Chem. Ges.*, 24, 2870, 1891.
7. Schimmel and Co., *Chem. Zentralbl.*, 2, 1907, 1901.
8. Power and Salvay, *J. Chem. Soc.*, 91, 2041, 1907.
9. Brooks, *J. Am. Chem. Soc.*, 33, 1764, 1911.
10. *Chem. Zentralbl.*, 1, 360, 1922.
11. Salgues, *C. R. Séances Acad. Sci. Paris*, 241, 677, 1956.
12. Goryaev and Pugachev, *Chem. Abstr.*, 50, 1684, 1956.
13. Willhalm et al., *Helv. Chim. Acta*, 49, 66, 1966.

	Isoeugenyl acetate	Isoeugenyl benzyl ether
Other names	Acetyl isoeugenol 2-Methoxy-4-propenylphenyl acetate	Benzyl isoeugenol 2-Methoxy-4-propenylphenyl ether
Empirical formula	$C_{12}H_{14}O_3$	$C_{17}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White crystals	White to ivory-colored crystalline powder
Assay	98% min[2]	
Molecular weight	206.24	254.33
Melting point	Approx. 80 C	58–59°C; 48°C
Boiling point		282°C
Congealing point	78 C	~57.0 C[2]
Isoeugenyl content		Not more than 1.0%[2]
Acid value	1.0 max[2]	
Solubility	Soluble in most organic solvents	Approx 1:50 in 90% alcohol[2]
Organoleptic characteristics	Weak, rose-carnation, somewhat spicy odor; initially burning, then sweet taste	Faint, floral odor of rose-carnation
Synthesis	From isoeugenol and acetic acid by esterification	By benzylation of isoeugenol; also by alkaline isomerization of benzyleugenol[6]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.44 ppm Ice cream, ices, etc. 2.1 ppm Candy 17 ppm Baked goods 17 ppm Chewing gum 100 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2470	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.

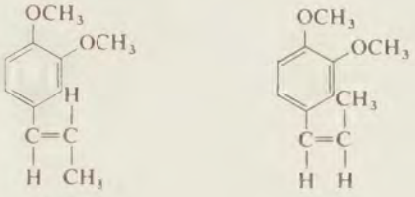
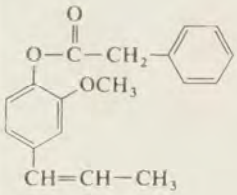
6. Pond and Beers, *J. Am. Chem. Soc.*, 19, 828, 1897.

	Isoeugenyl ethyl ether	Isoeugenyl formate
Other names	1-Ethoxy-2-methoxy-4-propenylbenzene 2-Ethoxy-5-propenylanisole Ethyl isoeugenol	2-Methoxy-4-propenyl phenyl formate 4-Propenyl-2-methoxyphenylformate
Empirical formula	$C_{12}H_{16}O_2$	$C_{11}H_{12}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Crystalline solid	Colorless to pale straw-yellow, viscous liquid
Molecular weight	192.26	192.22
Melting point	63–64°C (with sublimation)	
Boiling point	245°C	282°C
Congealing point		1.038 (1.12) at 15.5 C
Isoeugenol content		1.5660 at 20 C
Solubility	Highly soluble in ether and benzene; soluble in alcohol and acetic acid	Almost insoluble in water; soluble in alcohol; slightly soluble in propylene glycol
Organoleptic characteristics	Odor similar to isoeugenol	Faint, orris-like, green, sweet, woody odor with clove-like undertones; warm, spicy flavor
Synthesis	From isoeugenol by boiling with ethyl *p*-toluenesulfonate[6]	By formylation of isoeugenol
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 7.8 ppm Ice cream, ices, etc. 0.50 ppm Candy 17 ppm Baked goods 1.0–3.5 ppm	Condiments 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2472	FDA 121.1164; FEMA No. 2474

REFERENCES

For References 1–5, see end of Part III.

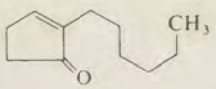
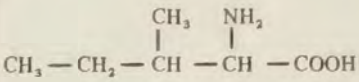
6. van Duin, *Recl. Trav. Chim. Pays-Bas*, 45, 351, 1926.

	Isoeugenyl methyl ether	Isoeugenol phenylacetate
Other names	1,2-Methoxy-4-propenylbenzene Methyl isoeugenol 4-Propenyl veratrole	Isoeugenol α-toluate 2-Methoxy-4-propenylphenyl phenylacetate 4-Propenylguaiacyl phenylacetate
Empirical formula	$C_{11}H_{14}O_2$	$C_{18}H_{18}O_3$
Structure	 *trans-* *cis-*	
Physical/chemical characteristics[5]		
Appearance	Colorless to pale-yellow liquid	Yellowish, viscous liquid
Molecular weight	178.23	95% min 282.34
Melting point	*trans-*, 16–17 C	
Boiling point	262–264 C; *cis-*, 138–140 C at 12 mm Hg; *trans-*, 143–144 C at 11 mm Hg	>100 C
Specific gravity	1.047–1.053 at 25°/25°C[2]	1.113–1.117
Refractive index	1.5660–1.5690 at 20°C[2]	1.575–1.577
Isoeugenol content		1 max
Acid value		
Solubility	1:2 in 70% alcohol;[2] 1:6.5–7.5 in 60% alcohol. Forms azeotropes with glycerin (75%), acetamide (31%), and phenylacetic acid (40%)	1:2 in 95% alcohol; insoluble in water
Organoleptic characteristics	Delicate, clove-carnation odor; burning, bitter taste	Intensely sweet odor reminiscent of carnation; vanilla, clove-like, and honey odor; sweet, spicy, slightly fruity flavor
Synthesis	By methylation of isoeugenol with methyl sulfate in alkaline solution[9]	From phenylacetyl chloride plus sodium isoeugenol
Natural occurrence	The natural and the commercial products are a mixture of *cis-* and *trans*-isomers. Originally isolated in the oil from roots of *Asarum arifolium* Michx.;[6] in the oil of *Cymbopogon javanensis*,[7] *Orthodon methylisoeugenoliferum* F. (approx 53%),[8] and others	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 4.0 ppm Ice cream, ices, etc. 7.7 ppm Candy 13 ppm Baked goods 18 ppm Gelatins and puddings 0.10 ppm Chewing gum 110 ppm	Non-alcoholic beverages 0.05 ppm Ice cream, ices, etc. 0.20 ppm Candy 3.0 ppm Baked goods 2.0–3.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2476	FDA 121.1164; FEMA No. 2477

REFERENCES

For References 1–5, see end of Part III.

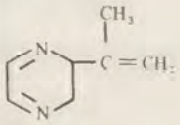
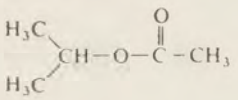
6. Miller, *Arch. Pharm.*, 240, 371, 1902.
7. Hoffman, *Chem. Zentralbl.*, 3, 886, 1919.
8. Fujita, *Chem. Abstr.*, 41, 3585, 1947.
9. Francesconi and Puxeddu, *Gazz. Chim. Ital.*, 1, 207, 1909.

	Isojasmone	DL-Isoleucine
Other names	2-Hexyl-cyclopenten-2-one-1	2-Amino-3-methylpentanoic acid α-Amino-β-methylvaleric acid
Empirical formula	$C_{11}H_{18}O$	$C_6H_{13}O_2N$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellow to yellow-brown liquid	Rhombic or monoclinic platelets (from diluted alcohol)
Assay	80% min	
Molecular weight	166.26	131.11
Melting point	144°C at 10 mm Hg	275°C (sealed tube) 292°C (decomposes)
Flash point	>100°C	
Specific gravity	0.908–0.920 at 25°C; 0.911 at 22°C	
Refractive index	1.4750–1.4800 at 20 C	
Acid value	2 max	
Solubility	1:10 in 70% alcohol; 1:1 in 80% alcohol	Slightly soluble in water
Organoleptic characteristics	Green odor reminiscent of jasmine	Flavorless
Synthesis		From the corresponding aldehyde by Bucherer's reaction[6]
Natural occurrence	Not reported found in nature	
Reported uses[3]		Non-alcoholic beverages 50.0 ppm Baked goods 50.0 ppm Condiments, pickles 50.0 ppm Meat, meat sauces, soups 50.0 ppm Milk, dairy products 50.0 ppm Cereals 50.0 ppm
Regulatory status	FDA 121.1164	FEMA No. 3295

REFERENCES

For References 1–5, see end of Part III.

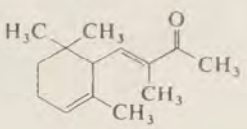
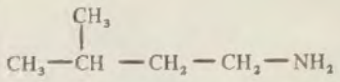
6. *Ullmanns Enzyklopädie der Technischen Chemie*, 3rd ed., Vol. 3, Urban and Schwarzenberg, 1952, 514.

	Isopropenylpyrazine	Isopropyl acetate
Other names	2-Isopropenyl-1,4-diazine 2-(1-Methylvinyl)pyrazine 2-Isopropenylpyrazine	
Empirical formula	$C_7H_8N_2$	$C_5H_{10}O_2$
Structure		
Physical/chemical characteristics		
Appearance		Colorless liquid
Assay	C: 69.97%; H: 6.71%; N: 23.31%	
Molecular weight	120.16	102.13
Boiling point		89.5°C
Specific gravity		0.8718 at 20 C
Refractive index		1.3773 at 20 C
Mass spectra[7]	39 (35), 41 (18), 52 (23), 67 (24), 94 (11), 119 (100), 120 (84)	
Organoleptic characteristics		Intense, fruity odor; on dilution a sweet apple-like flavor
Synthesis	By alkylation of the Mannich base obtained by reacting formaldehyde and dimethylamine with ethylpyrazine, followed by the Hoffmann degradation[8]	By direct acetylation of isopropyl alcohol in the presence of various catalysts: concentrated H_2SO_4, diethyl sulfate, chlorosulfonic acid, and boron trifluoride.[6,7,8]
Natural occurrence	Reported found as a steam-volatile component in roasted Spanish peanuts[6]	In pineapple, pear, and cocoa
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Gelatins and puddings 10.0 ppm Meat, meat sauces, soups 10.0 ppm Milk, dairy products 10.0 ppm Cereals 10.0 ppm	Non-alcoholic beverages 16 ppm Ice cream, ices, etc. 17 ppm Candy 58 ppm Baked goods 75 ppm
Regulatory status	FEMA No. 3296	FDA 121.1164; FEMA No. 2926

REFERENCES

For References 1–5, see end of Part III.

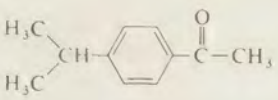
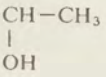
6. Walradt et al., *J. Agric. Food Chem.*, 19, 972, 1971.
7. Walradt et al., *J. Agric. Food Chem.*, 18, 926, 1971.
8. Kamal et al., *J. Org. Chem.*, 27, 1355, 1962.
9. Dow Chemical Co., U.S. Patent 2,021,851, 1932.
10. Dorris, Sowa and Nieuwland, *J. Am. Chem. Soc.*, 56, 2689, 1934.
11. Vogel, *J. Chem. Soc.*, p. 629, 1948.

	α-Isomethylionone	Isopentylamine
Other names	α-Cyclocitrylidene butanone Methyl-γ-ionone (so called) 4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-methyl-3-buten-2-one	Isoamylamine 3-Methylbutylamine Isoamino pentane Isobutyl carbylamine
Empirical formula	$C_{14}H_{22}O$	$C_5H_{13}N$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellowish liquid	Colorless to pale straw-colored mobile liquid
Assay	85–95% (98% min)	
Molecular weight	206.30	87.17
Boiling point	93°C at 3.1 mm Hg	96.5–97.5°C
Specific gravity	0.9304 at 22°C; 0.925–0.929 at 25°/25°C	0.7491 at 20°C
Refractive index	1.5000–1.5020 at 20°C; 1.4990 at 25°C	1.4083 at 20°C
Solubility		Miscible with water, alcohol, propylene glycol, glycerine, and oils
Organoleptic characteristics	Fine violet and orris-like odor	Unpleasant ammoniacal odor
Synthesis	By condensation of citral with methyl ethyl ketone controlling the ratio between the *n*- and the *iso*-forms. The methyl *pseudo*-ionone obtained is then subjected to ring closure, using strong alkali and high temperature (thus favoring the formation of the normal α- and β-methylionones) or with quaternary ammonium base (thus favoring the formation of *iso*-forms). See also monographs of α- and β-ionone and methyl α-, β-, and γ-ionones.	From isoamyl chloride and sodamide in liquid ammonia;[6,7] by reduction of isoamyl nitrile[8,9]
Natural occurrence	Not reported found in nature	Reported found in rye ergot and in many botanical sources (Rosaceae, Saxifragaceae, Umbelliferae, Caprifoliaceae);[10] also commonly found among the degradation products of proteins
Reported uses[3]	Non-alcoholic beverages 0.97 ppm Ice cream, ices, etc. 0.98 ppm Candy 4.9 ppm Baked goods 4.3 ppm Gelatins and puddings 0.05 ppm Chewing gum 0.80 ppm	Non-alcoholic beverages 0.10 ppm Ice cream, ices, etc. 0.10 ppm Candy 0.10 ppm Baked goods 0.10 ppm Gelatins and puddings 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2714	FEMA No. 3219

REFERENCES

For References 1–5, see end of Part III.

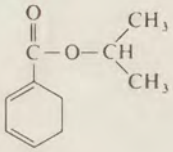
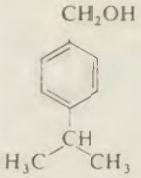
6. Shreve and Rothenberger, *Ind. Eng. Chem.*, 29, 1361, 1937.
7. Shreve and Burtsfield, *Ind. Eng. Chem.*, 33, 220, 1941.
8. Seigle and Hass, *Ind. Eng. Chem.*, 31, 649, 1939.
9. Miduno and Takayama, *Bull. Chem. Soc. Jap.*, 17, 137, 1942.
10. Steiner and Loffler, *Z. Wiss. Bot.*, 71, 523, 1929.

	p-Isopropylacetophenone	Isopropyl alcohol
Other names	Acetocumene *p*-Acetyl cumol 1,4-Acetyl-isopropyl benzol 1-Isopropyl-4-acetylbenzene *p*-Isopropyl acetylbenzol Methyl *p*-isopropylphenyl ketone	Dimethylcarbinol Isopropanol 2-Propanol
Empirical formula	$C_{11}H_{14}O$	C_3H_8O
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	162.23	60.09
Melting point		−81 to −83°C
Boiling point	252–254°C (250°C)	82.3–82.4°C
Flash point		15°C
Specific gravity	0.9755 at 15°C; 0.975 at 15.5°C	0.7854 at 20°C
Refractive index		1.37757 at 20°C
Solubility	Insoluble in water; soluble in alcohol	Miscible with water, alcohol, ether, and chloroform
Organoleptic characteristics	Odor reminiscent of orris and basil; warm, spicy flavor	Alcoholic, somewhat unpleasant odor; burning taste
Synthesis	By condensing cymene with acetyl chloride in the presence of $AlCl_3$;[6] also from benzol, acetyl chloride, and isopropyl chloride via Friedel-Crafts	Synthetically prepared from acetylene or propylene
Natural occurrence	In oil of lavandin	Reported found in apple and cognac aromas (esterified)
Reported uses[3]	Non-alcoholic beverages 0.08 ppm Ice cream, ices, etc. 0.10 ppm Candy 0.50 ppm Baked goods 1.0 ppm Pickles 5.0 ppm	Non-alcoholic beverages 25 ppm Candy 10–75 ppm Baked goods 75 ppm
Regulatory status	FDA 121.1164; FEMA No. 2927	FDA 121.1164; FEMA No. 2929

REFERENCES

For References 1–5, see end of Part III.

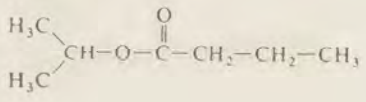
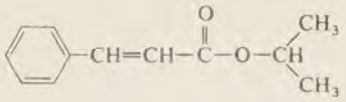
6. Widman, *Ber. Dtsch. Chem. Ges.*, 21, 225, 1888.

	Isopropyl benzoate		*p*-Isopropylbenzyl alcohol	
Other names			Cumic alcohol Cuminic alcohol Cuminol Cuminyl alcohol *p*-Cymen-l-ol	
Empirical formula	$C_{10}H_{12}O_2$		$C_{10}H_{14}O$	
Structure				
Physical/chemical characteristics[5]				
Appearance	Liquid		From colorless to yellow liquid	
Molecular weight	164.21		150.22	
Boiling point	218–219°C		248°C	
Specific gravity	1.0263 at 4°C		0.978 at 20°C	
Refractive index			1.522 at 24°C	
Solubility	Insoluble in water; readily soluble in alcohol and ether		Slightly soluble in water; miscible with alcohol and ether	
Organoleptic characteristics			Intense, persistent, caraway-like odor; aromatic, burning taste	
Synthesis	By heating benzoyl chloride and isopropyl alcohol[6]		From cuminaldehyde with H_2 or NH_3 under pressure in methanol solution and in the presence of Raney Ni catalyst; or by catalytic reduction of methyl *p*-isopropylbenzoate	
Natural occurrence	In apple, pear, cocoa and honey		Reported found in the oil from fruits of *Cuminum cyminum* and *Carum carvi* L.; also in the oils of *Eucalyptus bakeris* (esterified) and French lavender	
Reported uses[3]	Non-alcoholic beverages Ice cream, ices, etc. Candy Baked goods	0.50 ppm 1.0 ppm 1.0 ppm 1.0 ppm	Non-alcoholic beverages Ice cream, ices, etc. Candy Baked goods	11 ppm 0.47 ppm 33 ppm 35 ppm
Regulatory status	FDA 121.1164; FEMA No. 2932		FDA 121.1164; FEMA No. 2933	

REFERENCES

For References 1–5, see end of Part III.

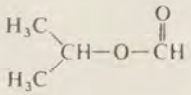
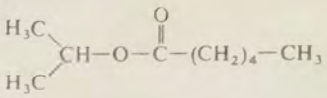
6. Perkin, *J. Chem. Soc.*, 69, 1174, 1896.

	Isopropyl butyrate	Isopropyl cinnamate
Other names		Isopropyl β-phenylacrylate Isopropyl 3-phenylpropenoate
Empirical formula	$C_7H_{14}O_2$	$C_{12}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, viscous liquid; solidifies when cold; tends to polymerize on becoming odorless
Molecular weight	130.18	190.24
Boiling point	129–131 C	268°–270°C
Specific gravity	0.8588 at 20 C	1.017 (1.03) at 18 C
Refractive index	1.3936 at 20°C	
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics	Pleasant odor reminiscent of butyric acid	Balsamic, sweet, dry amber-like odor; fresh, fruity flavor
Synthesis	From butyric acid and propylene in presence of concentrated H_2SO_4 at 125°C in sealed tube;[6,7] also from butyric acid and isopropyl alcohol in the presence of HCl[8] or *p*-toluenesulfonic acid[9]	By esterification of isopropanol with cinnamic acid
Natural occurrence	Reported found in strawberry	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 9.7 ppm Ice cream, ices, etc. 21 ppm Candy 39 ppm Baked goods 39 ppm	Non-alcoholic beverages 0.52 ppm Ice cream, ices, etc. 0.75 ppm Candy 1.3 ppm Baked goods 2.3 ppm
Regulatory status	FDA 121.1164; FEMA No. 2935	FDA 121.1164; FEMA No. 2939

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For References 1–5, see end of Part III.

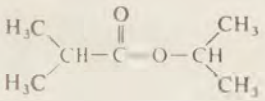
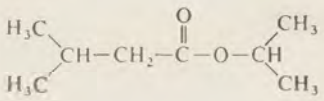
6. Dow Chemical Co., U.S. Patent 2,021,851, 1932.
7. **Fichter and Burgin,** *Helv. Chim. Acta,* 14, 95, 1931.
8. **Kohlrausch and Sabathy,** *Monatsh. Chem.*, 72, 310, 1939.
9. **Salmi and Leimu,** *Suom. Kemistil. B,* 20, 46, 1947.

	Isopropyl formate	Isopropyl hexanoate
Other names		Isopropyl caproate Isopropyl capronate Isopropyl hexylate
Empirical formula	$C_4H_8O_2$	$C_9H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	88.10	158.24
Boiling point	67–68°C	74°C (176°C) at 20 mm Hg
Specific gravity	0.8774 at 20°C; 0.883 at 0°C	0.8570 at 20°C
Refractive index	1.3678 at 20°C	
Solubility	Slightly soluble in water; completely miscible with alcohol, ether, and most organic solvents	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic fruity, ether-like odor; sweet taste reminiscent of plum	Sweet, delicate, fruity odor of pineapple; fresh, sweet, berry-like taste
Synthesis	By direct esterification	By esterification of hexanoic acid with isopropyl alcohol in benzene solution in the presence of trace amounts of concentrated H_2SO_4 and subsequent azeotropic distillation[6]
Natural occurrence	Reported found in several natural products	In strawberry; in bleu cheese
Reported uses[3]	Non-alcoholic beverages 18–25 ppm Ice cream, ices, etc. 18–25 ppm Candy 55–100 ppm Baked goods 60–100 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 5.5–10 ppm Candy 20–40 ppm Baked goods 20–40 ppm
Regulatory status	FDA 121.1164; FEMA No. 2944	FDA 121.1164; FEMA No. 2950

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For References 1–5, see end of Part III.

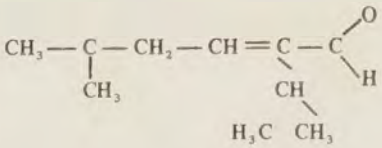
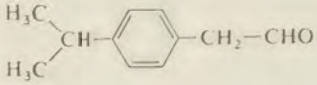
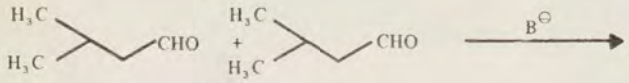
6. Commercial Solvents Corp., U.S. Patent 2,076,111, 1934.

	Isopropyl isobutyrate	Isopropyl isovalerate
Other names		
Empirical formula	$C_7H_{14}O_2$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	130.18	144.21
Boiling point	121°C	68–70°C at 55 mm Hg
Specific gravity	0.8687 at 0°C	
Refractive index		1.3960 at 20.5°C
Solubility	Insoluble in water; soluble in most organic solvents	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Intense, fruity, ether-like odor	Ether-like odor similar to the *n*-propyl ester; sweet, apple-like taste
Synthesis	By boiling isobutyryl chloride and isopropyl alcohol[6]	From isobutene and isopropyl alcohol in the presence of CO and HF under pressure[7]
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 12–25 ppm Ice cream, ices, etc. 18–25 ppm Candy 58–100 ppm Baked goods 60–100 ppm	Non-alcoholic beverages 3.4 ppm Ice cream, ices, etc. 3.4 ppm Candy 11 ppm Baked goods 11 ppm
Regulatory status	FDA 121.1164; FEMA No. 2937	FDA 121.1164; FEMA No. 2961

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For References 1–5, see end of Part III.

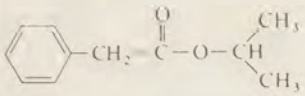
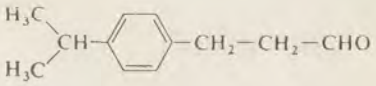
6. **Kohlrausch and Skrabal,** *Monatsh. Chem.*, 70, 393, 1937.
7. **Friedmann and Cotton,** U.S. Patent 3,052,698, 1962.

	2-Isopropyl-5-methyl-2-hexenal	*p*-Isopropylphenylacetaldehyde
Other names	*iso*-Dihydrovandulyl aldehyde	Cuminic acetaldehyde *p*-Cymen-7-carboxaldehyde Homo-cuminic aldehyde 4-Isopropyl phenylacetaldehyde
Empirical formula	$C_{10}H_{18}O$	$C_{11}H_{14}O$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Molecular weight	154.24	162.23
Boiling point		230°C (243°C)
Specific gravity		0.955 at 15.5°C
Refractive index		1.5200 at 20°C
Solubility		Almost insoluble in water; soluble in alcohol
Organoleptic characteristics		Characteristic bark odor; citrus, bittersweet, fruity flavor
Synthesis		From cumyl magnesium chloride and ethyl formate or triethyl *o*-formate followed by acid hydrolysis of the acetal
Natural occurrence	Reported found in cocoa[6]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm Gelatins and puddings 2.0 ppm Milk, dairy products 0.5 ppm	Non-alcoholic beverages 0.10 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50 ppm
Regulatory status	FEMA No. 3406	FDA 121.1164; FEMA No. 2954

REFERENCES

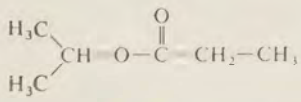
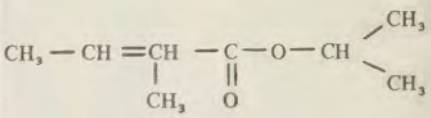
For References 1–5, see Introduction to Part II.

6. van Praag et al., *J. Agric. Food Chem.*, 16, 1005, 1968.

	Isopropyl phenylacetate	3-(*p*-Isopropylphenyl)-propionaldehyde
Other names	Isopropyl α-toluate	Cuminyl acetaldehyde *p*-Cymyl propanal *p*-Isopropylhydrocinnamaldehyde 3-(*p*-Isopropylphenyl)-propionic aldehyde
Empirical formula	$C_{11}H_{14}O_2$	$C_{12}H_{16}O$
Structure		
Physical chemical characteristics[5]		
Appearance	Liquid	Colorless, viscous liquid
Molecular weight	178.23	176.26
Boiling point	253 C	
Specific gravity	1.0096 at 20°C	
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics	Fragrant, rose-like scent; sweet, honey-like flavor with a wine undertone	Powerful, sweet, green, floral odor; peculiar, sweet, green, fruity flavor
Synthesis		By condensation of cumin aldehyde with acetaldehyde, followed by hydrogenation to the saturated aldehyde; also from cumyl magnesium chloride and propyl formate, followed by acid hydrolysis of the acetal
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.20–0.50 ppm Ice cream, ices, etc. 1.8 ppm Candy 0.50–8.0 ppm Baked goods 3.0–8.0 ppm	Non-alcoholic beverages 0.80 ppm Ice cream, ices, etc. 0.80 ppm Candy 1.3 ppm Baked goods 3.0 ppm Chewing gum 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2956	FDA 121.1164; FEMA No. 2957

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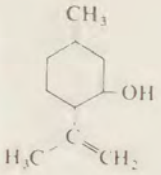
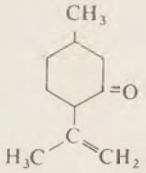
For References 1–5, see end of Part III.

	Isopropyl propionate	Isopropyl tiglate
Other names		Isopropyl-α-methyl crotonate Isopropyl-3-methyl-2-butenoate
Empirical formula	$C_6H_{12}O_2$	$C_8H_{15}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	
Molecular weight	116.16	143.20
Boiling point	108–110°C	
Specific gravity	0.8660 at 20°C	
Refractive index	1.3872 at 20°C	
Solubility	Completely miscible with alcohol and with diluted alcohol	
Organoleptic characteristics	Bittersweet taste reminiscent of plum	
Synthesis	By direct esterification in benzene solution and in the presence of *p*-toluenesulfonic acid[8]	By photolysis of 2,2,5,5-tetramethyldihydro-3-furanone in methanol;[6] also by esterification of 3-methyl-2-butenoic acid with isopropyl alcohol in the presence of concentrated sulfuric acid[7]
Natural occurrence	In raspberry and currant	
Reported uses[3]	Non-alcoholic beverages 9.7 ppm Ice cream, ices, etc. 5.0–50 ppm Candy 40–50 ppm Baked goods 30–50 ppm	Baked goods 5.0 ppm Gelatins and puddings 1.0 ppm Soups 1.0 ppm Salad oil 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2959	FEMA No. 3229

REFERENCES

For References 1–5, see end of Part III.

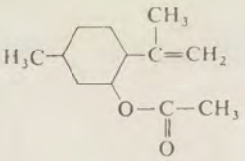
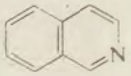
6. **Hagens, Wasacz, Joullie and Yates,** *J. Org. Chem.*, 35, 3682, 1970.
7. **Hagens et al.,** *J. Org. Chem.*, 35, 3682, 1970.
8. **Salmi and Leimu,** *Chem. Abstr.*, 42, 4031, 1948

	Isopulegol	Isopulegone
Other names	*p*-Menth-8-en-3-ol 1-Methyl-4-isopropenylcyclohexan-3-ol	*p*-Menth-8-en-3-one 1-Methyl-4-isopropenylcyclohexan-3-one 1-Methyl-4-isopropenyl-3-cyclohexanone
Empirical formula	$C_{10}H_{18}O$	$C_{10}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	154.24	152.23
Boiling point	*l*-iso, 94 C at 14 mm Hg; *d*-neoiso, 95 C at 17 mm Hg; *d*-neoiso, 96 C at 15 mm Hg	101–102°C at 17 mm Hg
Specific gravity	*l*-iso, 0.9110 at 20 C; *d*-neoiso, 0.9107 at 25 C	0.92177 at 20.4°C
Refractive index	*l*-iso, 1.4723 at 20 C; *d*-neoiso, 1.4686 at 25 C; *d*-neoiso, 1.4775 at 10°C	1.46787 at 20.4°C
Optical rotation	*l*-iso, −25.9°; *d*-neoiso, +39.3°	
Synthesis	Several stereoisomers are possible. Only *l*-isopulegol and *d*-neoisopulegol have been isolated from mixtures of alcohols obtained by cyclization of *d*-citronellal[6]	The structure of isopulegone was defined by Tiemann and Schmidt[7] as well as by Hugh, Kon, and Linstead;[8] usually prepared from isopulegol.[8]
Natural occurrence	*l*-Isopulegol has been reported found in the essences of lemongrass, East African geranium, and *Eucalyptus citriodora*. *d*-Isopulegol is present in the oils of *Backhousia* and *Baeckea citriodorae*. *d*-Neoisopulegol is found in *Mentha rotundifolia*.	Natural isopulegone is dextrorotatory. Reported found in the essential oils from leaves of *Bystropogon mollis*, *Mentha timija*, and others
Reported uses[3]	Non-alcoholic beverages 7.4 ppm Ice cream, ices, etc. 29 ppm Candy 23 ppm Baked goods 23 ppm	Non-alcoholic beverages 4.0 ppm Ice cream, ices, etc. 12 ppm Candy 16 ppm Baked goods 16 ppm
Regulatory status	FDA 121.1164; FEMA No. 2962	FDA 121.1164; FEMA No. 2964

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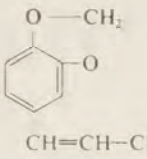
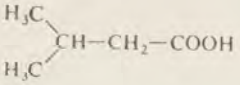
For References 1–5, see end of Part III.

6. **Pickard et al.**, *J. Chem. Soc.* (London), 117, 1248, 1920.
7. **Tiemann and Schmidt**, *Ber. Dtsch. Chem. Ges.*, 29, 914, 1896.
8. **Hugh, Kon and Linstead**, *J. Chem. Soc.*, (London), p. 2585, 1927.

	Isopulegyl acetate	Isoquinoline
Other names		2-Benzazine Benzo(*c*)pyridine
Empirical formula	$C_{12}H_{20}O_2$	C_9H_7N
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Low-melting, crystalline solid
Assay	95% min	
Molecular weight	196.29	129.15
Melting point		26.5°C
Boiling point	104–105°C at 10 mm Hg	243°C
Flash point	87°C	
Specific gravity	0.932–0.936 (0.9394) at 20°C	1.0980 at 20°C
Refractive index	1.4572 at 20°C	1.61478 at 20°C
Optical rotation	−1.1°	
Acid value	1 max	
Solubility	1:4 in 70% alcohol; 1:2 in 80% alcohol	Slightly soluble in water; soluble in most organic solvents
Organoleptic characteristics	Sweet, mint-like odor	Odor reminiscent of benzaldehyde and anise
Synthesis	By prolonged heating of citronellal with acetic anhydride (with or without sodium acetate)	Obtained from coal tar (238–250°C boiling fraction). It is isolated as the sulfate or as is by repeated freezing.[6]
Natural occurrence	Not reported found in nature	Not reported found in nature; occurs in coal tar, where it is formed during the dry distillation of coal
Reported uses[3]	Non-alcoholic beverages 5.8 ppm Ice cream, ices, etc. 22 ppm Candy 19 ppm Baked goods 19 ppm	Non-alcoholic beverages 0.25 ppm Ice cream, ices, etc. 0.25 ppm Candy 1.0 ppm Baked goods 0.004–1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2965	FDA 121.1169; FEMA No. 2978

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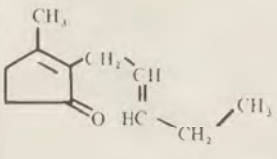
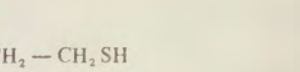
For References 1–5, see end of Part III.
6. Kjellman, U.S. Patent 2,483,420, 1949.

	Isosafrole	Isovaleric acid
Other names	3,4-Methylenedioxy-l-propenylbenzene	Delphinic acid Isobutyl formic acid Isopropylacetic acid β-Methyl butyric acid Valerianic acid
Empirical formula	$C_{10}H_{10}O_2$	$C_5H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Dense, colorless liquid
Molecular weight	162.18	102.13
Melting point	6.7–6.8 C	−30°C
Boiling point	252 C (127–128 C at 15 mm Hg)	176.5°C
Flash point		70°C
Specific gravity	1.122 at 20 C	0.93080 at 15°C
Refractive index	1.5777 at 20 C	1.4064 at 15°C
Solubility	Soluble in most organic solvents	Soluble in water (forms the hydrate $C_5H_{10}O_2 \cdot H_2O$ with 30 parts of water), alcohol, ether, and chloroform
Organoleptic characteristics	Anise odor	Characteristic disagreeable odor, extremely penetrating and persistent; sour taste
Synthesis	By alkaline isomerization of safrole using KOH at the boil[6] or an alcoholic NaOH solution at room temperature under pressure[7]	By oxidation of isoamyl alcohol or isovaleric aldehyde
Natural occurrence	Of the two isomers (*cis*- and *trans*-), the *trans*-form is the more stable and has been isolated in the pure state, probably occurring in the essential oil of ylang-ylang. It has been identified in the oils of *Illicium religiosum*[8] and *Ligusticum acutilobum* Sieb. and Zucc.[9]	Of the three possible isomers of *n*-valeric acid, only isovaleric acid finds extensive application in flavoring. Originally reported in seal and dolphin fat; subsequently isolated from valerian. Also reported found in the essential oils of: cypress, citronella, laurel leaves, cajeput, *Cymbopogon javanensis*, hops, *Persea pubescens*, geranium, American peppermint, niaouli, spearmint, rosemary, lemongrass, *Eucalyptus goniocalyx* and other sp., tobacco, *Monarda fistulosa*, *Thymus mastichina*, *Artemisia frigida*, and probably in lavender. Finally, reported among the constituents of petitgrain lemon[10]
Reported uses[3]		Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 14 ppm Candy 12 ppm Baked goods 5.5 ppm Cheese 2.4 ppm
Regulatory status	Use in foods is not permitted in U.S.A.	FDA 121.1164; FEMA No. 3102

REFERENCES

For References 1–5, see end of Part III.

6. **Wagner,** *Riechst. Aromen*, p. 52, 1926.
7. **Nagai,** *Soc. Chem. Ind.* (Japan), 29, 364, 1926.
8. **Chen,** *Chem. Zentralbl.*, 1, 1163, 1930.
9. **Noguchi et al.,** *Chem. Zentralbl.*, 2, 4050, 1937.
10. **Peuron,** *Riv. Ital. EPPOS*, 8, 413, 1965.

	Jasmone	2-Keto-4-butanethiol
Other names	3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one	4-Mercapto-2-butanone
Empirical formula	$C_{11}H_{16}O$	C_4H_8OS
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellow oil	
Molecular weight	164.25	104.17
Boiling point	134–135°C at 12 mm Hg 109–110°C at 5 mm Hg 257–258°C at 755 mm Hg	59–60°C at 15 mm Hg
Specific gravity	0.9437 at 22°C 0.9466 at 15°C	
Refractive index	1.4979 at 23°C 1.50058 at 15°C	
Solubility	Slightly soluble in water; soluble in alcohol, ether, and carbon tetrachloride	
Organoleptic characteristics	Jasmine odor	
Synthesis	A review and classification on the synthesis of jasmone is available[10]	By reduction of 4-bromo-2-butanone with NaHS;[6] by reacting methyl vinyl ketone with hydrogen sulfide;[7] from methyl vinyl ketone and thioacetamide;[8] from methyl vinyl ketone and hydrogen sulfide at 12 to 15°C by a patented process[9]
Natural occurrence	The *cis*-form is reportedly occurring naturally; it is found in the essential oils of jasmine (3%), jonquil, and *Pittosporum glabratum*, in neroli oil, in peppermint (*Mentha piperita*), and in bergamot	
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Gelatins and puddings 10.0 ppm	Baked goods 0.20 ppm Meat, meat sauces, soups 0.20 ppm
Regulatory status	FEMA No. 3196	FEMA No. 3357

REFERENCES

For References 1–5, see end of Part III.

6. Asinger, Thiel and Horingklee, *Annalen*, 610, 1, 1957.
7. Murata and Arai, *J. Chem. Soc. Jap.*, 59, 129, 1956.
8. Barrett et al., *J. Chem. Soc.*, p. 788, 1964.
9. Kostyukoskii and Slavachevskaya, U.S.S.R. Patent 319,591.
10. Anonymous, *Fr. Ses Parfums*, 1(3), 39, 1958.

	Lactic acid	Lauric aldehyde
Other names	2-Hydroxypropanoic acid	Aldehyde C-12 1-Dodecanal *n*-Dodecyl aldehyde Lauraldehyde
Empirical formula	$C_3H_6O_3$	$C_{12}H_{24}O$
Structure	$CH_3-CH(OH)-COOH$	$CH_3-(CH_2)_{10}-CHO$
Physical/chemical characteristics		
Appearance	Syrupy, rather hygroscopic liquid	Colorless to yellow liquid, solidifying at low temperature
Assay		92% min[2] (96.5%)
Molecular weight	90.08	184.32
Melting point	18°C; *d,l*: 52–53°C	11°C (8°C min)
Boiling point	122°C at 15 mm Hg	237°C; 99.5–100°C at 3.5 mm Hg
Flash point		82°C (119°C)
Specific gravity	1.249 at 15°C; *d*, 1.2485 at 20°C	0.826–0.836 at 25°/25°C;[2] 0.8352 at 15°C
Refractive index		1.4330–1.4390 at 20°C;[2] 1.4328 at 24.7°C
Optical rotation	*l*, −2.6°; *d*, +2.6 (from water) at 21–22°C	
Acid value		10 max[2] (3.8)
Solubility	Completely miscible with water, alcohol, and glycerin; readily soluble in ether	Insoluble in water; soluble in alcohol and most organic solvents; 1:2 in 80% alcohol; 1:0.5 in 90% alcohol
Organoleptic characteristics	Slightly sour odor and taste	Characteristic fatty odor reminiscent of violet on dilution; fatty, woody taste
Synthesis	By fermentation from sugar or starch. The commercial product is the racemic form.	By oxidation of the corresponding alcohol or reduction of the acid
Natural occurrence	Reported found in *Papaver somniferum* L., apples and other fruits, tomato juice, and several plants. It is a constituent of wine and sour milk. The two optically active isomers are found in muscular tissues and are formed by the action of lactic-acid bacteria in several fermentation processes.	Reported found in the essential oils of: lemon, sweet orange, bitter orange, mandarin, Mexican lime, and petitgrain bigarade and in the turpentine of some varieties of pine
Reported uses[3]	Non-alcoholic beverages 34 ppm Ice cream, ices, etc. 66 ppm Candy 130 ppm Baked goods 89 ppm Gelatins and puddings 14–25 ppm Chewing gum 610 ppm Toppings 300 ppm Pickles and olives 1,200–24,000 ppm	Non-alcoholic beverages 0.93 ppm Ice cream, ices, etc. 1.5 ppm Candy 2.4 ppm Baked goods 2.8 ppm Gelatins and puddings 0.10 ppm Chewing gum 0.20–110 ppm
Regulatory status	FDA GRAS (general); FEMA No. 2611	FDA 121.1164; FEMA No. 2615

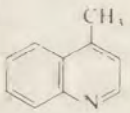
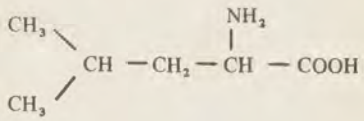
REFERENCES

For References 1–5, see end of Part III.

	Lauryl acetate	Lauryl alcohol
Other names	Acetate C-12 Dodecanyl acetate Dodecyl acetate	Alcohol C-12 Dodecyl *n*-Dodecyl alcohol 1-Dodecanol
Empirical formula	$C_{14}H_{28}O_2$	$C_{12}H_{26}O$
Structure	$CH_3-(CH_2)_{10}-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_3$	$CH_3-(CH_2)_{10}-CH_2OH$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid at room temperature; crystalline or flakes below 20 C
Assay	98% min	97% min[2] (98.5%)
Molecular weight	228.37	186.34
Melting point		26 C (21–24 C)
Boiling point		150°C at 20 mm Hg
Congealing point		>21°C[2]
Flash point		>82°C
Specific gravity	0.860–0.865 at 25°C	0.830–0.836 at 25°/25°C[2]
Refractive index	1.4320–1.4360 at 20°C	1.4400–1.4440 at 20°C[2]
Acid value		Not more than 1[2]
Solubility	1:4 in 80% alcohol; soluble in most organic solvents	1:3 and more in 70% alcohol;[2] 1:2 in 80% alcohol; insoluble in water but soluble in most organic solvents
Organoleptic characteristics	Characteristic citrus-rose odor; the corresponding flavor develops only on dilution	Characteristic fatty odor; unpleasant at high concentrations but delicate and floral on dilution; fatty, waxy flavor
Synthesis	By acetylation of lauryl alcohol	Commercially prepared by hydrogenation of lauric acid; normally employed as a replacement for the corresponding aldehyde
Natural occurrence	Reported found in several natural products	Reported found in the oil of Mexican lime and in the oil from flowers of *Furcraea gigantea*
Reported uses[3]	Non-alcoholic beverages 2.3 ppm Ice cream, ices, etc. 1.7 ppm Candy 4.6 ppm Baked goods 5.6 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.8 ppm Baked goods 1.7 ppm Chewing gum 16–27 ppm Syrups 7.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2616	FDA 121.1164; FEMA No. 2617

REFERENCES

For References 1–5, see end of Part III.

	Lepidine	L-Leucine
Other names	Cincholepidine 6-Methylquinoline* γ-Methylquinoline	α-Aminoisocaproic acid 2-Amino-4-methylpentanoic acid 2-Aminoisobutylacetic acid 2-Amino-4-methylvaleric acid
Empirical formula	$C_{10}H_9N$	$C_6H_{13}O_2N$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Hexagonal platelets (from diluted alcohol)
Molecular weight	143.18	131.18
Melting point		293–295°C (decomposes)
Boiling point	261–263°C	145–148°C (with sublimation)
Congealing point	0°C	
Specific gravity	1.086 at 20°C	1.293 at 18°C
Optical rotation		−10.42° at 20°C in water
Solubility	Slightly soluble in water; miscible with alcohol, benzene, and ether	Slightly soluble in water; insoluble in alcohol and ether
Organoleptic characteristics	Quinoline odor; tends to darken on exposure to light	Slightly bitter taste
Synthesis	From coal tar, by synthesis from *p*-aminobenzaldehyde and acetone	By bromination, followed by amination of isocaproic acid;[6] via the acetamidomalonic ester;[7] by isolation from gluten, casein, keratin;[8] from hydantoin[9]
Natural occurrence		Reported found as a constituent in proteins; also present in the free state in the human body
Reported uses[3]	In whisky 0.22 ppm Ice cream, ices, etc. 1.4 ppm Candy 1.8 ppm Baked goods 1.8 ppm	Non-alcoholic beverages 50.0 ppm Baked goods 50.0 ppm Condiments, pickles 50.0 ppm Meat, meat sauces, soups 50.0 ppm Milk, dairy products 50.0 ppm Cereals 50.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2744	FEMA No. 3295

*The term *p*-methylquinoline, although sometimes used, is a misnomer.

REFERENCES

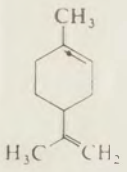
For References 1–5, see end of Part III.

6. Horning, *Organic Syntheses*, Coll. Vol. 3, Wiley & Sons, New York, 1955, 523.
7. Albertson and Archer, *J. Am. Chem. Soc.*, 67, 308, 1945.
8. Barnett, *J. Biol. Chem.*, 100, 543, 1933; U.S. Patent 2,009,868.
9. White, U.S. Patent 2,557,920, assigned to Dow Chemical Co., 1951.

	Levulinic acid
Other names	β-Acetylpropionic acid γ-Ketovaleric acid 4-Oxopentanoic acid
Empirical formula	$C_5H_8O_3$
Structure	$CH_3-\overset{\overset{O}{\|}}{C}-CH_2-CH_2-COOH$
Physical, chemical characteristics[2]	
Appearance	White, crystalline solid
Molecular weight	116.12
Melting point	37°C
Boiling point	139–140°C at 8 mm Hg
Specific gravity	1.147 at 18°C (over cooled liquid)
Refractive index	1.4342 at 40°C
Solubility	Readily soluble in water, alcohol, and ether
Synthesis	By action of more or less concentrated HCl on sucrose, glucose, or fructose; hence, its reported presence in caramels
Natural occurrence	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 14 ppm Ice cream, ices, etc. 14 ppm Candy 53 ppm Baked goods 53 ppm Gelatins and puddings 4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2627

REFERENCES

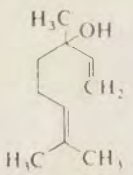
For References 1–5, see end of Part III.

	Limonene (*d*-, *l*-, and *dl*-)
Other names	Cajeputene Carvene Dipentene Kautschin 1,8(9)-*p*-Menthadiene *p*-Mentha-1,8-diene 1-Methyl-4-isopropenyl-1-cyclohexene
Empirical formula	$C_{10}H_{16}$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid
Molecular weight	136.23
Boiling point	*dl*-, 176–178°C
Specific gravity	*d*-, 0.838–0.843 at 25°/25°C;[2] *d*- and *l*-, 0.8403 at 20°C; *dl*-, 0.8481 at 15°C
Refractive index	*d*-, 1.4710–1.4740 at 20°C;[2] *d*- and *l*-, 1.4701–1.4706 at 25°C
Optical rotation	*d*-, +96° to +104°;[2] *d*-, +126.6°; *l*-, −126.3°
Peroxide value	*d*-, not more than 2.0
Solubility	Insoluble in water; miscible with alcohol
Organoleptic characteristics	Pleasant, lemon-like odor free from camphoraceous and turpentine-like notes[2]
Synthesis	*d*-Limonene may be obtained by steam distillation of citrus peels and pulp resulting from the production of juice and cold-pressed oils, or from deterpenation of citrus oils. It is sometimes redistilled.
Natural occurrence	The most important and widespread terpene. It is known in the *d*- and *l*- optically active forms and in the optically inactive *dl*-form (known as dipentene). It has been reported found in more than 300 essential oils in amounts ranging from 90–95% (lemon, orange, mandarin) to as low as 1% (palmarosa).[6] The most widespread form is the *d*-limonene, followed by the racemic form, and then *l*-limonene.
Reported uses[3]	Non-alcoholic beverages 31 ppm Ice cream, ices, etc. 68 ppm Candy 49 ppm Baked goods 120 ppm Gelatins and puddings 48–400 ppm Chewing gum 2,300 ppm
Regulatory status	FDA GRAS; FEMA No. 2633 (*d*-form)

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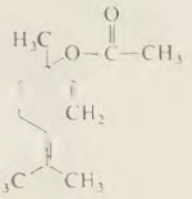
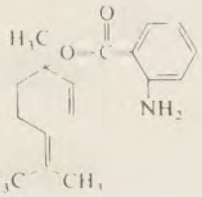
For References 1–5, see end of Part III.

6. Gildemeister and Hoffmann, *Die Aetherischen Oele*, Vol. IIIa, Akademie Verlag, 1960, pp. 45–46.

	Linalool
Other names	Coriandrol (*d*-linalool from coriander oil) 3,7-Dimethyl-1,6-octadien-3-ol Licarcol (*l*-linalool from bois de rose oil) *dl*-Linalool (synthetic)
Empirical formula	$C_{10}H_{18}O$
Structure	
Physical/chemical characteristics[5]	The following constants refer to the synthetic product. These may vary within an ample range for a product of natural origin, depending on the source.
Appearance	Colorless liquid
Assay	>95%[2]
Molecular weight	154.24
Boiling point	198 C
Flash point	78 C
Specific gravity	0.858–0.862 at 25 C[2]
Refractive index	1.4600–1.4630 at 20 C[2]
Saponification number	Not more than 1.5[2]
Solubility	1:4 in 60% alcohol;[2] insoluble in water; miscible with alcohol and ether
Organoleptic characteristics	Typical floral odor free from camphoraceous and terpenic notes.[2] Synthetic linalool exhibits a cleaner and fresher note than the natural product.
Synthesis	It can be prepared synthetically starting from myrcene or from dehydrolinalool. It can be obtained by fractional distillation and subsequent rectification from the oils of Cajenne rosewood (*Licasia guaianensis*, *Ocotea caudata*), Brazil rosewood (*Ocotea parviflora*), Mexican linaloe, shiu (*Cinnamomum camphora* Sieb. var. *linaloöifera*), and coriander seeds (*Coriandrum sativum* L.).
Natural occurrence	The optically active forms (*d*- and *l*-) and the optically inactive form occur naturally in more than 200 oils from herbs, leaves, flowers, and wood. The *l*-form is present in the largest amounts (80–85%) in the distillates from leaves of *Cinnamomum camphora* var. *orientalis* and *Cinnamomum camphora* var. *occidentalis* and in the distillate from Cajenne rosewood. It also has been reported in: champaca, ylang-ylang, neroli, Mexican linaloe, bergamot, lavandin, and others. A mixture of *d*- and *l*-linalool has been reported in Brazil rosewood (85%). The *d*-form has been found in palmarosa, mace, sweet orange-flower distillate, petitgrain, coriander (60–70%), marjoram, *Orthodon linaloöliferum* (80%), and others. The inactive form has been reported in clary sage, jasmine, and *Nectandra elaiophora*.
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 3.6 ppm Candy 8.4 ppm Baked goods 9.6 ppm Gelatins and puddings 2.3 ppm Chewing gum 0.80–90 ppm Condiments 40 ppm
Regulatory status	FDA GRAS; FEMA No. 2635

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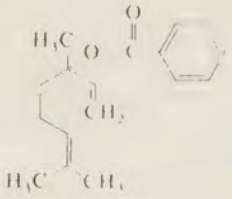
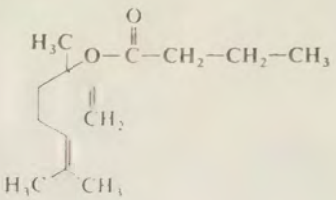
For References 1–5, see end of Part III.

	Linalyl acetate	Linalyl anthranilate
Other names	Bergamol 3,7-Dimethyl-1,6-octadien-3-yl acetate	3,7-Dimethyl-1,6-octadien-3-yl anthranilate Linalyl-2-aminobenzoate Linalyl-*o*-aminobenzoate
Empirical formula **Structure**	$C_{12}H_{20}O_2$ 	$C_{17}H_{23}NO_2$ 
Physical/chemical characteristics[5]	The physical constants differ within an ample range, depending on the natural source or on the synthetic route.	
Appearance	Colorless liquid	Liquid, almost colorless or very pale straw-yellow
Assay	95% (syn)	
Molecular weight	196.29	273.38
Boiling point	115–116°C at 25 mm Hg (nat)	350°C
Flash point	85°C (nat)	
Specific gravity	0.9060 at 15°C (nat); 0.895–0.905 at 25°C (syn)	1.055 at 15.5°C
Refractive index	1.4500 at 20°C (nat); 1.4495–1.4512 at 20°C (syn)	1.4970 at 20°C
Optical rotation	−7 42′ to +8 18′ (nat); ±0 (syn)	
Acid value	0.5 max (syn)	
Solubility	1:3–5 in 70% alcohol; soluble in essential oils and most common organic solvents	Insoluble in water; almost insoluble in propylene glycol; soluble in alcohol
Organoleptic characteristics	Characteristic bergamot-lavender odor and persistent sweet, acrid taste	Sweet orange-like flavor; fragrance varies, depending on the source of linalool
Synthesis	Normally prepared by direct acetylation of linalool;[6] another method starts from myrcene hydrochloride, anhydrous sodium acetate, and acetate anhydride in the presence of a catalyst.[7] All synthetic methods tend to avoid the simultaneous formation (because of isomerization) of terpenyl and geranyl acetate.	From linalool and isatoic anhydride with catalytic amounts of sodium hydroxide; from linalyl formate plus methylanthranilate with sodium linalool
Natural occurrence	Reported found in the essential oils of bergamot, lavender, clary sage, and lavandin; also identified among the constituents of the essential oils of: *Salvia officinalis*, petitgrain, sassafras, neroli, lemon, Italian lime, jasmine, *Mentha citrata*, *Mentha aquatica*, *Thymus mastichina*, etc. Also reported in abundant quantities in the essential oil from flowers, leaves, and stems of *Tagetes patula*,[8] in the distillate from leaves of *Citrus aurantifolia*[9] from India, and in the essential oil of *Mentha arvensis*.[10]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages, 1.9 ppm; ice cream, ices, etc., 3.8 ppm; candy, 11 ppm; baked goods, 8.9 ppm; gelatins and puddings, 3.8 ppm; chewing gum, 13 ppm	Non-alcoholic beverages, 1.8 ppm; ice cream, ices, etc., 0.72 ppm; candy, 4.7 ppm; baked goods, 0.20–8.0 ppm
Regulatory status	FDA GRAS; FEMA No. 2636	FDA 121.1164; FEMA No. 2637

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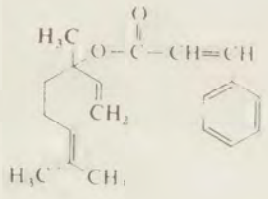
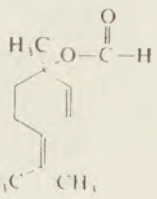
For References 1–5, see end of Part III.

6. Tiemann, *Chem. Ber.*, 31, 839, 1898.
7. U.S. Patent 2,794,826, 1957.
8. Dhingra and Dhingra, *Perfum. Essent. Oil Rec.*, 47, 391, 1956.
9. Banerji and Kumar, *Perfum. Essent. Oil Rec.*, 48, 343, 1957.
10. Chagawets and Borisyuk, *Miltizer Ber.*, p. 61, 1958.

	Linalyl benzoate	Linalyl butyrate
Other names		Linalyl-*n*-butyrate
Empirical formula	$C_{17}H_{22}O_2$	$C_{14}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellow or yellow-brownish liquid; high-quality grades almost colorless	Colorless or yellowish liquid
Assay	75% min	95% min
Molecular weight	258.37	224.34
Boiling point	263°C	232 C
Flash point	98°C	100 C
Specific gravity	0.980–0.999 at 25°C	0.893–0.904 at 25/25 C; 0.8890–0.8903 at 20 C
Refractive index	1.505–1.520 at 20°C	1.451–1.456 at 20 C; 1.4483–1.4492 at 25°C
Optical rotation		±1 (optically inactive if obtained from synthetic linalool)
Acid value	5 max	1 max
Solubility	1:1 in 90% alcohol	1:3 in 80% alcohol
Organoleptic characteristics	Heavy odor reminiscent of genet, bergamot, and lily	Fruity note with a bergamot-like undertone; flavor reminiscent of certain types of honey on dilution; moderately stable
Synthesis	From linalool and benzoyl chloride in the presence of pyridine	Analogous to that of geranyl butyrate
Natural occurrence	Reported found in the essential oils of ylang-ylang and tuberose[6]	Reported found in the oil of *Artemisia porrecta* var. *coerulea* and in lavender oil[7,8]
Reported uses[3]	Non-alcoholic beverages 0.31 ppm Ice cream, ices, etc. 0.42 ppm Candy 1.2 ppm Baked goods 1.6 ppm Gelatins and puddings 0.28 ppm	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 4.3 ppm Candy 2.2 ppm Baked goods 13 ppm Gelatins and puddings 0.09 ppm
Regulatory status	FDA 121.1164; FEMA No. 2638	FDA 121.1164; FEMA No. 2639

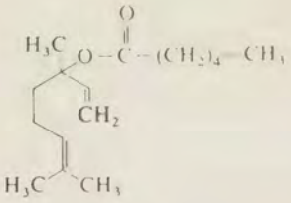
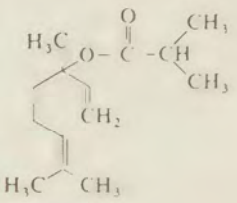
REFERENCES

For References 1–5, see end of Part III.
6. Labaune, *Traites Chim. Org.*, 22, 1047, 1953.
7. Burger, *Riechstoffindustrie*, p. 132, 1926.
8. Burger, *Riv. Ital. EPPOS*, 7, 450, 1966.

	Linalyl cinnamate	Linalyl formate
Other names	Linalyl β-phenylacrylate Linalyl 3-phenylpropenoate	3,7-Dimethyl-1,6-octadien-3-yl formate
Empirical formula	$C_{19}H_{24}O_2$	$C_{11}H_{18}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to yellowish liquid
Assay		90% min[2]
Molecular weight	284.40	182.26
Boiling point	353°C	102°C (202°C) at 10 mm Hg
Flash point		87.5°C
Specific gravity	0.980 at 15.5°C	0.910–0.918[2] (0.915–0.924) at 25/25°C
Refractive index	1.5330 at 20°C	1.453–1.458[2] (1.4550–1.4580) at 20°C
Acid value		Not more than 3.0[2] (1)
Solubility	Insoluble in water; soluble in alcohol	1:6 in 70% alcohol;[2] 1:1 in 80% alcohol; insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Sweet, persistent odor with soft floral notes; clearly balsamic; slightly fruity flavor	Fruity, floral (rose) odor reminiscent of bergamot and vervain; bittersweet flavor with pineapple-like undernote
Synthesis	From linalyl formate plus methylcinnamate and sodium linalool; by "Roche" method from dehydrolinalool and cinnamic acid via the dehydro ester, which is hydrolyzed to the subject compound	By the esterification of linalool with formic acid
Natural occurrence	Not reported found in nature	Reported found in nature: *Lavandula*, *Prunus armeniaca*, *Prunus persica*, and *Salvia sclarea*, peach, oil of lime, petitgrain
Reported uses[3]	Non-alcoholic beverages 0.57 ppm Ice cream, ices, etc. 0.59 ppm Candy 2.0 ppm Baked goods 2.1 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 12 ppm Candy 3.8 ppm Baked goods 13 ppm Chewing gum 1.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2641	FDA 121.1164; FEMA No. 2642

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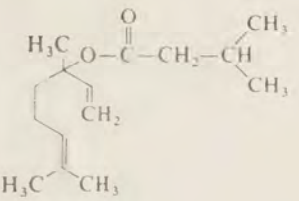
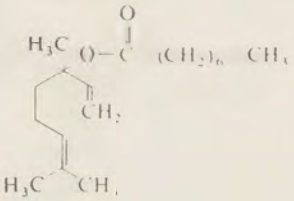
For References 1–5, see end of Part III.

	Linalyl hexanoate	Linalyl isobutyrate
Other names	Linalyl caproate Linalyl capronate Linalyl hexylate	3,7-Dimethyl-1,6-octadien-3-yl isobutyrate
Empirical formula	$C_{16}H_{28}O_2$	$C_{14}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless to slightly yellow liquid
Assay		95% min[2]
Molecular weight	252.40	224.34
Boiling point	252°C	
Flash point		>100°C
Specific gravity	0.90	0.882–0.888 at 25°/25°C;[2] 0.8926 at 15°C
Refractive index		1.446–1.451[2] (1.4490) at 20°C
Acid value		Not more than 1.0[2]
Optical rotation		−10.54° at 20°C (undiluted)
Solubility	Insoluble in water; soluble in alcohol	1:3 in 80% alcohol[2]
Organoleptic characteristics	Green, warm, fruity odor with an animal-like undertone; pineapple-pear flavor	Light, fruity odor with a lavender note; sweet flavor reminiscent of black currant
Synthesis	By esterification of dehydrolinalool with *n*-hexanoic acid followed by hydrogenation at the dehydro ester	By esterification of linalool with isobutyric anhydride
Natural occurrence		Reported found in the essential oil of Ceylon cinnamon and in lavender oil.[6,7] A *dextro*-rotatory form has been reported in the oil from leaves of *Agathosoma gnidioides* (Schlechter)[9]
Reported uses[3]	Non-alcoholic beverages 3.2 ppm Ice cream, ices, etc. 6.0 ppm Candy 11 ppm Baked goods 15 ppm	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 2.8 ppm Candy 4.9 ppm Baked goods 13 ppm
Regulatory status	FDA 121.1164; FEMA No. 2643	FDA 121.1164; FEMA No. 2640

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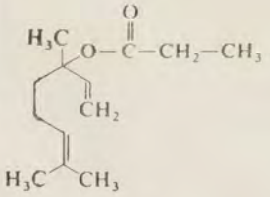
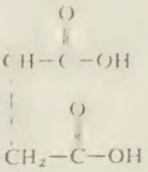
For References 1–5, see end of Part III.

6. Bürger, *Riechstoffindustrie*, p. 132, 1926.
7. Kauffmann and Kjelsberg, *Riechstoffindustrie*, 2, 171.
8. Smith and Roux, *Trans. R. Soc. S. Afr.*, 31, 340, 1947; *Chem. Abstr.*, 41, 7673, 1947.

	Linalyl isovalerate	Linalyl octanoate
Other names	Linalyl isopentanoate	Linalyl caprylate Linalyl octoate Linalyl octylate
Empirical formula	$C_{15}H_{26}O_2$	$C_{18}H_{32}O_2$
Structure		
Physical/chemical characteristics[4]		
Appearance	Liquid	Colorless, oily liquid
Assay	96% min	
Molecular weight	238.37	280.46
Boiling point		264 C
Specific gravity	0.8940–0.9000 at 15 C	0.88
Refractive index	1.4510–1.4540 at 20 C	
Acid value	0.09 max	
Solubility	1:5.5–7 in 80% alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Stable, suave, fruity odor; sweet, apple-like taste somewhat reminiscent of plum and peach	Dry, fruity, herbaceous odor; sweet apricot and plum-like taste with a perfumey note
Synthesis	From dehydrolinalool and isovaleric acid followed by hydrogenation; also from linalool and isovaleric acid by azeotropic esterification	By esterification of linalool with *n*-octanoic acid under azeotropic conditions; also by hydrogenation of dehydrolinalyl octanoate
Natural occurrence	Reported found in nature (*Salvia officinalis* and *Salvia spinosa*)	Reported found in lemongrass
Reported uses[3]	Non-alcoholic beverages 0.96 ppm Ice cream, ices, etc. 0.91 ppm Candy 5.7 ppm Baked goods 5.6 ppm Gelatins and puddings 0.10 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 0.50–3.0 ppm Candy 0.50 ppm Baked goods 0.60–15 ppm
Regulatory status	FDA 121.1164; FEMA No. 2646	FDA 121.1164; FEMA No. 2644

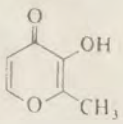
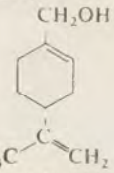
REFERENCES

For References 1–5, see end of Part III.

	Linalyl propionate	Malic acid
Other names	3,7-Dimethyl-1,6-octadien-3-yl propanoate	"Apple acid" (*l*-form found in apple) 2-Hydroxy-1,4-butanedioic acid Hydroxysuccinic acid
Empirical formula	$C_{13}H_{22}O_2$	$C_4H_6O_5$
Structure		
Physical/chemical characteristics[4]		
Appearance	Almost colorless liquid	Crystalline solid
Assay	92% min[2] (95%)	
Molecular weight	210.31	134.09
Melting point		*l*-, 99–100°C; *d*-, 99–101°C
Boiling point	115°C (226°C) at 10 mm Hg	*l*-, approx 140°C (with decomposition)
Specific gravity	0.895–0.902[2] (0.8940–0.8954) at 25°/25°C	*l*-, 1.595 at 20°C
Refractive index	1.4500–1.4550[2] (1.4495–1.4510) at 20°C	
Optical rotation	±1[2]	At 18°C (in acetone): *l*-, −5.7°; *d*-, +5.2°
Acid value	1 max[2] (0.5)	
Solubility	1:7 in 70% alcohol; very slightly soluble in water; slightly soluble in propylene glycol; insoluble in glycerin	Readily soluble in alcohol and water; slightly soluble in ether
Organoleptic characteristics	Sweet, floral odor reminiscent of bergamot oil; sweet taste reminiscent of black currant (also pear and pineapple)	Nearly odorless (sometimes a faint, acrid odor); tart, acidic taste; non-pungent
Synthesis	By esterification of linalool with propionic acid or propionic anhydride	By hydration of maleic acid; by fermentation from sugars
Natural occurrence	The *l*-form has been reported found in lavender and sage	Occurs in maple sap, apple, and many other fruits
Reported uses[3]	Non-alcoholic beverages 4.9 ppm Ice cream, ices, etc. 3.6 ppm Candy 5.3 ppm Baked goods 12 ppm Gelatins and puddings 4.4 ppm	Non-alcoholic beverages 380 ppm Ice cream, ices, etc. 390 ppm Candy 420 ppm Baked goods 0.60–1.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2645	FDA GRAS; FEMA No. 2655

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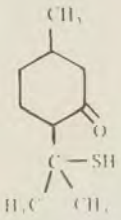
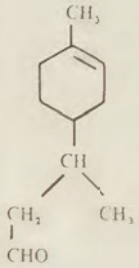
For References 1–5, see end of Part III.

	Maltol	*p*-Mentha-1,8-dien-7-ol
Other names	3-Hydroxy-2-methyl-(1,4-pyran) 3-Hydroxy-2-methyl-4H-pyran-4-one 3-Hydroxy-2-methyl-4-pyrone Larixinic acid 2-Methyl pyromeconic acid	1-Hydroxymethyl-4-isopropenyl-1-cyclohexene Perillyl alcohol
Empirical formula	$C_6H_6O_3$	$C_{10}H_{16}O$
Structure		
Physical/chemical characteristics[5]		The following values are for the *d*- and *l*-forms present in ginger grass oil; constants vary according to the source.[6,7,8]
Appearance	Monoclinic prisms from chloroform; orthorhombic bipyramidal crystals from alcohol; white crystals usually	Dense, oily liquid
Molecular weight	126.11	152.23
Melting point	159–162°C (164°C); volatile with steam; sublimes at 93°C	
Boiling point		*l*-, 92–93°C at 5 mm Hg; *d*-, 94–96°C at 4–5 mm Hg
Specific gravity		At 15°C: *l*-, 0.9510; *d*-, 0.9536
Refractive index		At 20°C: *l*-, 1.49629; *d*-, 1.49761
Optical rotation		*l*-, −13.9°; *d*-, +12.7°
Solubility	Soluble in alcohol and chloroform; 1.2% in water; sparingly soluble in benzene, ether, and petroleum ether. Soluble in NaOH solutions yielding CO_2; 1.2% in glycerin; 2.8% in propylene glycol	
Organoleptic characteristics	Warm, sweet, fruity odor; jam-like odor in solution	Characteristic odor similar to linalool and terpineol
Synthesis	By alkaline hydrolysis of streptomycin salts; also from piperidine to pyromeconic acid and subsequent methylation at the 2 position	The *l*-form is obtained starting from β-pinene or by reducing perillic aldehyde with zinc dust and acetic acid, followed by saponification of the acetate. For structural studies see reference 9.
Natural occurrence	Reported found in the bark of young larch trees (*Pinus larix*), pine needles (*Abies alba*), chicory, wood tars and oils, and roasted malt	The *d*- and *l*-forms occur naturally in ginger grass essential oil; the *l*-form is found in lavandin and bergamot, while the *d*-form is found in caraway; also reported found in either form in the essential oils of *Juniperus sabina* L., East Indian geranium, and others
Reported uses[3]	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 8.7 ppm Candy 31 ppm Baked goods 30 ppm Gelatins and puddings 7.5 ppm Chewing gum 90 ppm Jellies 15 ppm	Non-alcoholic beverages 0.50–1.0 ppm Ice cream, ices, etc. 0.50–1.0 ppm Candy 20 ppm Baked goods 10–50 ppm
Regulatory status	FDA 121.1164; FEMA No. 2656	FDA 121.1164; FEMA No. 2664

REFERENCES

For References 1–5, see end of Part III.

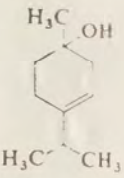
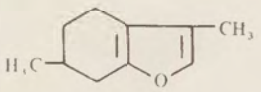
6. Semmler and Zaar, *Ber. Dtsch. Chem. Ges.*, 44, 460, 1911.
7. Semmler and Zaar, *Ber. Dtsch. Chem. Ges.*, 44, 54, 1911.
8. Elze, *Chem. Ztg.*, 34, 767, 1910.
9. Semmler and Zaar, *Ber. Dtsch. Chem. Ges.*, 44, 52, 460, 1911.

	p-Mentha-8-thiol-3-one		*p*-Menth-1-ene-9-al	
Other names	8-Mercapto-*p*-menthane-3-one		Carvomenthenal	
Empirical formula	$C_{10}H_{18}OS$		$C_{11}H_{18}O$	
Structure				
Physical/chemical characteristics				
Molecular weight	185.31			
Boiling point	62°C at 0.1 mm Hg (mixture of stereoisomers)			
Refractive index	1.4948–1.4951 (mixture of stereoisomers)			
Optical rotation	(*trans*-form), −32° at 20°C (c = 0.117 g/100 ml in CH_3OH) (*cis*-form), +40° at 20°C (c = 0.127 g/100 ml in CH_3OH)			
Organoleptic characteristics	Black-currant flavor			
Synthesis	By reaction of pulegone or isopulegone with hydrogen sulfide excess and ethanolic potassium hydroxide[6]			
Natural occurrence	In buchu leaf oil[7]			
Reported uses[3]	Non-alcoholic beverages	1.0 ppm	Non-alcoholic beverages	2.0 ppm
	Ice cream, ices, etc.	1.0 ppm	Ice cream, ices, etc.	2.0 ppm
	Candy	1.0 ppm	Candy	2.0 ppm
	Baked goods	1.0 ppm	Gelatins and puddings	2.0 ppm
	Gelatins and puddings	1.0 ppm		
	Chewing gum	1.0 ppm		
Regulatory status	FEMA No. 3177		FEMA No. 3178	

REFERENCES

For References 1–5, see end of Part III.

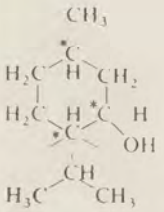
6. German Patent, 2,043,341.
7. Lamparsky and Schudel, *Tetrahedron Lett.*, 3, 3323, 1971.

	p-Menth-3-en-1-ol	Menthofuran
Other names	Δ_3-*para*-Menthen-1-ol 1-Methyl-4-isopropyl-3-cyclohexen-1-ol 1-Terpinenol	4,5,6,7-Tetrahydro-3,6-dimethylbenzofuran
Empirical formula	$C_{10}H_{18}O$	$C_{10}H_{14}O$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless, oily liquid	Bluish liquid
Assay	*Note*: This ingredient is considered an undesirable component of commercial terpineol.	
Molecular weight	154.24	150.22
Boiling point	92–97 C (210 C) at 14 mm Hg	80°C at 18 mm Hg 90–92°C at 3 mm Hg
Specific gravity	0.9210 at 24 C	0.965 at 15°C
Refractive index	1.4778 at 24 C	1.4807 at 20°C
Optical rotation		+92.5 at 25°C
Solubility	Slightly soluble in water; soluble in alcohol, propylene glycol, and various oils	
Organoleptic characteristics	Dry, woody, somewhat musty odor	Odor very similar to that of menthol
Synthesis	Prepared by Wallach[6]	By thermal decomposition of the sulfone of 3-hydroxy-3,8(9)-methadiene-9-sulfonic acid; the latter is obtained by the sulfonapulegone in acetic anhydride[6]
Natural occurrence	Reported found in camphor essential oil	Reported found in peppermint oil[7]
Reported uses[3]		Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm
Regulatory status	FDA 121.1164	FEMA No. 3235

REFERENCES

For References 1–5, see end of Part III.

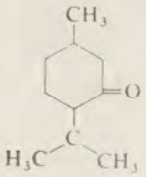
6. Wallach, *Annalen*, 356, 218, 1907; 362, 269, 1908.
7. Eastman, *J. Am. Chem. Soc.*, 72, 5313, 1950.
8. Wienhaus, *A. Angew. Chem.*, 47, 415, 1934.

	Menthol
Other names	Hexahydrothymol 3-*p*-Menthanol *p*-Menthan-3-ol *l*-Menthol 1-Methyl-4-isopropylcyclohexan-3-ol
Empirical formula	$C_{10}H_{20}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Crystals or granules
Assay	See Reference 6
Molecular weight	156.27
Melting point	42–43 C for *l*-form
Boiling point	216.5°C for *l*-form; 111°C at 20 mm Hg for *l*-form
Specific gravity	0.904 at 15°/15°C; 0.9007 at 20°C; 0.8911 at 30°C
Refractive index	1.461 at 20°C; 1.460 at 22°C; 1.4580 at 25°C; 1.4461 at 60°C
Optical rotation	-50°0′ (in alcohol) at 20°C; -49°0′ (c-2.0 in alcohol) at 16°C
Solubility	Slightly soluble in water; very soluble in alcohol, chloroform, ether, pet ether, glacial acetic acid, and liquid petrolatum
Organoleptic characteristics	Mint-like odor; fresh, cooling taste
Synthesis	By hydrogenation of thymol (see References 7 and 8). For a complete review of the various menthols, see Reference 9.
Natural occurrence	In peppermint and other mint oils (e.g., *M. arvensis*)
Reported uses[3]	Non-alcoholic beverages 35 ppm Ice cream, ices, etc. 68 ppm Candy 400 ppm Baked goods 130 ppm Chewing gum 1,100 ppm
Regulatory status	FDA 121.1164; FEMA No. 2665

REFERENCES

For Reference 1–5, see end of Part III.

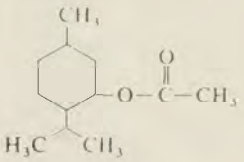
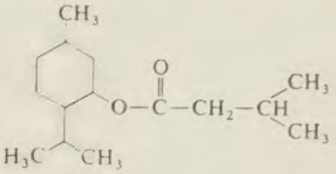
6. *Food Chemical Codes*, 1st ed., National Academy of Sciences, 1963, 423.
7. *Beilstein's Encyclopedia of Organic Chemistry*, B6², Springer Verlag, p. 49.
8. *Beilstein's Encyclopedia of Organic Chemistry*, B6², Springer Verlag, p. 39.
9. Guenther, *The Essential Oils*, Vol. 2, D. Van Nostrand Co., 1949, 216.

	Menthone	
Other names	2-Isopropyl-5-methyl-cyclohexanone *p*-Menthan-3-one	
Empirical formula	$C_{10}H_{18}O$	
Structure		
Physical/chemical characteristics	*Racemic form*	*Optically active form*
Appearance	Colorless liquid	Colorless liquid
Assay	98%	95%
Molecular weight	154.24	154.24
Boiling point	Approx 210 C	Approx 210 C
Specific gravity	0.890–0.894 at 25°C	0.888–0.895 at 25 C
Refractive index	1.4480–1.4520 at 20°C	1.4480–1.4530 at 20°C
Optical rotation	±2	−15 to +15
Solubility	Insoluble in water; soluble 1:3 in 70% alcohol; soluble in alcohol and most common organic solvents	
Organoleptic characteristics	Characteristic odor similar to menthol	
Synthesis[7]	By oxidation of menthol;[6] see also Reference 7 and 8	
Natural occurrence	Several stereoisomers are reported found in nature. *l*-Menthone is a constituent of the essential oils of Russian and American peppermint, geranium, *Andropogon fragrans, Mentha timija, Mentha arvensis,* and others. *d*-Menthone is present in the essential oils of *Barosma pulchellum, Nepeta japonica* Maxim., and others. *d*-Isomenthone has been reported isolated from *Micromeria abissinica* Benth., *Pelargonium tomentosum* Jacquin., etc. *l*-Isomenthone has been identified in Reunion geranium, *Pelargonium capitatum,* and others.	
Reported uses[3]	Non-alcoholic beverages 7.7 ppm Ice cream, ices, etc 33 ppm Candy 71 ppm Baked goods 52 ppm Chewing gum 8.7 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2667	

REFERENCES

For References 1–5, see end of Part III.

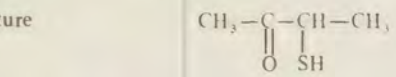
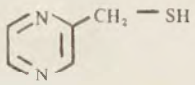
6. Moriya, *J. Chem. Soc.* (London), 39, 77, 1881.
7. Anders and Andreef, *Ber. Dtsch. Chem. Ges.*, 25, 617, 1892.
8. Beckmann and Pleissner, *Annalen*, 21, 262, 1891.

	l-Menthyl acetate	Menthyl isovalerate
Other names	*l-p*-Menth-3-yl acetate	*p*-Menth-3-yl isovalerate Validol
Empirical formula	$C_{12}H_{22}O_2$	$C_{15}H_{28}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Assay	95% min	96% min
Molecular weight	198.31	240.39
Boiling point	227–228°C	140–146°C (241°C) at 22 mm Hg
Flash point	92°C	120°C
Specific gravity	0.9220–0.9310 at 25°C; 0.9264 at 20°C	0.9040–0.9080 (0.907) at 15°C
Refractive index	1.4440–1.4500 (1.4472) at 20°C	1.4470–1.4480 at 20°C
Optical rotation	±2 (commercial product); *l*-, −72°47′ to 73°18′	Approx −36° (commercial product) (−64°12′)
Acid value		0.09 max
Solubility	Soluble in essential oils and most common solvents; 1:15 in 65% alcohol; 1:6 in 70% alcohol; 1:1 in 80% alcohol	Insoluble in water; 1:8 to 1:10 in 80% alcohol
Organoleptic characteristics	Fresh odor similar to mint and rose (on dilution); characteristic, fresh, pungent flavor, different from menthol (being much milder); cool mouthfeel with only a trace of mint flavor	Odor similar to both menthol and isovaleric acid—sweet and herbaceous, somewhat balsamic or root-like; bitter, wood-like taste
Synthesis	By reacting acetic anhydride with menthol in the presence of anhydrous sodium acetate	Prepared by heating a mixture of *l*-menthol and isovaleric acid at 100–110°C in the presence of trace concentrated H_2SO_4[6] or at 100°C in the presence of HCl[7]
Natural occurrence	Reported as a normal constituent of peppermint oil in varying amounts, depending on the source. The synthetic product is optically *laevo*-rotatory; the commercial product is optically inactive.	Reported found in several peppermint essential oils: American,[8] French,[9,10] English,[11] and Russian[12] peppermint oil
Reported uses[3]	Non-alcoholic beverages 5.5 ppm Ice cream, ices, etc. 4.0 ppm Candy 26 ppm Baked goods 24 ppm Chewing gum 5.2 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 2.9 ppm Candy 7.4 ppm Baked goods 18 ppm
Regulatory status	FDA 121.1164; FEMA No. 2668	FDA 121.1164; FEMA No. 2669

REFERENCES

For References 1–5, see end of Part III.

6. Senderens and Aboulenc, *Ann. Chim. Paris*, 9(18), 184, 1922.
7. Bobranski, *J. Pharm. Chim.*, 8(20), 437, 1934.
8. Power and Kleber, *Arch. Pharm.*, 232, 652, 1894.
9. Charabot, *Bull Soc. Chim. Fr.*, 3(19), 117, 1898.
10. Roure-Bertrand fils, *Giornale*, p. 17, March 1900.
11. Umney, *Chem. Zentralbl.*, 1, 710, 1896.
12. Schindelmeiser, *Chem. Zentralbl.*, 2, 1764, 1906.

	3-Mercapto-2-butanone	2-Mercaptomethylpyrazine
Other names		Pyrazine methanethiol Pyrazinyl methylmercaptan
Empirical formula	C_4H_8OS	$C_5H_6N_2S$
Structure		
Physical/chemical characteristics		
Appearance	Becomes cloudy after short storage; forms water droplets within 5 hrs at room temperature	
Assay		C: 47.59%; H: 4.79%; N: 22.20%; S: 25.41%
Molecular weight	104.17	126.18 (calculated = 126.025171)
Melting point		
Boiling point	46–70°C at 15 mm Hg 50°C at 18 mm Hg	44–45°C at 0.07 mm Hg
Specific gravity	1.0156 at 20°C	
Refractive index	1.4694 at 20°C	
Solubility	With difficulty soluble in water; easily soluble in alcohol, ether, pyridine, and aqueous alkalis	
Organoleptic characteristics		Roasted, meat-like flavor
Synthesis	From 2,4,5-trimethyl-2-ethyl-3-thiazoline with butyl and hydrolysis.[6] From oxo-compound with sulfur or polysulfides and ammonia at room temperature[7]	Chloromethylpyrazine is added to sodium hydrogen sulfide[8]
Reported uses[3]	Non-alcoholic beverages 0.2 ppm Candy 0.2 ppm Baked goods 0.2 ppm Meat, meat sauces, soups 0.2 ppm Milk, dairy products 0.2 ppm Cereals 0.2 ppm	Baked goods 10.0 ppm Condiments 10.0 ppm Meat, meat sauces, soups 10.0 ppm
Regulatory status	FEMA No. 3298	FEMA No. 3299

REFERENCES

For References 1–5, see end of Part III.

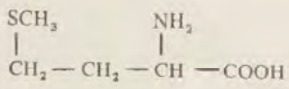
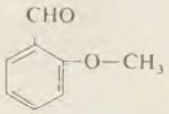
6. **Thiel et al.**, *Ann. Chem.*, 613, 128, 1958.
7. **Asinger, Thiel and Pallas**, East German Patent 13,954, 1957; *Chem. Abstr.*, 53, 11235e, 1959.
8. **Winter et al.**, U.S. Patent 3,702,253, 1972.

	3-Mercapto-2-pentanone		Mesityl oxide	
Other names			4-Methyl-3-penten-2-one Isopropylidene acetone Methyl isobutenyl ketone	
Empirical formula	$C_5H_{10}OS$		$C_6H_{10}O$	
Structure	$CH_3-CH_2-\underset{\displaystyle SH}{\underset{\vert}{CH}}-CO-CH_3$		H_3C, H_3C $\diagdown$ $\diagup$ $C=CH-C(=O)-CH_3$	
Physical/chemical characteristics				
Appearance			Colorless oily liquid	
Molecular weight	118.19		98.15	
Melting point			-52.85°C	
Boiling point			129.76°C 72.1°C at 100 mm Hg 41°C at 23 mm Hg -8.7°C at 1 mm Hg	
Flash point			+30.6°C	
Specific gravity			0.8653 at 20°C	
Refractive index			1.4440 at 20°C	
Solubility			Slightly soluble in water, acetone, and propylene glycol; soluble in alcohol and ether in all proportions	
Organoleptic characteristics			The commercial grade exhibits an unpleasant odor; the pure material has a pleasant honey-like odor	
Synthesis			By reacting acetone or diacetone alcohol with iodine or other dehydrating agent;[6,7] by condensation of acetone over sulfonated polystyrene-divinylbenzene resin used as an ion exchange catalyst[8]	
Natural occurrence			Reported found as a constituent in coffee aroma[9]	
Reported uses[3]	Non-alcoholic beverages	0.2 ppm	Ice cream, ices, etc.	0.75 ppm
	Candy	0.2 ppm	Candy	1.12 ppm
	Baked goods	0.2 ppm	Baked goods	2.25 ppm
	Meat, meat sauces, soups	0.2 ppm	Gelatins and puddings	0.50 ppm
	Cereals	0.2 ppm	Milk, dairy products	0.40 ppm
	Milk, dairy products	0.2 ppm		
Regulatory status	FEMA No. 3300		FEMA No. 3368	

REFERENCES

For References 1–5, see end of Part III

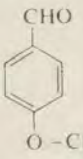
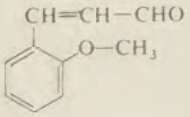
6. **Conant and Tuttle,** *Organic Syntheses,* Coll. Vol. 1, Gilman, H. and Blatt, A. H., Eds., Wiley & Sons, New York, 1941, 345.
7. *Ullmanns, Enzyklopädie der Technischen Chemie,* 3rd ed., Vol. 9, Urban and Schwarzenberg, 1958, 555.
8. **Klein and Banchero,** *Ind. Eng. Chem.,* 48, 1278, 1956.
9. **Stoll et al.,** *Helv. Chim. Acta,* 50, 628, 1967.

	D,L-Methionine	*o*-Methoxybenzaldehyde
Other names	2-Amino-4-(methylthio)butanoic acid 2-Amino-γ-(methylthio)butyric acid	*o*-Anisaldehyde Methyl salicylaldehyde Salicylaldehyde methyl ether
Empirical formula	$C_5H_{11}O_2NS$	$C_8H_8O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Platelets (from alcohol)	Crystals, colorless or cream-colored
Molecular weight	149.21	136.15
Melting point	281°C (decomposes)	35–37°C (38°C)
Boiling point		243–244°C; 122°C at 20 mm Hg
Specific gravity	1.340	1.1326 at 20°C
Refractive index		1.560 at 20°C
Solubility	Very soluble in water; insoluble in ether, benzene, and petroleum ether; soluble in diluted acids and alkalis; slightly soluble in alcohol	Insoluble in water; soluble in alcohol and benzene; very soluble in ether and chloroform
Organoleptic characteristics		Faint, sweet, floral odor; blends well with cassia; spice-like flavor, quite bitter above 30–40 ppm
Synthesis	By addition of methanethiol to acrolein;[6] by chemical conversion of methylthiopropionic aldehyde[7–9]	Prepared from salicylaldehyde and dimethyl sulfate in weak alkaline solution
Natural occurrence		Reported found in the oil of *Cinnamomum cassia* Nees ex Bl.[10]
Reported uses[3]	Non-alcoholic beverages 50.0 ppm Baked goods 50.0 ppm Condiments, pickles 50.0 ppm Meat, meat sauces, soups 50.0 ppm Milk, dairy products 50.0 ppm Cereals 50.0 ppm	
Regulatory status	FEMA No. 3301	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.

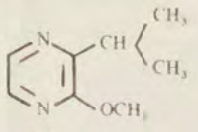
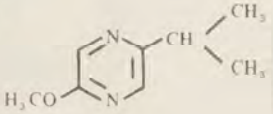
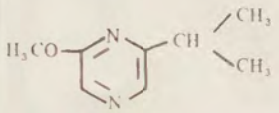
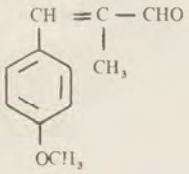
6. British Patent 605,311, 1948; *Chem. Abstr.*, 43, 677a, 1949.
7. **Pierson et al.**, *J. Am. Chem. Soc.*, 70, 1450, 1948.
8. **Pierson and Tishler**, U.S. Patent, 2,584, 496, assigned to Merck & Co., 1952.
9. **Weiss**, U.S. Patent 2,732,400, assigned to American Cyanamid Co., 1956.
10. **Dodge**, *Chem. Zentralbl.*, 1, 747, 1919.

	p-Methoxybenzaldehyde	*o*-Methoxycinnamaldehyde
Other names	*p*-Anisaldehyde Anisic aldehyde Aubepine	*o*-Cumaric aldehyde methyl ether β-(*o*-Methoxyphenyl)-acrolein 3-(*o*-Methoxyphenyl)-propenal 3-(*o*-Methoxyphenyl)propen-2-al-1
Empirical formula	$C_8H_8O_2$	$C_{10}H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow liquid	Pale-yellow crystal flakes (from alcohol)
Assay	97.5% min[2] (97–99%)	
Molecular weight	136.15	162.19
Melting point	2.5 C	45–46 C
Boiling point	247 C	295 C with decomposition; 160–161°C at 12 mm Hg
Congealing point	1 C min	
Flash point	121 C	
Specific gravity	1.119–1.123 at 25/25 C;[2] 1.123 at 20 C	
Refractive index	1.5710–1.5740 at 20°C[2]	
Acid value	6 max[2]	
Solubility	1:7 in 50% alcohol; soluble in most organic solvents; at least 99% soluble in sodium bisulfite solution[2]	Soluble in alcohol, ether, and chloroform; very slightly soluble in water
Organoleptic characteristics	Characteristic hawthorn odor; pungent, anise-like flavor; bitter flavor above 30–40 ppm	Sweet, warm, spicy-floral odor with fruity undertones; sweet, spicy, warm flavor; somewhat pungent above 200–300 ppm
Synthesis	By methylation and oxidation of *p*-cresol and also by oxidation of anethol	It is formed after a long contact period between salicylaldehyde and acetaldehyde in diluted alkaline solution.[7] It can be formed by condensation of salicylaldehyde methylether with acetaldehyde under alkaline conditions. From the corresponding oxime[9]
Natural occurrence	Reported found in essential oils and extracts: vanilla, *Acacia farnesiana* Willd., *Magnolia salicifolia* Maxim., *Erica arborea*, *Pirus communis*, *Boswellia serrata*, and others;[6] also in anise, fennel, star anise (especially when aged due to the oxidation of anethol)	Reported found in cinnamon essential oil[8] (*Cinnamomum cassia* Nees ex Bl.), from which it is separated as stearoptene; in cinnamon[10]
Reported uses[3]	Non-alcoholic beverages 6.3 ppm Ice cream, ices, etc. 5.6 ppm Candy 14 ppm Baked goods 16 ppm Gelatins and puddings 0.50–30 ppm Chewing gum 18–76 ppm	Candy 80.0 ppm Baked goods 40.0 ppm Chewing gum 450.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2670	FDA 121.1164; FEMA No. 3181

REFERENCES

For References 1–5, see end of Part III.

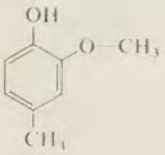
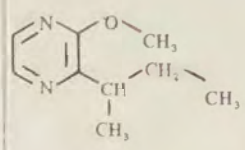
6. Honda, *Miltizer Ber.*, p. 36, 1958.
7. Darlington and Christensen, *J. Am. Pharm. Assoc.*, 33, 298, 1944.
8. Bertrams and Kurstens, *J. Prakt. Chem.*, 2(51), 316, 1895.
9. Brady et al., *J. Chem. Soc.*, 125, 1418, 1924.
10. Heide, *J. Agric. Food Chem.*, 20, 747, 1972.

	2-Methoxy-3 or 5 or 6-isopropyl pyrazine	*p*-Methoxy-α-methyl cinnamaldehyde
Other names	(a) 2-Isopropyl-3-methoxypyrazine (b) 2-Isopropyl-5-methoxypyrazine (c) 2-Isopropyl-6-methoxypyrazine 2-Methoxy-3 or 5 or 6-(1-methylethyl)pyrazine	3-(*p*-Methoxyphenyl)-2-methyl-2-propenal
Empirical formula	$C_8H_{12}N_2O$	$C_{11}H_{12}O_2$
Structure	 (a)  (b)  (c)	
Physical chemical characteristics		
Assay	C: 63.1345%; H: 7.9473%; N: 18.4059%; O: 10.5123%	
Molecular weight	152.20	176.21
Boiling point		106–109°C at 0.1 mm Hg
Refractive index		1.6290 at 25°C
Mass spectra[9]	(a): 41 (25), 43 (14), 52 (12), 53 (9), 54 (10), 68 (12), 95 (11), 105 (13), 124 (21), 137 (100), 152 (38)	
IR spectra[9]	(a): S (6.5, 6.85, 6.9, 7.16, 7.2, 7.5, 8.6, 8.9, 9.9) M (7.7, 7.9, 8.4, 9.1, 9.2, 11.9) W (6.3, 9.4, 9.6, 11.2, 13.7) VW (5.3, 5.6, 10.5, 1.08, 12.5)	
Synthesis	(a) From 2-hydroxy-3-propylyprazine by methylation with diazomethane; the 2-hydroxy-3-propylpyrazine was prepared by condensing norvaline amide hydrochloride with glyoxal[9] (a + b + c) A mixutre can be obtained by methoxylation of isopropylchloropyrazine[10]	By formylation of the corresponding olefin[11]
Natural occurrence	In *Pisum sativum*;[6] tentatively identified in potatoes[7]	Non-alcoholic beverages 1.0 ppm Candy 10.0 ppm
Reported uses[3]	Gelatins and puddings 0.05 ppm Condiments 0.02 ppm Meat, meat sauces 0.02 ppm Olives, relishes 0.05 ppm Found effective in increasing flavor levels of potatoes and potato products[8]	
Regulatory status	FEMA No. 3358	FEMA No. 3182

REFERENCES

For References 1–5, see end of Part III.

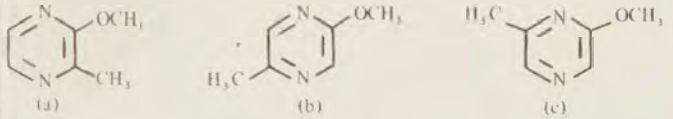
6. **Murray et al.,** *Chem. Ind.* (London), 27, 897, 1970.
7. **Buttery et al.,** *J. Agric. Food Chem.*, 18, 538, 1970.
8. **Guadagni et al.,** *J. Food Chem.*, 36, 363, 1971.
9. **Seifert et al.,** *J. Agric. Food Chem.*, 18(2), 246, 1970.
10. **Winter,** U.S. Patent 3,622,346, 1967.
11. **Schimdle and Barnett,** *J. Am. Chem. Soc.*, 78, 3209, 1956.

	2-Methoxy-4-methylphenol	2-Methoxy-3-(1-methylpropyl)pyrazine
Other names	Creosol 4-Hydroxy-3-methyl-1-methyl benzene 2-Methoxy-*p*-cresol 4-Methylguaiacol	2-Methoxy-3-*sec*-butylpyrazine
Empirical formula	$C_8H_{10}O_2$	$C_9H_{14}N_2O$
Structure		
Physical/chemical characteristics		
Appearance	Colorless to yellowish liquid; solidifies when cold	
Assay		C: 65.03%; H: 8.49%; O: 9.63%; N: 16.85%
Molecular weight	138.16	166.22 (calculated = 166.110612)
Melting point	5.5°C	
Boiling point	220–221°C (222°C)	
Specific gravity	1.098 (1.10) at 20°C	
Refractive index	1.5353 at 25°C	
Mass spectra[1,2]		105(14), 123(12), 124(100), 137(50), 138(90), 151(46), 152(12)
IR spectra[1,2]		S (3.4, 6.9, 7.2, 7.4, 8.6) M (3.5, 6.5, 7.7, 8.4, 8.9, 9.9, 11.9) W (3.3, 6.4, 7.9, 9.0, 11.5)
Solubility	Slightly soluble in water; soluble in alcohol, ether, benzene, chloroform, and acetic acid	
Organoleptic characteristics	Characteristic aromatic odor (sweet, spicy, slightly vanilla-like); somewhat bitter taste (vanilla-like)	
Synthesis	By methylation of homopyrocatechin using dimethyl sulfate and alkali;[6,7] also by hydrogenation of vanillin	By condensation of isolencine amide with glyoxal, followed by methylation with CH_2N_2.[11]
Natural occurrence	Occurs in beechwood tar; also identified in the essential oils of ylang-ylang,[8] jasmine,[9] and anise seeds. It is one of the active constituents of creosote.[10]	
Reported uses[3]	Non-alcoholic beverages 10–21 ppm Alcoholic beverages 0.02 ppm Ice cream, ices, etc. 0.05 ppm Candy 0.77 ppm Baked goods 1.0 ppm	Non-alcoholic beverages 0.05 ppm Alcoholic beverages 20.0 ppm Ice cream, ices, etc. 0.05 ppm Candy 0.05 ppm Baked goods 0.05 ppm Gelatins and puddings 0.05 ppm Vegetables 0.05 ppm
Regulatory status	FDA 121.1164; FEMA No. 2671	FEMA No. 3433

REFERENCES

For References 1–5, see end of Part III.

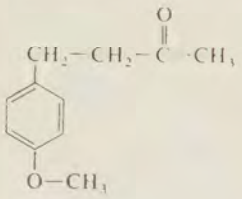
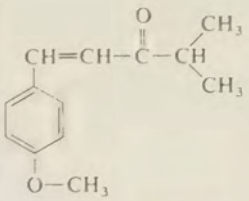
6. Fachberg, List and Co., German Patent 258,185.
7. Fachberg, List and Co., *Chem. Zentralbl.*, 1, 1481, 1913.
8. Schimmel and Co., *Chem. Zentralbl.*, 1, 1087, 1913.
9. **Naves and Grampoloff,** *Helv. Chim. Acta*, 25, 1500, 1942.
10. **Monod et al.,** *Chem. Abstr.*, 45, 3124, 1951.
11. **Buttery et al.,** *Chem. Ind.*, 15, 490, 1969.
12. **Kolor et al.,** personal communication, 1973.

	2 or 5 or 6-Methoxy-3-methylpyrazine (mixture of isomers)
Other names	(a) 2-Methoxy-3-methylpyrazine (b) 2-Methoxy-5-methylpyrazine (c) 2-Methoxy-6-methylpyrazine
Empirical formula	$C_6H_8N_2O$
Structure	 (a) (b) (c)
Physical/chemical characteristics	
Assay	C: 58.05%; H: 6.50%; N: 22.57%; O: 12.89%
Molecular weight	124.14
Boiling point	48–50° C at 15 mm Hg (mixture)
Refractive index	n_D^{23} 1.5055 d_4^{23} 1.082 (mixture)
Mass spectra[8]	(a): 40 (3), 52 (4), 53 (3), 67 (3), 68 (12), 80 (8), 81 (2), 94 (15), 95 (23), 106 (33), 108 (36), 123 (28), 124 (100)
NMR spectra[9]	(a): δ 2.42 (3, S, $-CH_3$), 3.91 (3, S, $-O-CH_3$), 7.87 (1, d, ring $-H$), 7.95 (1, d, ring $-H$) (b): δ 2.40 (3 S, $-CH_3$), 3.86 (3, S, $-O-CH_3$), 7.86 (1, d, ring $-H$), 8.04 (1, d, ring $-H$) (c): δ 2.37 (3, S, $-CH_3$), 3.86 (3, S, $-O-CH_3$), 7.88 (1, S, ring $-H$), 7.94 (1, S, ring $-H$)
Organoleptic characteristics	Aroma reminiscent of hazelnut, almond, and peanut
Synthesis	From 2-methylpyrazine by various routes[6]
Reported uses[3]	Ice cream, ices, etc. 2.0 ppm Candy 4.0 ppm Baked goods 4.0 ppm Gelatins and puddings 2.0 ppm The methyl methoxypyrazines are used as nut-like flavoring agents for foods and beverages;[6] the 2-methoxy-3-methyl derivative is used as a coffee aroma enhancing agent[7]
Regulatory status	FEMA No. 3183

REFERENCES

For References 1–5, see end of Part III.

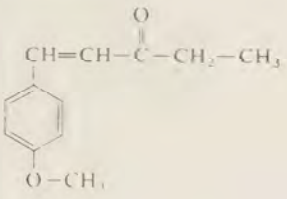
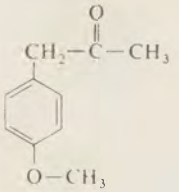
6. **Winter**, U.S. Patent 3,622,346, 1967.
7. **Parliment et al.**, French patent 2,062,168.
8. **Friedel et al.**, *J. Agric. Food Chem.*, 19, 530, 1971.
9. **Nakel and Haynes**, *J. Agric. Food Chem.*, 20(3), 683, 1972.

	4-(*p*-Methoxyphenyl)-2-butanone	1-(4-Methoxyphenyl)-4-methyl-1-penten-3-one
Other names	Anisyl acetone "Frambinone methylether" *p*-Methoxy phenylbutanone (common commercial name) "Raspberry ketone methylether"	α,α-Dimethylanisylacetone "Homo e'hone" *p*-Methoxystyryl isopropyl ketone
Empirical formula	$C_{11}H_{14}O_2$	$C_{13}H_{16}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid; solidifies below 10 C	Colorless, oily liquid
Molecular weight	178.23	204.27
Melting point	9–10°C	28°C
Boiling point	277°C (160°C at 22 mm Hg)	217–219°C at 40 mm Hg
Specific gravity	1.0504 at 22°C	
Solubility	Very slightly soluble in water; soluble in alcohol, poorly soluble in propylene glycol	Very slightly soluble in water; soluble in alcohol; poorly soluble in propylene glycol
Organoleptic characteristics	Intensely sweet, floral, fruity odor; cherry-raspberry flavor at low concentrations	Caramel, fruity odor with buttery top-note; sweet taste with fruity note
Synthesis	By condensing acetone with anisaldehyde to yield anisylidene acetone and subsequent hydrogenation in the presence of Pd catalyst[6]	By condensing methyl isopropyl ketone with anisaldehyde in the presence of diluted alkali solution[8]
Natural occurrence	Contained (approximately 53% level) in the odorous principle obtained by extraction and hydrolysis from aloe wood (*Aquilaria agallocha* Roxb.)[7]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 12 ppm Ice cream, ices, etc. 10–12 ppm Candy 28 ppm Baked goods 26 ppm Gelatins and puddings 25 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2672	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.

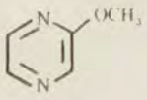
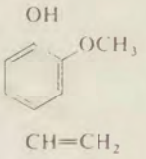
6. Zemplén, Bognár and Boskovitz, *Ber. Dtsch. Chem. Ges. B.*, 77, 784, 1944.
7. Itikawa and Heiken Yo, *J. Chem. Soc. Jap.*, 60, 1247, 1939.
8. Vorländer and Knotzsch, *Ann. Chem.*, 294, 334, 1897.

	1-(*p*-Methoxyphenyl)-1-penten-3-one	1-(*p*-Methoxyphenyl)-2-propanone
Other names	"Ethone" *p*-Methoxystyryl ethyl ketone α-Methyl anisylacetone α-Methylanisylidene acetone	Anisic ketone Anisketone Anisyl methyl ketone *p*-Methoxyphenylacetone
Empirical formula	$C_{12}H_{14}O_2$	$C_{10}H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White-yellowish crystals	Colorless, oily liquid
Assay	99% min	
Molecular weight	190.24	164.21
Melting point	60 C (min)	
Boiling point	278°C at 12 mm Hg	264–265°C; 136–138°C at 12 mm Hg
Specific gravity		1.0814 at 0°C; 1.067 at 18°C
Refractive index		1.5253 at 20°C
Solubility	1 gm in 5 ml of 95% alcohol; insoluble in water; soluble in alcohol; poorly soluble in propylene glycol	Almost insoluble in water; soluble in alcohol and ether
Organoleptic characteristics	Odor similar to butter, sweet and lasting; sweet, fruity taste at low levels; slightly burning taste at higher levels	Odor and taste similar to anise
Synthesis	By saturation at room temperature of a mixture of anisaldehyde and methyl ethyl ketone with HCl,[6] or by treating α-methyl-α-(4-hydroxy)benzylidene acetone with methyl iodide in alkaline solution[7]	Obtained by boiling α- or β-anetholglycol with a 20% solution of sulfuric acid,[8] or from 1-(*p*-methoxyphenyl)-propan-1,2-ol by treatment with diluted sulfuric acid
Natural occurrence	Not reported found in nature	Reported found in Chinese star anise[9] and in Russian star anise;[10] also reported found in sweet and common fennel
Reported uses[3]	Non-alcoholic beverages 2.3 ppm Ice cream, ices, etc. 2.3 ppm Candy 28 ppm Baked goods 12 ppm	Non-alcoholic beverages 0.60–2.8 ppm Ice cream, ices, etc. 1.2–2.8 ppm Candy 4.4–6.0 ppm Baked goods 4.4–6.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2673	FDA 121.1164; FEMA No. 2674

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For References 1–5, see end of Part III.

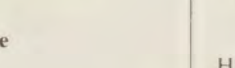
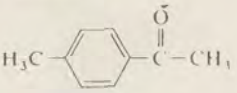
6. Iwamoto, *Chem. Zentralbl.*, 1, 2730, 1927; *Bull. Chem. Soc. Jap.*, 2, 54, 1927.
7. Iwamoto, *Bull. Chem. Soc. Jap.*, 2, 55, 1927.
8. Toenies, *Ber. Dtsch. Chem. Ges.*, 20, 2982, 1887.
9. Tardy, *Bull. Soc. Chim. Fr.*, 3(27), 990, 1902.
10. Bouchard and Tardy, *C. R. Séances Acad. Sci. Paris*, 122, 198, 1896.

	Methoxypyrazine		2-Methoxy-4-vinylphenol	
Other names	2-Methoxy-1,4-diazine 2-Methoxypyrazine		4-Hydroxy-3-methoxystyrene *p*-Vinylguaiacol	
Empirical formula	$C_5H_6N_2O$		$C_9H_{10}O_2$	
Structure				
Physical/chemical characteristics				
Assay	C: 54.54%; H: 5.49%; N: 25.44%; O: 14.53%			
Molecular weight	110.12		150.18	
Boiling point	60–61°C at 29 mm Hg		100°C at 5 mm Hg	
Organoleptic characteristics	Odor threshold: 700 ppb in water[7]			
Synthesis	From 2-hydroxypyrazine by various routes[6]		From vanillin by reacting with acetic anhydride and sodium acetate yielding 3-methoxy-4-hydroxycinnamic acid on subsequent hydrolysis; the latter, heated with quinoline in the presence of hydroquinone, is decarboxylated to 4-vinylguaiacol[8]	
Natural occurrence			Reported found among the steam-distillable phenols from the alcoholic fermentation of cereal grains, especially corn; probably formed from ferulic acid[9]	
Reported uses[3]	Non-alcoholic beverages	10.0 ppm	Non-alcoholic beverages	0.25–3.0 ppm
	Ice cream, ices, etc.	10.0 ppm	Ice cream, ices, etc.	0.25–11 ppm
	Candy	10.0 ppm	Candy	1.0–8.0 ppm
	Baked goods	10.0 ppm	Baked goods	1.0–8.0 ppm
	Gelatins and puddings	10.0 ppm		
	Meat, meat sauces, soups	10.0 ppm		
	Milk, dairy products	10.0 ppm		
	Cereals	10.0 ppm		
Regulatory status	FEMA No. 3302		FDA 121.1164; FEMA No. 2675	

REFERENCES

For References 1–5, see end of Part III.

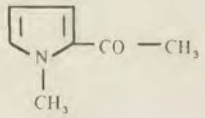
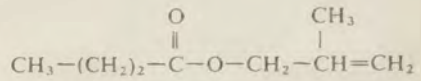
6. Phillips and Phillips, *J. Chem. Soc.*, p. 1294, 1956.
7. Seifert et al., *J. Agric. Food Chem.*, 18, 246, 1970.
8. Toshiyuki et al., *Nippon Kagaku Zasshi*, 80, 1337, 1959.
9. Steinke and Paulson, *J. Agric. Food Chem.*, 4(12), 381, 1964.

	Methyl acetate	4′-Methylacetophenone
Other names		*p*-Acetotoluene *p*-Methylacetophenone 1-Methyl-4-acetyl benzene Methyl *p*-tolyl ketone
Empirical formula	$C_3H_6O_2$	$C_9H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless or nearly colorless liquid; tends to solidify at room temperature
Assay	96% min	98% min[2]
Molecular weight	74.08	134.17
Melting point	−98°C	−23°C
Boiling point	56°C	222–226°C at 756 mm Hg
Flash point	Approx 15°C (−16°C)	
Specific gravity	0.9415–0.9455 at 15°C; 0.933 at 20°C	1.001–1.004 at 25/25°C;[2] 1.0016 at 20°C
Refractive index	1.3610–1.3630 (1.3619) at 20°C	1.5320–1.5345[2] (1.5335) at 20°C
Acid value	0.9 max	
Solubility	Soluble in water; completely miscible with alcohol and ether	1:10 in 50% alcohol;[2] 1:3 in 60% alcohol; insoluble in water; sparingly soluble in most organic solvents
Organoleptic characteristics	Pleasant, fruity odor and slightly bitter flavor	Fruity, floral odor resembling acetophenone; sweet, strawberry-like flavor
Synthesis	By boiling acetic acid and methanol in the presence of acid catalysts; or by heating methanol with an excess carbon monoxide under pressure in the presence of a catalyst (phosphoric acid, cobalt salts)	By slow addition of acetyl chloride to a mixture of toluene and $AlCl_3$ in an ice bath and under vacuum, maintaining the temperature at +5°C and then letting it increase to +20°C
Natural occurrence	Reported found in several fruits, such as grape, banana, and *Citrus maxima*, and in coffee; also identified in rum ether[6]	Reported found in the essential oil distilled from the wood of *Myrocarpus fastigiatus*,[7,8] *Myrocarpus frondosus*,[9] bois de rose, and probably mimosa extracts[10,11]
Reported uses[3]	Non-alcoholic beverages 28 ppm Alcoholic beverages 0.20 ppm Ice cream, ices, etc. 29 ppm Candy 11 ppm Baked goods 14 ppm Gelatins and puddings 0.10 ppm	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 1.6 ppm Candy 5.2 ppm Baked goods 4.9 ppm Chewing gum 870 ppm Condiments 5.8 ppm Maraschino cherries 8.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2676	FDA 121.1164; FEMA No. 2677

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For References 1–5, see end of Part III.

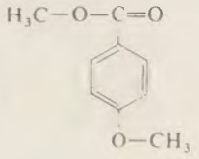
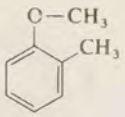
6. **Fenaroli et al.**, *Riv. Ital. EPPOS*, 9, 484, 1965; 2, 75, 1966.
7. **Verley**, *Bull. Soc. Chim. Fr.*, 3(17), 909, 1897.
8. **Verley**, *Bull. Soc. Chim. Fr.*, 3(19), 138, 1898.
9. **Naves**, *Helv. Chim. Acta*, 31, 44, 1948.
10. *Parfum. Mod.*, 5, 99, 1926.
11. *Chem. Drug.*, 105, 201, 1926.

	1-Methyl-2-acetyl pyrrole	2-Methylallyl butyrate
Other names	Methyl 1-methylpyrrol-2-yl ketone	Isopropenyl carbinyl-*n*-butyrate Methallyl butyrate β-Methylallyl-*n*-butyrate 2-Methyl-2-propen-1-yl butyrate
Empirical formula	C_7H_9NO	$C_8H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Molecular weight	123.15	142.19
Boiling point	88–93°C at 22 mm Hg	168°C
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics		Powerful, penetrating, fruity, ethereal odor; sharp, acrid taste above 20 ppm, becoming sweet, pineapple-, apple-, and plum-like
Synthesis	From N-methyl pyrrole and Grignard reagent;[6] by acetylation of 1-methylpyrrole[7]	By direct esterification of β-methylallyl alcohol with butyric acid
Natural occurrence	Reported found as a component in coffee aroma[8]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Gelatins and puddings 10.0 ppm	Non-alcoholic beverages 0.20 ppm Baked goods 0.20 ppm
Regulatory status	FEMA No. 3184	FDA 121.1164; FEMA No. 2678

REFERENCES

For References 1–5, see end of Part III.

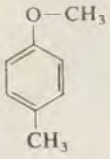
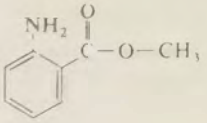
6. Hertz, *J. Org. Chem.*, 22, 1260, 1957.
7. Anderson, *Can. J. Chem.*, 35, 21, 1957.
8. Gianturco, Gianmarino, Friedel and Flanagan, *Tetrahedron Lett.*, 20, 2951, 1964.

	Methyl anisate	*o*-Methylanisole
Other names	Methyl *p*-methoxybenzoate	*o*-Cresyl methyl ether 2-Methoxy toluene *o*-Methoxy toluene Methyl *o*-tolyl ether
Empirical formula	$C_9H_{10}O_3$	$C_8H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Low-melting solid	Colorless liquid
Molecular weight	166.18	122.17
Melting point	48–49°C	
Boiling point	254–255°C	166–167°C; 63–64°C at 14 mm Hg (172°C)
Specific gravity		0.9853 at 15.5°C
Refractive index		1.5199 at 15.3°C
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Herbaceous, anise-like odor; sweet taste similar to melon	Pungent, warm, floral odor with earthy, walnut undertones; sweet, fruity, nut-like flavor at low levels
Synthesis	By esterification of anisic acid with methanol or from sodium anisate, dimethyl sulfate, and small amounts of methanol	By methylation of *o*-cresol using dimethyl-sulfate in caustic soda at 40°C[7]
Natural occurrence	Reported found in the mushroom variety *Trametes graveolens*[6]	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 3.0 ppm Candy 8.0 ppm Baked goods 6.2 ppm	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.3–4.0 ppm Baked goods 4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2679	FDA 121.1164; FEMA No. 2680

REFERENCES

For References 1–5, see end of Part III.

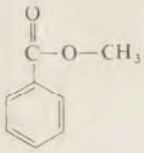
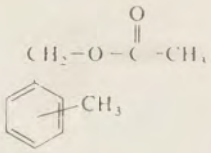
6. Aye, *Arch. Pharm.*, p. 246, 1931.
7. Boyd and Hardy, *J. Chem. Soc.*, p. 637, 1928.

	p-Methylanisole	Methyl anthranilate
Other names	*p*-Cresyl methyl ether *p*-Methoxy toluene Methyl *p*-cresol Methyl *p*-tolyl ether	Methyl 2-aminobenzoate Methyl *o*-aminobenzoate
Empirical formula	$C_8H_{10}O$	$C_8H_9NO_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to pale-yellow liquid with bluish fluorescence
Assay		98% min[2]
Molecular weight	122.17	151.17
Melting point		24–25 C
Boiling point		132 C at 14 mm Hg
Congealing point		23.8 C (24 C)
Specific gravity	0.966–0.970 at 25°/25°C[2]	1.161–1.169 at 25 /25 C;[2] 1.1640 at 25 C
Refractive index	1.5100–1.5130 at 20°C[2]	1.5820–1.5840 at 20 C;[2] 1.5802 at 25 C
Cresol content	Not more than 0.5%[2]	
Solubility	1:3 in 80% alcohol;[2] soluble in most organic solvents; 1:7 in 70% alcohol	1:5 in 60% alcohol;[2] soluble in water and most organic solvents
Organoleptic characteristics	Pungent odor suggestive of ylang-ylang	Characteristic orange-flower odor, and slightly bitter, pungent taste
Synthesis	By methylation of *p*-cresol	By heating anthranilic acid and methyl alcohol in the presence of sulfuric acid and subsequent distillation
Natural occurrence	Reported found in the oils of ylang-ylang, cananga, and others	Reported found in several essential oils: neroli, orange, bergamot, lemon, mandarin, jasmine, tuberose, gardenia, champaca, ylang-ylang, and others; also in the juice and oil of *Vitis labrusca*[6]
Reported uses[3]	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 2.7 ppm Candy 4.8 ppm Baked goods 7.6 ppm Gelatins and puddings 0.50–4.0 ppm Condiments 2.0 ppm Syrups 8.0 ppm	Non-alcoholic beverages 16 ppm Alcoholic beverages 0.20 ppm Ice cream, ices, etc. 21 ppm Candy 56 ppm Baked goods 20 ppm Gelatins and puddings 23 ppm Chewing gum 2,200 ppm
Regulatory status	FDA 121.1164; FEMA No. 2681	FDA GRAS; FEMA No. 2682

REFERENCES

For References 1–5, see end of Part III.

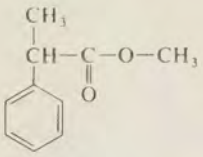
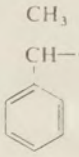
6. Mattick et al., *J. Agric. Food Chem.*, 4, 334, 1963.
7. Roger, *Food Technol.*, 6, 309, 1961.

	Methyl benzoate	Methylbenzyl acetate (mixed *o*-,*m*-,*p*-)
Other names	Niobe oil Oil niobe	Tolyl acetate
Empirical formula	$C_8H_8O_2$	$C_{10}H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	98% min[2]	98% min[2]
Molecular weight	136.15	164.20
Melting point	−12 to −13 C	
Boiling point	199–200 C	
Flash point	82 C	
Specific gravity	1.082–1.088 at 25 /25 C;[2] 1.0785 at 30 C	1.030–1.035 at 25°/25°C[2]
Refractive index	1.5140–1.5180 at 20 C;[2] 1.5181 at 16 C	1.5015–1.5040 at 20°C[2]
Acid value	Not more than 1[2]	Not more than 1[2]
Solubility	1:4 and more in 60% alcohol;[2] 1:1.5 in 70% alcohol; insoluble in water; miscible with alcohol and ether	1:2 in 70% alcohol;[2] soluble in benzyl benzoate, mineral oil, and most fixed oils; partly soluble in propylene glycol; insoluble in glycerin
Organoleptic characteristics	Fruity odor, also similar to cananga	
Synthesis	By heating benzoic acid and dimethyl sulfate to high temperature;[6] or by exchange between ethyl benzoate and methanol in KOH solution[7]	By acetylation of the alcohol
Natural occurrence	Reported in the oils of tuberose (flowers),[8] ylang-ylang,[9] clove,[10] *Polianthes tuberosa* L. (flowers),[11] and *Narcissus jonquilla* L. (flowers)[12]	
Reported uses[3]	Non-alcoholic beverages 2.2 ppm Ice cream, ices, etc. 4.5 ppm Candy 8.4 ppm Baked goods 9.9 ppm Chewing gum 61 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2683	FDA 121.1164

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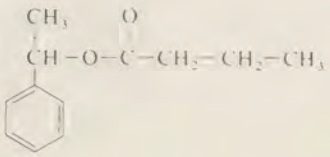
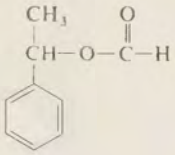
For References 1–5, see end of Part III.

6. Simon, *Compt. Rend.*, 176, 585, 1923.
7. Reimer and Downes, *J. Am. Chem. Soc.*, 43, 949, 1921.
8. *Schimmel Ber.*, April 1903.
9. *Schimmel Ber.*, October 1901.
10. *Schimmel Ber.*, April 1903.
11. Elze, *Chem. Zentralbl.*, 2, 2198, 1928.
12. Soden, *J. Prakt. Chem.*, 110, 277, 1925.

	α-Methylbenzyl acetate	α-Methylbenzyl alcohol
Other names	Gardenol Methyl phenylcarbinyl acetate Styralyl acetate Styrolene acetate	Methylphenylcarbinol 1-Phenylethanol α-Phenylethyl alcohol Phenyl methyl carbinol Styralyl alcohol Styrolyl alcohol
Empirical formula	$C_{10}H_{12}O_2$	$C_8H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid congealing below room temperature
Assay	97% min[2]	97% min[2]
Molecular weight	164.21	122.17
Melting point		20°C
Boiling point	213°C	205°C
Congealing point		19°C min[2]
Flash point	81°C	93°C
Specific gravity	1.023–1.026 at 25°/25°C;[2] 1.024 at 25°C	1.009–1.014 at 25°/25°C;[2] 1.013 at 20°C
Refractive index	1.4935–1.4970 (1.4948) at 20°C[2]	1.5250–1.5290 at 20°C[2]
Acid value	2.0 max[2]	
Ketone content		1% max[2] (as acetophenone)
Solubility	1:7 in 60% alcohol;[2] soluble in most organic solvents	1:3 in 50% alcohol;[2] 1:16 in 30% alcohol; insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Intensive green odor suggestive of gardenia; bitter, acrid taste, interesting on dilution	Mild hyacinth-gardenia odor
Synthesis	By acetylation of methyl phenyl carbinol; from benzaldehyde by reacting with magnesium methyl bromide and subsequent acetylation; from 1-bromoethylbenzene and silver acetate in acetic acid	By oxidation of ethylbenzene or by reduction of acetophenone
Natural occurrence	Reported found in gardenia flower oil	Not reported found in natural oils. Two optically active isomers exist. The commercial product is the racemic form
Reported uses[3]	Non-alcoholic beverages 3.9 ppm Ice cream, ices, etc. 5.4 ppm Candy 12 ppm Baked goods 17 ppm Chewing gum 0.80 ppm Topping 30 ppm	Non-alcoholic beverages 4.6 ppm Ice cream, ices, etc. 3.8 ppm Candy 6.8 ppm Baked goods 9.0 ppm Gelatins and puddings 4.0 ppm Chewing gum 0.30 ppm
Regulatory status	FDA 121.1164; FEMA No. 2684	FDA 121.1164; FEMA No. 2685

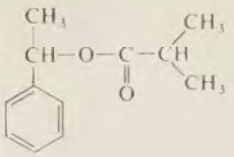
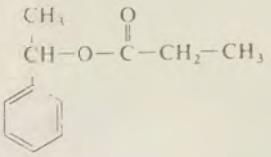
REFERENCES

For References 1–5, see end of Part III.

	α-Methylbenzyl butyrate	α-Methylbenzyl formate
Other names	Methyl phenylcarbinyl-*n*-butyrate Styralyl butyrate	Methyl phenylcarbinyl formate "Styralyl formate"
Empirical formula	$C_{12}H_{16}O_2$	$C_9H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Molecular weight	192.26	150.18
Solubility	Almost insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Fruital-floral, jasmine-like odor; apricot/apple-like flavor notes	Woody odor of mimosa and gardenia; dry notes and fruity taste
Synthesis	From methylphenylcarbinol and *n*-butyric acid by esterification	By esterification of methylphenylcarbinol with formic acid in the presence of acetic anhydride
Natural occurrence		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 4.0–5.0 ppm Ice cream, ices, etc. 4.0–10 ppm Candy 10–20 ppm Baked goods 10–20 ppm	Non-alcoholic beverages 2.0–5.0 ppm Ice cream, ices, etc. 3.0–5.0 ppm Candy 10–20 ppm Baked goods 10–20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2686	FDA 121.1164; FEMA No. 2688

REFERENCES

For References 1–5, see end of Part III.

	α-Methylbenzyl isobutyrate	α-Methylbenzyl propionate
Other names	Methyl phenylcarbinyl isobutyrate Styralyl isobutyrate	Methyl phenylcarbinyl propionate Styralyl propionate
Empirical formula	$C_{12}H_{16}O_2$	$C_{11}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	192.26	178.23
Solubility	Very slightly soluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Jasmine-like, floral odor	Floral, sweet, green odor typical of gardenia and jasmine
Synthesis	By esterification (under azeotropic conditions) of methylphenylcarbinol with isobutyric acid	By direct esterification of methylphenylcarbinol with propionic acid under azeotropic conditions
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 10 ppm Candy 10 ppm Baked goods 10 ppm	Non-alcoholic beverages 4.0–5.0 ppm Ice cream, ices, etc. 4.0–5.0 ppm Candy 10–15 ppm Baked goods 10–15 ppm
Regulatory status	FDA 121.1164; FEMA 2687	FDA 121.1164; FEMA No. 2689

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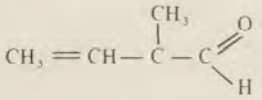
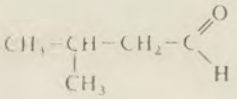
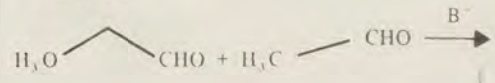
For References 1–5, see end of Part III.

	2-Methyl-1-butanethiol	3-Methyl-2-butanethiol
Other names	Amyl mercaptan 2-Methylbutyl mercaptan Thioamyl alcohol	Isopentyl mercaptan Isoamyl mercaptan Isopentanethiol Isoamyl thioalcohol Isoamyl sulfhydrate
Empirical formula	$C_5H_{12}S$	$C_5H_{12}S$
Structure	$CH_3-CH_2-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-CH_2SH$	$CH_3-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-CH_2-CH_2-SH$
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Molecular weight	104.22	104.22
Boiling point	118.2°C	118°C
Specific gravity	0.8420 at 20°C	0.8350 at 20°C
Refractive index	1.4440 at 20°C	1.4418 at 20°C
Optical rotation	+3.21° at 23°C	
Solubility		Insoluble in water; soluble in alcohol and ether in all proportions
Organoleptic characteristics		Repulsive, characteristic mercaptan-like odor
Synthesis	From 2-methyl-1-butyl isothiourea picrate by conversion to bis [(s)-2-methylbutyl] disulfide, followed by reduction to the corresponding thiol, using sodium metal in liquid ammonia[6]	From isoamyl chloride and potassium sulfhydrate[8] also, the corresponding sodium salt can be prepared from diisopentyl-disulfide and sodium metal in liquid ammonia[9]
Natural occurrence	Reported as occurring in the petroleum fraction boiling between 111°C and 150°C[7]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.8 ppm Candy 0.8 ppm Baked goods 0.8 ppm Meat, meat sauces, soups 0.8 ppm Milk, dairy products 0.8 ppm Cereals 0.8 ppm	Non-alcoholic beverages 1.2 ppm Candy 1.2 ppm Baked goods 1.2 ppm Meat 1.2 ppm Milk, dairy products 1.2 ppm Cereals 1.2 ppm
Regulatory status	FEMA No. 3303	FEMA No. 3304

REFERENCES

For References 1–5, see end of Part III.

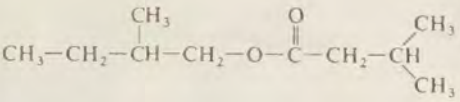
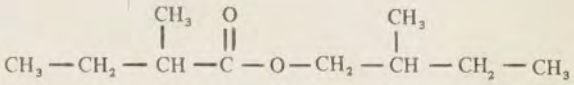
6. **Polak, Bregant and Balenovic,** *Bull. Sci. Cons. Acad. RSF Yougosl. Sect. A*, 13(1–2), 1968; *Chem. Abstr.*, 69, 43345h, 1968.
7. **Colenian, Thompson, Hopkins and Rall,** *J. Chem. Eng. Data*, 10(1), 80, 1965.
8. *Merck Index*, 8th ed., Merck & Co., Rahway, N.J., 1968, 579.
9. **Williams and Gebauer-Fuelnegg,** *J. Am. Chem. Soc.*, 53, 355, 1931.

	2-Methyl-2-butenal	3-Methylbutyl aldehyde
Other names	2-Methyl crotonaldehyde Tiglic aldehyde 2,3-Dimethylacrolein	Isovaleraldehyde 3-Methylbutanal 3-Methylbutyraldehyde
Empirical formula	C_5H_8O	$C_5H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid; readily oxidizes in the presence of air	Colorless liquid
Molecular weight	84.11	86.14
Boiling point	118°C 116.5–117.5°C at 738 mm Hg 63–65°C at 119 mm Hg	92.5°C
Specific gravity	0.8710 at 20°C	0.7977 at 20°C
Refractive index	1.4475 at 20°C	1.3902 at 20°C
Solubility	Slightly soluble in water; miscible with alcohol and ether; soluble in oils	Very slightly soluble in water; soluble in alcohol, propylene glycol, and oils
Organoleptic characteristics	Penetrating, powerful green-ethereal odor	Powerful, penetrating, acrid odor; at very low levels the flavor is warm, herbaceous, slightly fruity, and nut-like
Synthesis	By condensation of acetaldehyde and propionaldehyde[6,7] 	
Natural occurrence	Reported found in geranium oil;[8] also found in onion, garlic, mint, cooked chicken, coffee, roasted filberts, and roasted peanuts[9]	
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 5.0 ppm Chewing gum 5.0 ppm Meat, meat sauces, soups 2.5 ppm	
Regulatory status	FEMA No. 3407	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.

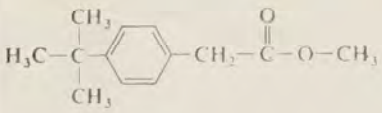
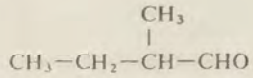
6. Morgan et al., *Chem. Ind.*, p. 519, 1933.
7. Bernhauer et al., *J. Prakt. Chem.*, 155, 315, 1940.
8. Timmer et al., *J. Agric. Food Chem.*, 19(6), 1066, 1971.
9. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Centraal Instituut voor Voedingsonderzoek, Zeist, Netherlands.

	2-Methylbutyl isovalerate	2-Methylbutyl-2-methyl butyrate
Other names	*d-sec*-Butylcarbinyl isopentanoate	α,β-Methylbutyl-*dl*-2-methyl butanoate
Empirical formula	$C_{10}H_{20}O_2$	$C_{10}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Molecular weight	172.27	172.27
Boiling point		184–187°C
Solubility	Insoluble in water; soluble in alcohol	
Organoleptic characteristics	Herbaceous, fruity, somewhat earthy fragrance; sweet, herbaceous, fruity flavor	
Synthesis	By direct esterification of 2-methylbutanol with isovaleric acid	By esterification of 2-methylbutanoic acid with 2-methyl-1-butanol;[6] by condensation of isobutyraldehyde at 120°C[7]
Natural occurrence		Reported found as a component in the essential oil of hops (*Humulus lupulus*);[8-10] also as the odorous component in *Vaccinium vitis idaea*[11] and in cocoa beans[12]
Reported uses[3]	The compound has been reported used in fabricating artificial peppermint essential oil, contributing the "non-minty" portion of the flavor	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 8.0 ppm Baked goods 8.0 ppm Gelatins and puddings 5.0 ppm Preserves 5.0 ppm
Regulatory status	FDA 121.1164	FEMA No. 3359

REFERENCES

For References 1–5, see end of Part III.

6. Bailey and Hass, *J. Am. Chem. Soc.*, 91, 63, 1969.
7. Hagemeyer, Jr. and Wright, Jr., U.S. Patent 3,081,344, 1963.
8. Naya and Kotake, *Nippon Kagaku Zasshi*, 88(12), 1302, 1967.
9. Buttery, Black, Guadagni and Kealy, *Am. Soc. Brew. Chem. Proc.*, 103, 1965.
10. Buttery, Black, Kealy and McFadden, *Nature*, 202(4933), 701, 1964.
11. Anjou and von Sydow, *Acta Chem. Scand.*, 21(4), 945, 1967.
12. Dietrich, Lederer, Winter and Stoll, *Helv. Chim. Acta*, 47(6), 1581, 1964.

	Methyl *p-tert*-butylphenylacetate	2-Methyl butyraldehyde
Other names	*p-tert*-Butylphenylacetic acid, methyl ester	2-Methylbutanal-l α-Methyl butyraldehyde Methyl ethyl acetaldehyde
Empirical formula	$C_{13}H_{18}O_2$	$C_5H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Molecular weight	206.28	86.13
Boiling point		93°C
Specific gravity		0.80
Solubility	Almost insoluble in water; soluble in alcohol	Slightly soluble in water; soluble in alcohol and propylene glycol
Organoleptic characteristics	Sweet, woody, and camphoraceous odor; roasted, chocolate-like flavor	Powerful, choking odor; peculiar cocoa and coffee-like flavor when diluted; sweet, slightly fruity, chocolate-like taste
Synthesis	By esterification of *p-tert*-butylphenylacetic acid with methanol	By oxidation of *sec*-butylcarbinol isolated from fermented fusel oil; the *dl*-form from *sec*-butyl magnesium bromide and formaldehyde; by reduction of methylethylacetic acid
Natural occurrence		
Reported uses[3]	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.35–1.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm	Non-alcoholic beverages 1.5–2.0 ppm Ice cream, ices, etc. 2.0–8.0 ppm Candy 6.6 ppm Baked goods 5.7 ppm
Regulatory status	FDA 121.1164; FEMA No. 2690	FDA 121.1164; FEMA No. 2691

REFERENCES

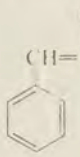
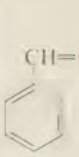
For References 1–5, see end of Part III.

	Methyl butyrate	2-Methyl butyric acid
Other names		Butane-2-carboxylic acid 2-Methylbutanoic acid α-Methyl butyric acid Methylethyl acetic acid Optically active isovaleric acid
Empirical formula	$C_5H_{10}O_2$	$C_5H_{10}O_2$
Structure	$CH_3-O-\overset{\overset{O}{\|\|}}{C}-(CH_2)_2-CH_3$	$CH_3-CH_2-\underset{\underset{CH_3}{\|}}{CH}-COOH$
Physical/chemical characteristics[5]		
Appearance	Colorless, mobile liquid	Colorless liquid
Assay		Exists in the *d*- (natural), *l*-, and *dl*-forms
Molecular weight	102.13	102.13
Melting point		*d*-, 176°C; *l*-, 176–177°C; *dl*-, 173–174°C
Boiling point	102°C (103°C)	
Flash point	14°C	
Specific gravity	0.8981 at 20°C; 0.905 at 15.5°C	At 20°C: *d*-, 0.934; *l*-, 0.934; *dl*-, 0.9332
Refractive index	1.3873 (1.3900) at 20°C	At 21.2°C: *d*-, 1.4044 *d*-, +16 to +21°; *l*-, −6° to −18°
Solubility	1:60 in water; miscible in alcohol and ether	Slightly soluble in water; soluble in alcohol and propylene glycol; slightly soluble in glycerin
Organoleptic characteristics	Apple-like odor and corresponding sweet taste; not very powerful; below 100 ppm may have banana-pineapple flavor	Pungent, acrid odor similar to roquefort cheese; acrid taste; at low dilutions pleasant, fruity taste
Synthesis	From methyl alcohol and butyric acid in the presence of concentrated H_2SO_4[6]	By decarboxylation of methyl ethyl malonic acid (with heat); also by oxidation of fermentation amyl alcohol (fusel oil)
Natural occurrence	Reported found in wood oil[7]	Occurring as the *d*-, *l*-, and *dl*-isomers. The racemic form has been reported found in angelica root oil and coffee. The *d*-isomer in the ester form has been identified in lavender oil.[8]
Reported uses[3]	Non-alcoholic beverages 17 ppm Ice cream, ices, etc. 31 ppm Candy 86 ppm Baked goods 48–200 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 3.0 ppm Candy 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2693	FDA 121.1164; FEMA No. 2695

REFERENCES

For References 1–5, see end of Part III.

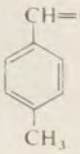
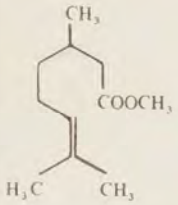
6. Vogel, *J. Chem. Soc.*, p. 629, 1948.
7. Fraps, *Am. Chem. J.*, 25, 37, 1901.
8. Seidel et al., *Helv. Chim. Acta*, 27, 663, 1944.

	α-Methylcinnamaldehyde	Methyl cinnamate
Other names	α-Methylcinnamal α-Methyl cinnamic aldehyde 2-Methyl-3-phenyl-2-propen-1-al 3-Phenyl-2-methyl acrolein	Methyl-3-phenyl propenoate
Empirical formula	$C_{10}H_{10}O$	$C_{10}H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellow, oily liquid	White to slightly yellow, crystalline solid; the *cis*- form (which is not a commercial material) is a liquid
Assay	97% min[2]	98% min[2]
Molecular weight	146.18	162.18
Melting point		*trans*-, 36°C; *cis*-, −3°C
Boiling point	137–138°C at 22 mm Hg	*trans*-, 254–255°C; *cis*-, 49°C
Congealing point		−33.8°C[2]
Specific gravity	1.035–1.039 at 25/25°C;[2] 1.0538 at 20°C	At 50°C: *trans*-, 1.0573
Refractive index	1.6025–1.6070[2] (1.6081) at 20°C	At 20°C: *trans*-, 1.5670; *cis*-, 1.5582
Acid value	Not more than 5[2]	Not more than 2[2]
Solubility	1:2 in 70% alcohol;[2] insoluble in water and glycerin	1:4 and more in 80% alcohol;[2] insoluble in water; soluble in propylene glycol, mineral oil, and other oils
Organoleptic characteristics	Characteristic cinnamon-type odor; soft, spicy flavor	Fruity, balsamic odor similar to strawberry; corresponding sweet taste
Synthesis	By condensing benzaldehyde with propionic aldehyde in the presence of a 1% caustic soda solution; also by the controlled hydrogenation of α-methylcinnamic aldehyde	By esterification of cinnamic acid with methanol using HCl as catalyst;[6] or by adding HCl to a boiling solution of cinnamyl nitrile in methanol[7]
Natural occurrence		Reported found in the oil from rhizomes of *Alpinia malaccensis*;[8] in the oil from leaves of *Ocimum canum* Sims.;[9,10] in the oil of *Narcissus jonquilla* L.;[11] in the oil from rhizomes of *Gastrochilus panduratum* Ridl.[12] Two isomers (*cis*- and *trans*-) are known.
Reported uses[3]	Non-alcoholic beverages 0.50–11 ppm Ice cream, ices, etc. 1.0–15 ppm Candy 26 ppm Baked goods 27 ppm Chewing gum 430 ppm	Non-alcoholic beverages 1.9 ppm Ice cream, ices, etc. 3.8 ppm Candy 8.7 ppm Baked goods 13 ppm Gelatins and puddings 1.7–14 ppm Chewing gum 2.7–40 ppm Condiments 0.40 ppm
Regulatory status	FDA 121.1164; FEMA No. 2697	FDA 121.1164; FEMA No. 2698

REFERENCES

For References 1–5, see end of Part III.

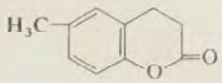
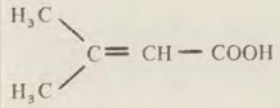
6. Weger, *Chem. Ann.*, 27, 74, 1885.
7. Pfeiffer, Engelhardt and Alfuss, *Chem. Ann.*, 467, 178, 1928.
8. Van Romburgh, *K. Ned. Akad. Wet. Versl. Gewone Vergad. Afd. Natuurkd.*, p. 445, 1900.
9. Roure-Bertrand fils, *Chem. Zentralbl.*, 1, 1654, 1914.
10. Schimmel and Co., *Chem. Ber.*, 1, 1654, 1914.
11. Soden, *J. Prakt. Chem.*, 2(110), 277, 1925.
12. Ultee, *Versl. Akad. Amsterdam*, 36, 1262, 1927; *Chem. Zentralbl.*, 99, 2018, 1928.

	p-Methylcinnamic aldehyde	Methyl citronellate
Other names	3-(*p*-Methylphenyl)-propenal	Methyl-3,7-dimethyl-6-octenoate
Empirical formula	$C_{10}H_{10}O$	$C_{11}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Crystals from diluted alcohol	Colorless mobile liquid
Molecular weight	146.18	184.28
Melting point	41.5°C	216°C
Boiling point	154°C at 25 mm Hg	78°C at 3 mm Hg
Specific gravity		0.8973 at 20°C
Refractive index		1.4415 at 20°C
Optical rotation		+5.45°
Solubility		Very slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics		Fruity (apple), brandy-like odor
Synthesis		From citronellic acid, methanol, and sulfuric acid;[6] from citronellic acid treated with diazomethane in ether solution[7]
Natural occurrence		Reported as naturally occurring in the oil from the leaves of *Calytrix tetragona*[8]
Reported uses[3]		Non-alcoholic beverages 1.5 ppm Baked goods 3.0 ppm Condiments, pickles 1.5 ppm
Regulatory status	FDA 121.1164	FEMA No. 3361

REFERENCES

For References 1–5, see end of Part III.

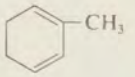
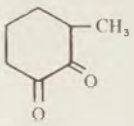
6. Tatsuzo and Okazawa *J. Chem. Soc Jap.*, 64, 501, 1943.
7. Lukeš, Zobáčová and Plešek, *Croat. Chem. Acta*, 29, 201, 1957; *Chem. Abstr.*, 53, 17898, 1959.
8. Panfold, Ramage and Simonsen, *J. Proc. R. Soc. N. S. W.*, 68, 80, 1935.

	6-Methyl coumarin	3-Methylcrotonic acid
Other names	Cocodescol 6-Methylbenzopyrone Pralina Toncair Toncarine (Tonkarin)	Senecioic acid 3,3-Dimethylacrylic acid β,β-Dimethylacrylic acid
Empirical formula	$C_{10}H_8O_2$	$C_5H_8O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White, crystalline solid	Prisms (from water)
Molecular weight	160.17	100.12
Melting point	74.6–75 C	70°C (sublimes)
Boiling point	303 C (305 C) at 725 mm Hg	199°C 114°C at 40 mm Hg
Congealing point	73.5 C	
Solubility	Very slightly soluble in hot water; insoluble in petroleum ether; soluble in oils	Soluble in most common organic solvents
Organoleptic characteristics	Somewhat dry, herbaceous (tonka-like) odor; also characterized as a delicate fig or date sweetness; almost bitter taste above 50 ppm, turning sweet and vanilla-like at lower levels	
Synthesis	By heating 6-methyl coumarin-3-carboxylic acid to 300–340 C; by condensation of *p*-cresoldisulfonic acid with fumaric acid in the presence of H_2SO_4; by condensation of *p*-homosalicylic aldehyde with malonic acid in the presence of aniline, followed by heating to form the lactone; from salicylaldehyde with propionic anhydride and sodium propionate	By the action of alkalis or bases on the ester of α-bromoisovaleric acid; by condensation of acetone with malonic acid or bromoacetic ester;[6] by oxidation of mesityl oxide with sodium hypochlorite
Natural occurrence	Not reported found in nature	Reported found in the rhizomes of *Senecio kaempferi* Sieb.,[7] the corresponding ester occurs naturally in wasteswort
Reported uses[3]	Non-alcoholic beverages 5.2 ppm Ice cream, ices, etc. 4.8 ppm Candy 21 ppm Baked goods 24 ppm Gelatins and puddings 39 ppm Chewing gum 0.80–15 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm Gelatins and puddings 5.0 ppm
Regulatory status	Status not fully defined by FDA; FEMA No. 2699	FEMA No. 3187

REFERENCES

For References 1–5, see end of Part III.

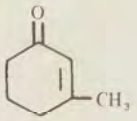
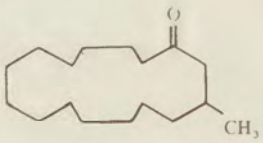
6. Kon and Linstead, *J. Chem. Soc.*, 127, 624, 1925.
7. Asahina, *Arch. Pharm.*, 251, 355, 1913.

	2-Methyl-1, 3-cyclohexadiene	1-Methyl-2,3-cyclohexadione
Other names	Dihydrotoluene (1,3) Dihydrotoluene (Δ1,3)	3-Methyl-1,2-cyclohexanedione 2-Methyl-3,4-cyclohexanedione
Empirical formula	C_7H_{10}	$C_7H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	
Molecular weight	94.16	126.15
Melting point	107–108°C (110°C)	61–63°C
Boiling point		69–72°C at 1 mm Hg
Specific gravity	0.8354 (0.835) at 20°C	
Refractive index	1.4662 at 18°C	
Solubility	Insoluble in water; very soluble in alcohol; soluble in ether	
Synthesis		By the method described by Wallach;[9] from the ethyl ester of γ-propionylbutyric acid and sodium ethylate[10]
Natural occurrence	By dehalogenation of 1,2-dibromo-1-methyl cyclohexane with sodium ethoxide;[6,7,8] purified by distillation over metallic sodium.	Reported found as a volatile constituent in coffee[11]
Reported uses[3]		Non-alcoholic beverages 0.6 ppm Candy 9.0 ppm Baked goods 6.0 ppm Gelatins and puddings 0.2 ppm
Regulatory status	FDA 121.1164	FEMA No. 3305

REFERENCES

For References 1–5, see end of Part III.

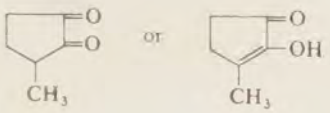
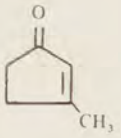
6. **Mousseron and Winternitz,** *Bull. Soc. Chim.*, 12, 70, 1945.
7. **Mousseron and Winternitz,** *Compt. Rend.*, 219, 210, 1944.
8. *Beilstein's Encyclopedia of Organic Chemistry*, Vol. 5, Springer Verlag, p. 115.
9. **Wallach,** *Liebigs Ann. Chem.*, 414, 314, 1916–1917; 437, 180, 1924.
10. **Lapin and Horeau,** *Chimia*, 15, 551, 1961.
11. **Gianturco, Gianmarino and Friedel,** *Nature*, 210(5043), 1358, 1966.

	3-Methyl-2-cyclohexen-1-one	3-Methyl-1-cyclopentadecanone
Other names	3-Methyl-Δ^2-cyclohexenone	*d, l*-Muscone Methyloxaltone
Empirical formula	$C_7H_{10}O$	$C_{16}H_{30}O$
Structure		
Physical/chemical characteristics[5]		
Molecular weight	110.05	238.42
Melting point	Approximately -21°C	
Boiling point	94.5–95.5°C at 22 mm Hg 78–79°C at 12 mm Hg 53–53.5°C at 2 mm Hg	130°C at 0.5 mm Hg
Specific gravity	0.9693 at 20°C	0.9221 at 17°C
Refractive index	1.4947 at 20°C	1.4802 at 17°C
Optical rotation		-13°, O' at 17°C
Solubility		Very slightly soluble in water; miscible with alcohol
Organoleptic characteristics	Miscible with water in all proportions	Soft, sweet, tenacious musky odor
Synthesis	By acid hydrolysis and decarboxylation of the corresponding 4-carbetoxy derivative;[6] by oxidation of 1-methyl-cyclohex-1-ene with chromium trioxide in acetic acid;[7] by cyclization of 3-carbetoxy-6-chlorohept-5-en-2-one with sulfuric acid[8]	From the condensation of dodecamethylene-α,ω-dimethylketone hexadecane);[10,11] for preparation of *d*- and *l*-forms, see References 12 and 13
Natural occurrence	Reported found in the oil of *Mentha pulegium*[9]	In natural musk
Reported uses[3]	Non-alcoholic beverages 0.02 ppm Ice cream ices, etc. 0.05 ppm Candy 0.08 ppm Baked goods 0.15 ppm Gelatins and puddings 0.05 ppm Milk, dairy products 0.02 ppm	Non-alcoholic beverages 0.03 ppm Alcoholic beverages 0.02 ppm Ice cream, ices, etc. 0.03 ppm Candy 0.05 ppm Baked goods 0.05 ppm Gelatins and puddings 0.02 ppm
Regulatory status	FEMA No. 3360	FEMA No. 3434

REFERENCES

For References 1–5, see end of Part III.

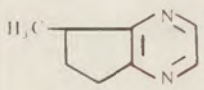
6. Smith and Ronalt, *J. Am. Chem. Soc.*, 65, 631, 1943.
7. Whitmore and Pedlow, *J. Am. Chem. Soc.*, 63, 758, 1941.
8. Wichterle et al., *Chem. Abstr.*, 42, 8162, 1948.
9. Naves, *Helv. Chim. Acta*, 26, 162, 1943.
10. Stoll et al., *Helv. Chim. Acta*, 30, 2019, 1947.
11. Blonquist et al., *J. Am. Chem. Soc.*, 70, 34, 1948.
12. Stallberg-Stenhagen, *Ark. Kemi*, 3, 517, 1951.
13. Felix et al., *Helv. Chim. Acta*, 54, 2896, 1971.

	Methylcyclopentenolone	1-Methyl-1-cyclopenten-3-one
Other names	Cyclotene 2-Hydroxy-3-methyl-2-cyclopenten-1-one Kentonareme 3-Methylcyclopentan-1,2-dione	3-Methyl-2-cyclopenten-1-one
Empirical formula	$C_6H_8O_2$	C_6H_8O
Structure		
Physical/chemical characteristics[5]		
Appearance	Crystalline solid	
Molecular weight	112.13	96.12
Melting point	105–107 C (anhydrous)	
Boiling point		157–158°C
Specific gravity		0.9712 at 26°C
Refractive index		1.4714 at 26°C
Solubility	Readily soluble in boiling water, alcohol, acetone, and chloroform; slightly less soluble in ether	Very soluble in water
Organoleptic characteristics	Sweet flavor somewhat similar to licorice	
Synthesis	See references 6 and 7. Sublimes and distills at atmospheric pressure with decomposition	By dehydrohalogenation of 2-chloro-1-methyl-cyclopentan-3-one[10]
Natural occurrence	Reported formed during the dry distillation of wood; found also in the corresponding tar oil;[8] identified in fenugreek[9]	
Reported uses[3]	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 5.6 ppm Candy 18 ppm Baked goods 13 ppm Gelatins and puddings 14 ppm Chewing gum 8.0–15 ppm Syrups 10–30 ppm	Non-alcoholic beverages 2.0 ppm Baked goods 3.0 ppm Condiments 2.0 ppm Meat, sauces, soups 2.0 ppm Cereals 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2700	FEMA No. 3435

REFERENCES

For References 1–5, see end of Part III.

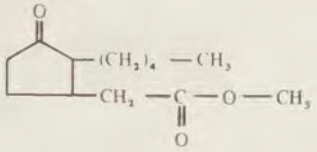
6. Nazarov and Akbrem, *Izv. Akad. Nauk SSSR Otd. Khim. Nauk*, p. 1383, 1956.
7. Krimen and Norman, U.S. Patent 2,856,962, 1958.
8. Meyerfeld, *Chem. Ztg.*, 36, 549, 1912.
9. Ruys, *Fr. Ses Parfums*, 47(9), 34, 1966.
10. Godchot et al., *Compt. Rend.*, 156, 1780, 1913.

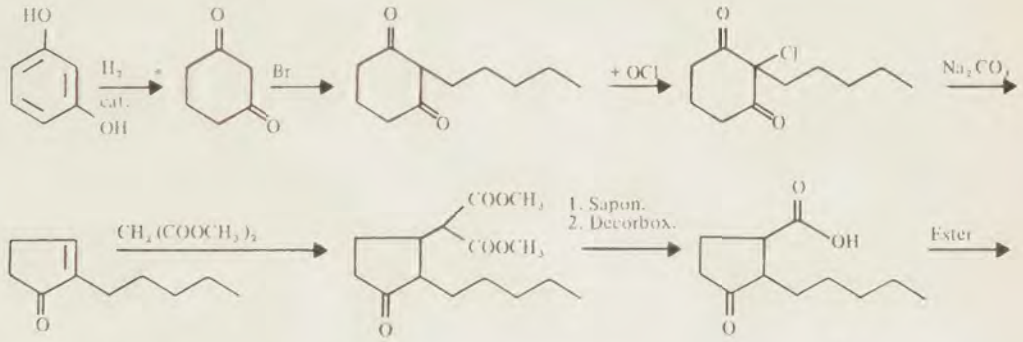
	5H-5-Methyl-6,7-dihydrocyclopentapyrazine
Other names	
Empirical formula	$C_8H_{10}N_2$
Structure	
Physical/chemical characteristics	
Appearance	Colorless crystals
Assay	C: 68.82%; H: 8.25%; N: 22.93%
Molecular weight	134.18
Melting point	121–123°C at 1 atm
Boiling point	47°C at 0.7 mm Hg 78–80°C at 10 mm Hg
Mass spectra[7]	119 (100), 134 (48), 133 (25), 39 (21), 27 (18), 52 (16), 78 (12), 41 (12)
IR spectra[7]	3050, 2960, 2930, 2870, 1455, 1430, 1385, 1330, 1155, 1125, 1090, 1075, 1015, 870, 845
UV spectra[7]	λ_{max} (MeOH): 277, 282, ($E = 9.7 \times 10^{-3}$), 308 nm
Synthesis	From condensation of 2-hydroxy-3-methyl-2-cyclopentene-1-one and ethylene diamine.[7] By condensing a cyclopentenolone with alkylenediamines, or alternatively, an aliphatic α-diketone with 1,2-diamino cyclopentane; the resulting product is dehydrogenated in the presence of palladium over activated charcoal or copper chromite[8]
Natural occurrence	Reported to be present in peanuts and filberts[6]
Reported uses[3]	Non-alcoholic beverages 0.045 ppm Ice cream, ices, etc. 0.25 ppm Candy 1.0 ppm Chewing gum 0.15 ppm Protein foods 0.5 ppm
Regulatory status	FEMA No. 3306

REFERENCES

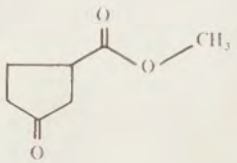
For References 1–5, see end of Part III.

6. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
7. Pittet et al., *J. Agric. Food Chem.*, 22(2), 275, 1974.
8. Flament et al., *Helv. Chim. Acta*, 56(2), 610, 1973.

	Methyl dihydrojasmonate
Other names	2-Amylcyclopentanone acetic acid, methyl ester Methyl hydrojasmonate Methyl-92-amyl-3-oxocyclopentyl) Methyl-2(-pentyl-3-oxo-1-cyclopentyl) acetate
Empirical formula	$C_{13}H_{22}O_3$
Structure	
Physical/chemical characteristics[5]	
Appearance	Pale-straw-colored to yellowish oily liquid
Molecular weight	226.32
Boiling point	> 300°C 109–112°C at 0.2 mm Hg[6] 100°C at 0.03 mm Hg[7]
Specific gravity	0.9968 at 21°C
Refractive index	1.4583 at 20°C
Solubility	Very slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics	Powerful sweet-floral, jasmine-like, somewhat fruity odor[8]
Synthesis	By condensation of 2-pentyl-2-cylcopenten-1-one with ethyl malonate, followed by hydrolysis, decarboxylation, and methylation;[6] also[9]



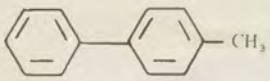
Natural occurrence	The odoriferous component in jasmine oil (*Jasminum gradiflorum* L.)	
Reported uses[3]	Non-alcoholic beverages	1.0 ppm
	Ice cream, ices, etc.	1.0 ppm
	Candy	1.0 ppm
	Baked goods	1.0 ppm
	Gelatins and puddings	1.0 ppm
	Condiments, pickles	1.0 ppm
	Preserves and spreads	1.0 ppm
Regulatory status	FEMA No. 3408	



REFERENCES

For References 1–5, see end of Part III.

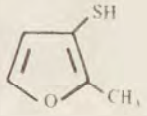
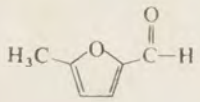
6. Demole et al., *Helv. Chim. Acta*, 45, 685, 1962.
7. Hikino et al., *Yakugaku Zasshi*, 83, 219, 1963; 85, 179, 1965; *Chem. Abstr.*, 62, 12969, 1965.
8. Arctander, *Perfume and Flavor Chemicals*, Montclair, N.J., 1969, No. 2076.
9. German Patent 2,160,646.

	p-Methyl diphenyl	Methyl disulfide
Other names	4-Methyl biphenyl Phenyl-*p*-tolyl *p*-Phenyltoluene	Dimethyl disulfide *Note:* Do not confuse with dimethyl sulfide
Empirical formula	$C_{13}H_{12}$	$C_2H_6S_2$
Structure		$H_3C-S-S-CH_3$
Physical/chemical characteristics[5]		
Appearance	Platelets (from methanol or ligroin)	Pale-yellow liquid
Molecular weight	168.24	94.19
Melting point	49–50°C	
Boiling point	267–268°C 134–136°C at 15 mm Hg	116–118°C (112°C)
Specific gravity	1.015 at 27°C	1.0647 at 20°C
Refractive index		1.5260 at 20°C
Solubility	Insoluble in water; soluble in alcohol and ether; very soluble in organic solvents	Very slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics		Diffuse intense onion odor; nonlachrymatory
Synthesis	By catalytic reduction of *p*-phenyl benzyl alcohol obtained from *p*-phenyl benzoic acid[6]	From magnesium methyl iodide and S_2Cl_2,[7] or from Na_2S_2 and sodium methyl sulfate,[8] also from methyl bromide and sodium thiosulfate, after which the resulting sodium methylthiosulfate is heated to yield dimethyl disulfide
Natural occurrence		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm Gelatins and puddings 5.0 ppm	
Regulatory status	FEMA No. 3186	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.

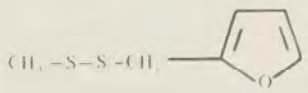
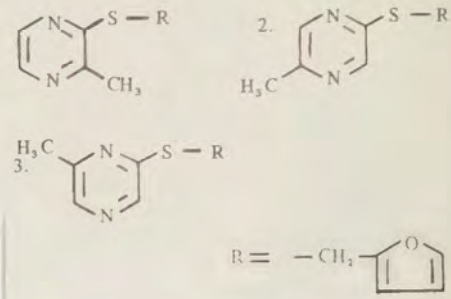
6. Newman, Eberwein and Wood, *J. Am. Chem. Soc.*, 81, 6454, 1959.
7. Ferrario, *Bull. Soc. Chim. Fr.*, 4(7), 524, 1910.
8. Ray and Gupta, *Z. Anorg. Chem.*, 187, 40, 1930.

	2-Methyl-3-furanthiol	5-Methyl furfural
Other names		5-Methyl-2-furaldehyde α-Methylfurfural
Empirical formula	C_5H_6OS	$C_6H_6O_2$
Structure		
Physical/chemical characteristics		
Appearance		Colorless liquid
Molecular weight	114.16	110.11
Boiling point		187°C; 79–81°C at 12 mm Hg
Specific gravity		1.1072 at 18°C
Refractive index		1.5263 at 20°C
Solubility		Soluble in water (3.3%); very soluble in alcohol; soluble in propylene glycol and oils
Organoleptic characteristics	Odor and taste of roasted meat	Sweet, spicy, warm odor; sweet caramel-like flavor
Synthesis	By a patented process[6]	See *Beilstein* B 17², 315; from sucrose with HCl, followed by treating with stannous chloride; from various methylpentoses by distillation with acid
Reported uses[3]	Baked goods 0.25 ppm Condiments 0.25 ppm Meat, meat sauces, soups 0.25 ppm	Non-alcoholic beverages 0.13 ppm Ice cream, ices, etc. 0.13 ppm Candy 0.03–0.13 ppm Baked goods 0.03 ppm
Regulatory status	FEMA No. 3188	Status not fully defined by FDA; FEMA No. 2702

REFERENCES

For References 1–5, see end of Part III.

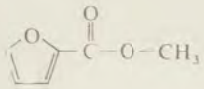
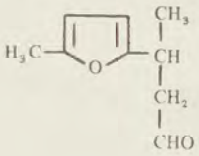
6. Evers, International Flavors and Fragrances, Inc., German Patent 2,003,525, 1970.

	Methyl furfuryl disulfide		2-Methyl-3 or 5 or 6-furfuryl thiopyrazine	
Other names			1. 2-Furfurylthio-3-methylpyrazine 2. 2-Furfurylthio-5-methylpyrazine 3. 2-Furfurlythio-6-methylpyrazine	
Empirical formula	$C_6H_8OS_2$		$C_{10}H_{10}N_2OS$	
Structure				
Physical/chemical characteristics				
Assay			C: 58.23%; H: 4.89%; N: 13.58%; O: 7.76%; S: 15.54%	
Molecular weight	128.19		206.27 (calculated = 206.051385)	
Boiling point			153–156 °C at 10 mm Hg (mixture)[6]	
Refractive index			n_D^{20} = 1.5970 n_D^{20} = 1.2164	
Organoleptic characteristics			Roasted, coffee-like flavor	
Synthesis			A mixture of 2-methyl 3-, 5-, and 6-chloropyrazine is prepared by chlorination of 2-methylpyrazine;[7] sodium furfuryl mercaptide is added to this mixture to give the three isomers[6]	
Natural occurrence	In bread (unpublished communication)			
Reported uses[3]	Non-alcoholic beverages	1.0 ppm	Non-alcoholic beverages	1.0 ppm
	Ice cream, ices, etc.	1.0 ppm	Ice cream, ices, etc.	1.0 ppm
	Candy	2.0 ppm	Baked goods	1.0 ppm
	Baked goods	2.0 ppm	Condiments	1.0 ppm
	Gelatins and puddings	1.0 ppm	Sauces	1.0 ppm
	Meat, meat sauces, soups	1.0 ppm		
Regulatory status	FEMA No. 3362		FEMA No. 3189	

REFERENCES

For References 1–5, see end of Part III.

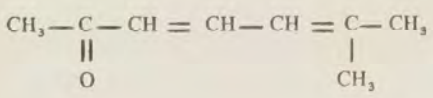
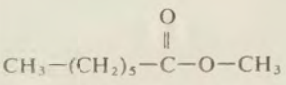
6. Winter et al., U.S. Patent 3,702,253, 1972.
7. Hirschberg and Spoerri, *J. Org. Chem.*, 26, 2356, 1961.

	Methyl furoate	3-(5-Methyl-2-furyl) butanal
Other names	Furan-2-carboxylic acid, methyl ester Methyl-2-furoate Methyl pyromucate	3-(5-Methyl-2-furyl) butyraldehyde
Empirical formula	$C_6H_6O_3$	$C_9H_{12}O_2$
Structure		
Physical/chemical characteristics[2]		
Appearance	Colorless liquid; tends to yellow on exposure to light	
Molecular weight	126.11	152.19
Boiling point	181–182°C; 81–82°C at 20 mm Hg	
Specific gravity	1.1786 at 21.4°C	
Refractive index	1.4860 at 20°C	
Solubility	Insoluble in water; soluble in alcohol and most organic solvents	
Organoleptic characteristics	Pleasant, fruity odor similar to mushroom, fungus or tobacco; sweet, tart, fruity taste, quite heavy	
Synthesis	From 2-furoic acid in methanol solution in the presence of HCl as catalyst[6] (oxidation or Carmizzaro reaction)	
Natural occurrence	Not reported found in nature	Reported not found in nature
Reported uses[3]	Non-alcoholic beverages 0.61 ppm Ice cream, ices, etc 0.06–1.3 ppm Candy 0.66 ppm Baked goods 1.0–1.3 ppm Condiments 0.02 ppm	Non-alcoholic beverages 0.1 ppm Ice cream, ices, etc. 0.4 ppm Candy 1.2 ppm Chewing gum 2.5 ppm Protein foods 0.1 ppm
Regulatory status	Status not fully defined by FDA; FEMA No. 2703	FEMA No. 3307

REFERENCES

For References 1–5, see end of Part III.

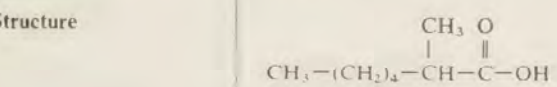
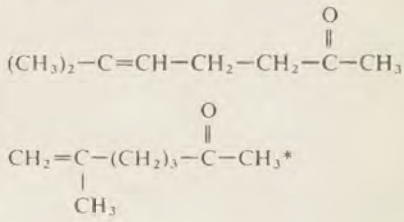
6. Gennari, *Gazz. Chim. Ital.*, 24(1), 249, 1894.

	6-Methyl-3,5-heptadien-2-one	Methyl heptanoate
Other names	2-Methyl-hepta-2,4-dien-6-one Methyl heptadienone 1-Acetyl-4-methyl-1,3-pentadiene	Methyl heptoate Methyl heptylate
Empirical formula	$C_8H_{12}O$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to pale yellow oily liquid	Colorless liquid
Molecular weight	124.18	144.21
Melting point		−55.8°C
Boiling point	190°C 83.5°C at 9 mm Hg	173.8°C
Specific gravity	0.8980 at 20°C	0.87115 at 20°C
Refractive index	1.5306 at 20°C	1.41334 at 20°C
Solubility	Almost insoluble in water; soluble in alcohol and oils	Soluble in most common organic solvents
Organoleptic characteristics	Cinnamon-like odor with a coconut undertone	Strong, almost fruity, orris-like odor; currant-like flavor
Synthesis	By reacting 2-methylbuten-2-al with acetone in the presence of sodium ethylate or sodium hydroxide;[6] by pyrolysis of tertiary acetylenic carbinyl acetoacetates in the presence of an acid catalyst[7]	By treating heptanoic acid with methyl alcohol in the presence of HCl or H_2SO_4[9-11]
Natural occurrence	Reported as occurring in the oil of lavandin[8]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.05 ppm Ice cream, ices, etc. 0.10 ppm Candy 0.15 ppm Baked goods 0.30 ppm Gelatins and puddings 0.05 ppm Milk, dairy products 0.05 ppm	Non-alcoholic beverages 0.80 ppm Ice cream, ices, etc. 0.83 ppm Candy 0.33 ppm Baked goods 0.50–0.60 ppm
Regulatory status	FEMA No. 3363	FDA 121.1164; FEMA No. 2705

REFERENCES

For References 1–5, see Introduction to Part II.

6. Fischer and Löwenberg, *Annalen.*, 494, 279, 1932.
7. Lacey, British Patent 741,047; *Chem. Abstr.*, 50, 16839, 1956.
8. Stadler, *Helv. Chim. Acta*, 43, 1601, 1960.
9. Gartenmeister, *Justus Liebigs Ann. Chem.*, 233, 281, 1886.
10. Bilterys and Gisseleire, *Bull. Soc. Chim. Belg.*, 44, 572, 1935.
11. Vogel, *J. Chem. Soc.* (London), p. 638, 1948.

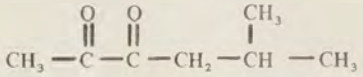
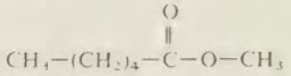
	2-Methylheptanoic acid	6-Methyl-5-hepten-2-one
Other names	Hexane-2-carboxylic acid Isocaprylic acid Isooctanoic acid Methylamylacetic acid 2-Methyloenanthic acid	2-Methyl heptenone 2-Methyl-2-hepten-6-one Methyl hexenyl ketone
Empirical formula	$C_8H_{16}O_2$	$C_8H_{14}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid; solidifies in the cold to colorless or white scaly crystals	Colorless to slightly yellow liquid
Assay		97% min[2]
Molecular weight	144.21	126.19
Melting point	15°C	−67.1°C
Boiling point	*dl*-, 121–122°C at 13 mm Hg; *d*-, 94–96°C at 1 mm Hg; 220°C	173.1°C (174°C)
Specific gravity	*l*-, 0.902 at 25°C	0.846–0.854 at 25°/25°C;[2] 0.8602 at 20°C
Refractive index	At 25°C: *l*-, 1.4233; *d*-, 1.4235	1.4380–1.4420[2] (1.4445) at 20°C
Optical rotation	*d*-, +8°9′; *l*-, −15°6′	
Solubility	Very slightly soluble in water; soluble in alcohol and oils	1:2 in 70% alcohol;[2] insoluble in water; soluble in most common organic solvents. Yields azeotropes with pentachloroethane (93%), *o*-cresol (15%), cineol (52%), and others
Organoleptic characteristics	Fatty, sour odor (rancid-like); sour, fruity, and nut-like flavor	Strong, fatty, green, citrus-like odor, and bittersweet taste reminiscent of pear
Synthesis	By decarboxylation of methylamyl malonic acid. Two optically active isomers and an optically inactive form can be prepared	From oil of lemongrass or from citral by refluxing for 12 hours in aqueous solution containing K_2CO_3, and subsequent distillation and vacuum fractionation; from acetoacetic ester and methylbuten-3-ol-2 with aluminum alcoholate in Carroll's reaction followed by pyrolysis of the ester.
Natural occurrence	Not reported found in nature	Originally identified in lemongrass.[6,7] It has been reported found in the essential oils of palmarosa, lemon, citronella, vervain, geranium, *Ocimum canum*, *Artemisia scoparia*, *Urtica dioica*, and others.
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 10 ppm Candy 10 ppm Baked goods 10 ppm	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 1.1 ppm Candy 1.1 ppm Baked goods 1.3 ppm Gelatins and puddings 1.3 ppm
Regulatory status	FDA 121.1164; FEMA No. 2706	FDA 121.1164; FEMA No. 2707

* Some products are 80% 6-methyl-5-hepten-2-one with 20% 2-methyl-1-hepten-6-one.

REFERENCES

For References 1–5, see end of Part III.

6. **Barbier and Bouveault,** *C. R. Séances Acad. Sci. Paris*, 118, 983, 1894.
7. **Tiemann, et al.,** *Ber. Dtsch. Chem. Ges.*, 28, 2126, 1895.

	5-Methyl-2,3-hexanedione	Methyl hexanoate
Other names	2-Methyl-4,5-hexanedione Acetyl isovaleryl Isobutyl methyl diketone Isobutyl methyl glyoxal Acetyl isopentanoyl	Methyl caproate Methyl capronate Methyl hexylate
Empirical formula	$C_7H_{12}O_2$	$C_7H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellowish liquid	Liquid
Molecular weight	128.17	130.18
Melting point		−71°C
Boiling point	138°C	151 C; 56°C at 20 mm Hg
Specific gravity	0.908 at 22°C	0.8850 at 20 C
Refractive index	1.4119 at 20°C	1.4049 at 20 C
Solubility	Slightly soluble in water; miscible with alcohol, propylene glycol, and glycerine	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Powerful oily-buttery odor; sweet taste in aqueous solution	Ether-like odor reminiscent of pineapple
Synthesis	By bromination of mesityl oxide, followed by treatment of the resulting dibromide with sulfuric acid[6]	By reacting methyl alcohol with hexanoic acid at 130–140°C in the presence of concentrated H_2SO_4 and distilling the ester from the reaction mixture[7,8]
Natural occurrence		Reported found in pineapple and *Fragaria vesca*
Reported uses[3]	Non-alcoholic beverages 20.0 ppm Candy 20.0 ppm	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 8.5 ppm Candy 5.3 ppm Baked goods 20 ppm
Regulatory status	FEMA No. 3190	FDA 121.1164; FEMA No. 2708

REFERENCES

For References 1–5, see end of Part III.

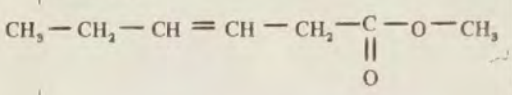
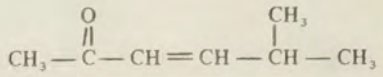
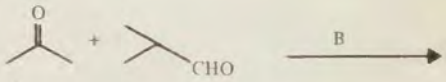
6. Dufraisse and Moureu, *Compt. Rend.*, 184, 99, 1927; *Bull. Soc. Chim. Fr.*, 41(4), 855, 1375, 1927.
7. Commercial Solvents Corp., U.S. Patent 2,029,694, 1934.
8. Vogel, *J. Chem. Soc.*, p. 630, 1948.

	2-Methylhexanoic acid	Methyl 2-hexenoate
Other names	2-Methylcaproic acid 2-Butylpropionic acid Butyl methylacetic acid Hexane-2-carboxylic acid	Methyl-α,β-hexenoate Methyl-β-propylacrylate
Empirical formula	$C_7H_{14}O_2$	$C_7H_{12}O_2$
Structure	$CH_3-CH_2-CH_2-CH_2-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-COOH$	$CH_3-(CH_2)_2-CH=CH-\overset{\displaystyle O}{\overset{\Vert}{C}}-O-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless oil	Colorless, mobile liquid
Molecular weight	130.19	128.17
Boiling point	105°C at 5 mm Hg	56–58 C at 13 mm Hg; 53–56 C at 7 mm Hg; 169 C
Specific gravity	0.909 at 25°C	
Refractive index	1.4189 at 25°C	
Optical rotation	*d*-, +19.6 at 22°C in ether *l*-, −15.25 at 25°C in ether	
Solubility	Either optically active form is miscible with water, ether, alcohol, and chloroform, as well as with other solvents	Very slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics		Green, musty, earthy, sweet, fruity odor; very powerful, sharp, green-fruity flavor
Synthesis	By catalytic hydrogenation of hexadien-2-carboxylic acid[6]	By boiling the corresponding acid with methanol in the presence of concentrated H_2SO_4 in chloroform and subsequent elimination of water from the vapors using $MgSO_4$;[7] also from 3-chloropropionic acid methyl ester and anhydrous sodium acetate in acetic acid[8]
Natural occurrence		Not reported found in nature
Reported uses[3]	Candy 8.0 ppm Baked goods 2.0 ppm Gelatins and puddings 2.0 ppm	Non-alcoholic beverages 0.03–0.12 ppm Candy 0.03 ppm
Regulatory status	FEMA No. 3191	FDA 121.1164; FEMA No. 2709

REFERENCES

For References 1–5, see end of Part III.

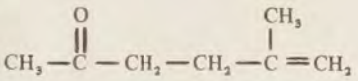
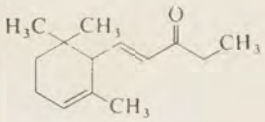
6. Reichstein and Trivelli, *Helv. Chim. Acta*, 15, 528, 1932.
7. Baker et al., *J. Org. Chem.*, 12, 144, 1947.
8. Guest, *J. Am. Chem. Soc.*, 69, 301, 1947.

	Methyl-3-hexenoate	5-Methyl-3-hexen-2-one
Other names	Methyl hydrosorbate	Isobutylidene acetone
Empirical formula	$C_7H_{12}O_2$	$C_7H_{12}O$
Structure		
Physical/chemical characteristics[5]		
Molecular weight	128.17	112.17
Boiling point		77.5°C at 50 mm Hg
Specific gravity		0.8407 at 22°C
Refractive index		1.4395 at 22°C
Synthesis	By selective hydrogenation of methyl sorbate;[6] from 3-hexenoic acid and methanol in the presence of BF_3.[7]	
Natural occurrence	Reported found as a volatile component in smooth Cayenne pineapple[8]	Reported found in roasted filberts[6]
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 4.0 ppm Baked goods 4.0 ppm Gelatins and puddings 2.0 ppm Preserves and spreads 2.0 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 4.0 ppm Baked goods 4.0 ppm Gelatins and puddings 4.0 ppm Milk, dairy products 1.0 ppm Cereals 2.0 ppm
Regulatory status	FEMA No. 3364	FEMA No. 3409

REFERENCES

For References 1–5, see end of Part III.

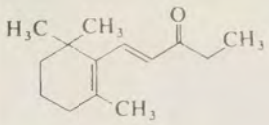
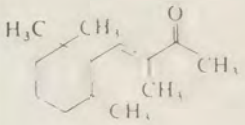
6. Frankel, Selke and Glass, *J. Am. Chem. Soc.*, 90(9), 2446, 1968.
7. Fell, Bendel, Lauscher and Huebner, *J. Chromatogr.*, 24(1), 161, 1966.
8. Flath and Forrey, *J. Agric. Food Chem.*, 18(2), 306, 1970.
9. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Central Instituut voor Voedingsonderzoek, Zeist, Netherlands.

	5-Methyl-5-hexen-2-one	Methyl-α-ionone
Other names	Methallyl acetone 4-Acetyl-2-methyl-1-butene	α-Cetone α-Cyclocitrylidene butanone α-Cyclocitrylidene methyl ethyl ketone α-*n*-Methylionone Raldeine 5-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-4-penten-3-one
Empirical formula	$C_7H_{12}O$	$C_{14}H_{22}O$
Structure		
Physical/chemical characteristics[5]		
Appearance		Yellowish, oily liquid
Molecular weight	112.17	206.30
Boiling point	148–149°C	97°C at 2.6 mm Hg; 238°C
Specific gravity	0.8475 at 25°C	0.9210 at 25°C
Refractive index	1.4279 at 25°C	1.4938 at 25°C
Organoleptic characteristics		Odor similar to α-ionone but lighter and more rounded; pleasant, fruity, and sweet nuance
Synthesis	From methallyl alcohol, the corresponding methallyl acetoacetone is prepared, dissolved in diphenyl ether, and finally heated to 200–215°C[6]	By condensation of citral with methyl ethyl ketone (see methyl γ-ionone or α-iso-methylionone)
Natural occurrence		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.12 ppm Ice cream, ices, etc. 0.25 ppm Candy 0.40 ppm Baked goods 0.75 ppm Gelatins and puddings 0.25 ppm Milk, dairy products 0.12 ppm	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 2.4 ppm Candy 6.6 ppm Baked goods 6.5 ppm Chewing gum 0.60 ppm Jellies 0.21 ppm
Regulatory status	FEMA No. 3365	FDA 121.1164; FEMA No. 2711

REFERENCES

For References 1–5, see end of Part III.

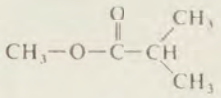
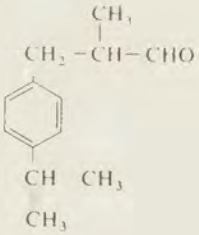
6. Kimel and Cope, *J. Am. Chem. Soc.*, 65, 1922, 1943.

	Methyl-β-ionone	*iso*-Methyl-β-ionone
Other names	β-Cetone β-Cyclocitrylidene butanone β-*n*-Methylionone Raldeine 5-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-4-penten-3-one	Isomethyl-β-ione γ-Isomethylionone "*delta*"-Methylionone 4-(2,6,6-Trimethyl-3-cyclohexen-1-yl)-3-methyl-3-buten-2-one
Empirical formula	$C_{14}H_{22}O$	$C_{14}H_{22}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellowish liquid	Almost colorless to slightly yellow oil
Molecular weight	206.30	206.33
Boiling point	102 C at 2.6 mm Hg; 242 C	232 C; 76 C at 0.3 mm Hg
Specific gravity	0.9338 at 25°C	
Refractive index	1.5140 at 25°C	1.4969 at 25°C
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics	Odor similar to β-ionone with a Bulgarian leather note	Light, warm, floral odor; berry-like flavor
Synthesis	By condensation of citral with methyl ethyl ketone (see γ-isomethylionone). It is usually present in low levels (6–7%) in commercial products.	See Reference 6
Natural occurrence	Not reported in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.2 ppm Candy 7.5 ppm Baked goods 5.9 ppm	Non-alcoholic beverages 0.61 ppm Ice cream, ices, etc. 0.89 ppm Candy 3.2 ppm Baked goods 2.8 ppm
Regulatory status	FDA 121.1164; FEMA No. 2712	FDA 121.1164; FEMA No. 2713

REFERENCES

For References 1–5, see end of Part III.

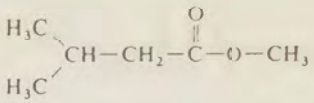
6. **Bedoukian,** *Perfumery and Flavoring Synthetics,* American Elsevier, 1967.

	Methyl isobutyrate	2-Methyl-3-(*p*-isopropylphenyl)-propionaldehyde
Other names	Methyl dimethylacetate Methyl-2-methylpropanoate	Cyclamen aldehyde *p*-Isopropyl-α-methylhydrocinnamaldehyde *p*-Isopropyl-α-methylphenylpropylaldehyde α-Methyl-*p*-isopropylhydrocinnamaldehyde
Empirical formula	$C_5H_{10}O_2$	$C_{13}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, mobile liquid	Colorless to pale-yellow liquid
Assay		90% min[2] (50–96%)
Molecular weight	102.13	190.28
Melting point	−85 C	
Boiling point	92–93 C	270 C
Specific gravity	0.891 at 20 C	0.946–0.952 at 25 /25 C;[2] 0.950 at 20 C
Refractive index	1.3840 at 20 C	1.5030–1.5080[2] (1.500) at 20 C
Acid value		Not more than 5[2]
Solubility	Slightly soluble in water; miscible with most common organic solvents	1:1 in 80% alcohol;[2] soluble in most common organic solvents
Organoleptic characteristics	Fruity (apple-pineapple) odor; sweet flavor reminiscent of apricot	Strong, flowery odor
Synthesis	By direct esterification of methanol with isobutyric acid	By condensation of cuminic aldehyde and propionaldehyde followed by hydrogenation in the presence of a catalyst[8]
Natural occurrence	Reported found in Russian champagnes[6] and among the volatile components of strawberry juice[7]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 22 ppm Ice cream, ices, etc. 38 ppm Candy 48–200 ppm Baked goods 48–200 ppm	Non-alcoholic beverages 0.30 ppm Ice cream, ices, etc. 0.45 ppm Candy 0.99 ppm Baked goods 1.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2694	FDA 121.1164; FEMA No. 2743

REFERENCES

For References 1–5, see end of Part III.

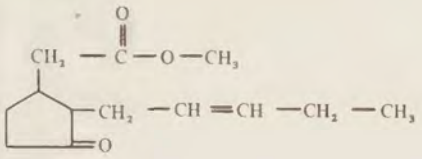
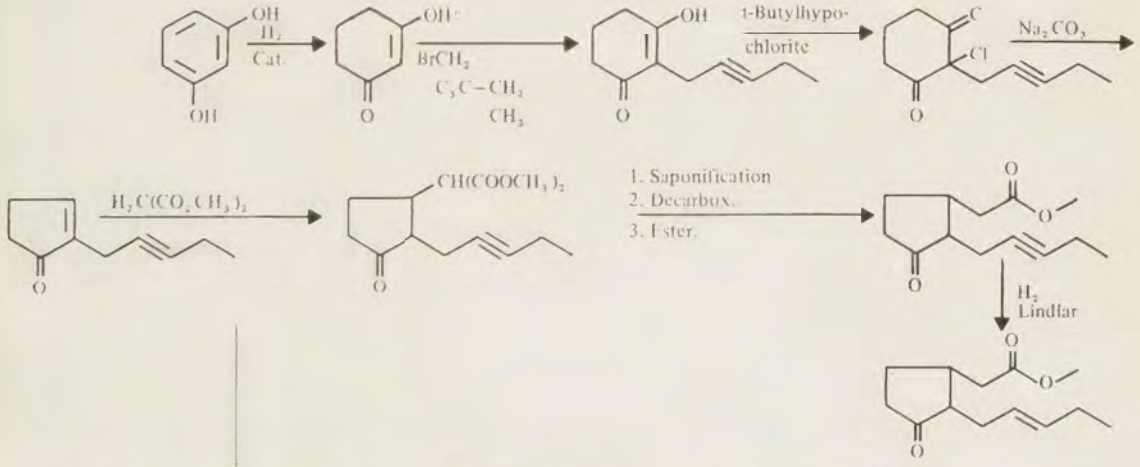
6. **Rodopulo and Egorov,** *Chem. Abstr.*, 61, 11291g, 1964.
7. **Roy et al.,** *J. Food Sci.*, 28, 478, 1963.
8. **Mousseron et al.,** *Fr. Ses Parfums*, 3, 28, 1958.

	Methyl isovalerate
Other names	
Empirical formula	$C_6H_{12}O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid
Molecular weight	116.16
Melting point	
Boiling point	116–117 C
Specific gravity	0.8807 at 20 C
Refractive index	1.3927 at 20 C
Solubility	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Strong, pungent, apple-like odor; bitter flavor
Synthesis	By esterification of isovaleric acid with methyl alcohol at the boil in the presence of concentrated H_2SO_4[6]
Natural occurrence	Reported found in pineapple fruits[7,8] and in the juice of a few varieties of Florida oranges[9]
Reported uses[3]	Non-alcoholic beverages 9.3 ppm Ice cream, ices, etc. 26 ppm Candy 26 ppm Baked goods 30 ppm Chewing gum 35 ppm
Regulatory status	FDA 121.1164; FEMA No. 2753

REFERENCES

For References 1–5, see end of Part III.

6. Vogel, *J. Chem. Soc.*, p. 630, 1948.
7. Haagen-Smit et al., *J. Am. Chem. Soc.*, 67, 1647, 1945.
8. Connel, *Aust. J. Chem.*, 1(17), 130, 1964.
9. Wolford et al., *J. Food Sci.*, 28, 320, 1963.

	Methyl jasmonate
Other names	2-Pentenyl cyclopentanone-3-acetic acid, methyl ester 2-(*cis*-Penten-2′-yl)-3-oxo-cyclopentane acetic acid, methyl ester Methyl (2-pent-2-enyl-3-oxo-1-cyclopentyl) acetate
Empirical formula	$C_{13}H_{20}O_3$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless oily liquid
Molecular weight	224.30
Boiling point	94°C at 0.05 mm Hg
Specific gravity	1.021 at 22.6°C
Refractive index	1.4730 at 31.8°C
Optical rotation	−76.5° (c = 3.5 in methanol)
Solubility	Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Powerful, floral-herbaceous, sweet-persistent odor[9]
Synthesis	Can be isolated from jasmine oil;[6] synthetically it can be prepared (probably in the *trans*-form) from muconic acid via the methyl-3-oxo-cyclopenthyl acetate[7]; also[10]
	
Natural occurrence	Reportedly identified in jasmin oil (*Jasminum grandiflorum* L.) and in Tunisian rosemary[8]
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm Gelatins and puddings 1.0 ppm Condiments, pickles 1.0 ppm Perserves and spreads 1.0 ppm
Regulatory status	FEMA No. 3410

REFERENCES

For References 1–5, see end of Part III.

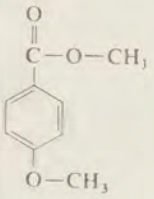
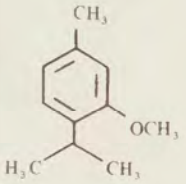
6. Demole et al., *Helv. Chim. Acta*, 45, 675, 1962.
7. Demole et al., *Helv. Chim. Acta*, 45, 692, 1962.
8. Crabalone, *Compt. Rend.* Paris, C264, 2074, 1967; *Chem. Abstr.*, 67, 84752r, 1967.
9. Arctander, *Perfume and Flavor Chemicals*, Montclair, N.J., 1969, No. 2093.
10. German Patent 2,160,646.

	Methyl laurate	Methyl mercaptan
Other names	Methyl dodecanoate Methyl dodecylate	Methanethiol
Empirical formula	$C_{13}H_{26}O_2$	CH_4S
Structure	$CH_3-(CH_2)_{10}-\overset{\overset{O}{\|}}{C}-O-CH_3$	H_3C-SH
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless gas; liquid under compression. The hydrate is a white crystalline material.
Molecular weight	214.35	48.11
Melting point	5°C	121 C
Boiling point	261–262°C; 127°C at 8 mm Hg	6.1–6.2 C at 727 mm Hg
Specific gravity	0.8695 at 20 C	0.894 (liquid)
Refractive index	1.4320 at 20°C	
Solubility	Insoluble in water; soluble in most common organic solvents	Gas is slightly soluble in water (decomposes slowly); soluble in alcohol, ether, and most common organic solvents
Organoleptic characteristics	Fatty, floral odor reminiscent of wine	Objectionable odor of decomposing cabbage
Synthesis	By prolonged boiling of lauric acid with methanol in the presence of sulfuric acid[10]	By heating an aqueous solution of potassium methyl sulfate and KHS; from sodium methyl sulfate and potassium sulfhydrate; also from methanol and hydrogen sulfide in the presence of a catalyst.
Natural occurrence	Reported found in orris absolute[11]	Originally identified in the fresh roots of *Rafanus sativus* L.;[6] reported found in the red algae of *Polysiphonia fastigiata*.[7] Also reported in the leaves of *Coprosma foetidissima* Forst.[8] and the seeds of *Brassica napus* var. *oleifera*[9]
Reported uses[3]	Non-alcoholic beverages 0.50–5.0 ppm Ice cream, ices, etc. 0.50–5.0 ppm Candy 0.02–0.50 ppm Baked goods 1.0 ppm	Non-alcoholic beverages 0.56 ppm Ice cream, ices, etc. 0.13–1.0 ppm Candy 0.13–1.0 ppm Baked goods 0.15–1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2715	FDA 121.1164; FEMA No. 2716

REFERENCES

For References 1–5, see end of Part III.

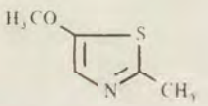
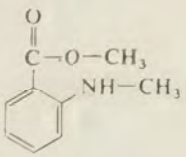
6. Nakamura, *Biochem. Z.*, 164, 31, 1925.
7. Haas, *Biochem. J.*, 29, 1297, 1935.
8. Sutherland, *Br. Abstr. A3*, p. 645, 1949.
9. Andre, *Chem. Abstr.*, 44, 2262, 1950.
10. Vogel, *J. Chem. Soc.*, p. 631, 1948.
11. Naves, *Helv. Chem. Acta*, 32, 2306, 1949.

	Methyl *o*-methoxybenzoate	1-Methyl-3-methoxy-4-isopropylbenzene
Other names	Dimethyl salicylate Methyl *o*-anisate	3-Methyl-*p*-cymene Thymol methylether
Empirical formula	$C_9H_{10}O_3$	$C_{11}H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Low-melting solid	
Molecular weight	166.18	164.24
Boiling point	48–49°C 254–255°C	215°C 94–96° C at 15 mm Hg
Specific gravity		0.9388 at 14°C
Refractive index		1.5062 at 20°C
Solubility	Insoluble in water; soluble in alcohol	
Organoleptic characteristics	Herbaceous, anise-like odor; sweet taste reminiscent of melon	
Synthesis	By esterification of anisic acid with methanol; or from sodium anisate and dimethylsulfate in the presence of methanol	From thymol and dimethylsulfate in alkaline solution;[6] from sodium thymolate with dimethylsulfate in water[7]
Natural occurrence	Reported found in a mushroom variety, *Trametes graveolens*[15]	In the oils of French *Christinium maritinium*,[8] *Orthodon madai*,[9] *O. hirtum*,[10] *O. tenuicaule*,[11] *O. japonicum albiflorum*,[12] *O. pseudohirtum*,[12] *O. goshizanese*,[12] *Eupatorium fortunei*,[13] and *Monarda punctata*[14]
Reported uses[3]	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 3.0 ppm Candy 8.0 ppm Baked goods 6.2 ppm	Non-alcoholic beverages 2.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm Condiments 2.0 ppm Meat, meat sauces, soups 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2679	FEMA No. 3436

REFERENCES

For References 1–5, see end of Part III.

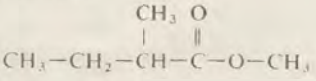
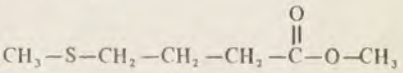
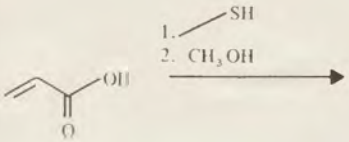
6. **Kuroda et al.**, *Sci. Pap. Inst. Phys. Chem. Res.*, 18, 61, 1932.
7. **Caujolle et al.**, *Compt. Rend.*, 218, 571, 1944.
8. **Delepine**, *Compt. Rend.*, 150, 1061, 1910; *Bull. Soc. Chim. Fr.*, [4] 7, 468, 1910.
9. **Fujita**, *J. Chem. Soc. Jap.*, 65, 166, 1944; *Chem. Abstr.*, 41, 3585, 1947.
10. **Fujita**, *J. Chem. Soc. Jap.*, 59, 500, 1938; *Chem. Abstr.*, 61, 137, 1940.
11. **Fujita**, *J. Chem. Soc. Jap.*, 61, 782, 1940.
12. **Fujita**, *Report of the Osaka Industrial Research Institute* No. 306, 1955, 8.
13. **Liang et al.**, *Chem. Abstr.*, 54, 5019, 1960.
14. **Schimmel and Co.**, *Ber. Schimmel*, No. 46, 1922.
15. **Aye**, *Arch. Pharm.*, p. 246, 1931.

	2-Methyl-5-methoxy thiazole		Methyl-*n*-methylanthranilate	
Other names			Dimethyl anthranilate Methyl 2-methylaminobenzoate Methyl *o*-methylaminobenzoate	
Empirical formula	C_5H_7NOS		$C_9H_{11}O_2N$	
Structure				
Physical/chemical characteristics[5]				
Appearance			Pale-yellow liquid with slight bluish fluorescence	
Assay			98% min[2] (99%)	
Molecular weight	141.18		165.19	
Melting point			18.5–19.5 C	
Boiling point			256 C; 130–131 C at 13 mm Hg	
Congealing point			>12.0 C[2] (12.5–15.5 C)	
Flash point			91 C	
Specific gravity			1.126–1.132 at 25°/25°C;[2] 1.3545–1.1375 at 15 C	
Refractive index			1.5785–1.5810[2] (1.5800–1.5810) at 20°C	
Acid value			0.2 max	
Solubility			1:3 in 80% alcohol;[2] 1:8–11 in 70% alcohol; insoluble in water; soluble in most common organic solvents	
Organoleptic characteristics			Orange and mandarin-peel-like odor; musty, grape-like flavor; somewhat more berry-like than grape	
Synthesis	Can be prepared from chloro- (or bromo-) methoxyacetaldehyde and thioacetamide[1,2]		By methylation of methyl anthranilate or esterification of *N*-methylanthranilic acid	
Natural occurrence			Reported found in mandarin essential oil[6] and mandarin-leaves essential oil (50–76.5%);[7,8] also reported in the oil from bulbs of *Kaempferia ethelae* L.,[9] in orange petitgrain,[10] and in the oil from hyacinth flowers[11]	
Reported uses[3]	Non-alcoholic beverages	2.0 ppm	Non-alcoholic beverages	5.1 ppm
	Baked goods	4.0 ppm	Ice cream, ices, etc.	5.0 ppm
	Meat, soups	2.0 ppm	Candy	18 ppm
			Baked goods	17 ppm
			Jellies	4.0 ppm
Regulatory status	FEMA No. 3192		FDA 121.1164; FEMA No. 2718	

REFERENCES

For References 1–5, see end of Part III.

6. Walbaum, *Chem. Zentralbl.*, 2, 677, 1900.
7. Charabot, *Chem. Zentralbl.*, 2, 879, 1903.
8. Schimmel and Co., *Chem. Zentralbl.*, 2, 1785, 1930.
9. Goulding and Roberts, *J. Chem. Soc.* (London), 107, 314, 1915.
10. Glichitch and Naves, *Chem. Zentralbl.*, 1, 604, 1930.
11. Hoejenbons and Coppens, *Chem. Zentralbl.*, 2, 2746, 1932.
12. Pitten et al., German Patent 2,152,557; *Chem. Abstr.*, 55, 88488, 1972.

	Methyl-2-methylbutyrate	Methyl-4-(methylthio) butyrate
Other names	Methyl-2-methylbutanoate Methyl methylethylacetate	Mixture of methyl 9,12-octadecadienoate and methyl 9,12,15- octadecatrienoate Methyl γ-methyl mercapto butyrate
Empirical formula	$C_6H_{12}O_2$	$C_6H_{12}O_2S$
Structure		
Physical/chemical characteristics		
Appearance	Colorless liquid	
Molecular weight	116.16	148.21
Boiling point	115–116°C	
Specific gravity	0.8851 at 20°C	
Refractive index	1.3942 at 20°C	
Solubility	Very slightly soluble in water; soluble in alcohol	
Organoleptic characteristics	Pungent, fruity odor; sweet, fruity, apple-like taste at low levels	
Synthesis	A mixture of esters including methyl 2-methylbutyrate is obtained from isobutene, CO, and methanol under pressure, or from butene, CO, and an acid catalyst under pressure[6]	
Natural occurrence	Reported found in fresh strawberry juice.[7] The laevorotatory and the racemic forms are known.	
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 10 ppm Candy 10 ppm Baked goods 10 ppm	Baked goods 10.0 ppm Meat, meat sauces 10.0 ppm Sauces 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2719	FEMA No. 3412

REFERENCES

For References 1–5, see end of Part III.

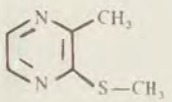
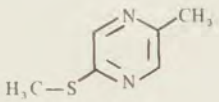
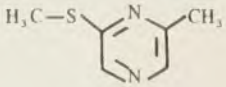
6. **Eidus and Kaal,** *Zh. Obshch. Khim.*, 33, 3283, 1963; 35, 120, 1965.
7. **Willhalm, Pauly and Winter,** *Helv. Chim. Acta*, 49, 65, 1966.

	Methyl-3-methylthiopropionate
Other names	Methylmercaptomethylpropionate Methyl-β-methylmercaptopropionate Methyl-β-methylthiopropionate β-Methylthiopropionic acid, methyl ester
Empirical formula	$C_4H_{10}O_2S$
Structure	$CH_2(SCH_3)-CH_2-C(=O)-OCH_3$
Physical/chemical characteristics[5]	
Appearance	Liquid
Molecular weight	134.20
Boiling point	69°C (181°C) at 11 mm Hg
Refractive index	1.4600 at 32°C
Solubility	Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Extremely powerful, penetrating, sweet odor; onion-like at high concentrations; sweet, pineapple flavor at high dilutions
Synthesis	Obtained in 84% yields by reacting $CH_2=CH-C(=O)-OCH_3$ with CH_3SH.[6] The corresponding acid also has been synthesized.[7]
Natural occurrence	Reported found in pineapple fruits[8]
Reported uses[3]	Non-alcoholic beverages 0.35 ppm Ice cream, ices, etc. 0.37 ppm Candy 0.74 ppm Baked goods 1.0 ppm Syrups 0.05 ppm
Regulatory status	FDA 121.1164; FEMA No. 2720

REFERENCES

For References 1–5, see end of Part III.

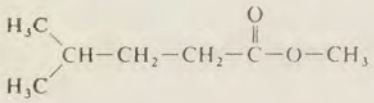
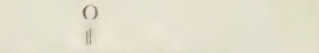
6. Haagen-Smit et al., *J. Am. Chem. Soc.*, 67, 1646, 1945.
7. Lester et al., *J. Am. Chem. Soc.*, 70, 3667, 1948.
8. Barger and Coyne, *Biochem. J.*, 22, 1417, 1928.

	2-Methyl-3 or 5 or 6-methylthiopyrazine
Other names	(a) 2-Methyl-3-methylthiopyrazine (b) 2-Methyl-5-methylthiopyrazine (c) 2-Methyl-6-methylthiopyrazine (Methylthio) methylpyrazine
Empirical formula	$C_6H_8N_2S$
Structure	 (a)  (b)  (c)
Physical/chemical characteristics	
Appearance	Colorless liquid
Assay	C: 51.40%; H: 5.75%; N: 19.98%; S: 22.87%
Molecular weight	140.21
Boiling point	105 -106°C at 12 mm Hg
Specific gravity	1.142 - 1.145
Refractive index	1.579 -1.583
Mass spectra	(a): 84 (14), 93 (14), 94 (10), 106 (18), 107 (31), 125 (27), 140 (100)
IR spectra[7]	(a) 9.15, 7.37, 7.26, 9.07, 8.53, 9.40, 11.88 μm
Solubility	Soluble in 1 part 70% alcohol or 5 parts 50% alcohol
Organoleptic characteristics	Roasted almonds, hazelnuts
Synthesis	From 2-methylchloropyrazine; a mixture of 2-methyl-3-methylthiopyrazine, 2-methyl-5-methylthiopyrazine, and 2-methyl-6-methylthiopyrazine is obtained[6]
Reported uses[3]	Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Baked goods 4.0 ppm Gelatins and puddings 2.0 ppm Coffee aroma enhancing agent[8]
Regulatory status	FEMA No. 3208

REFERENCES

For References 1–5, see end of Part III.

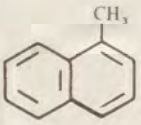
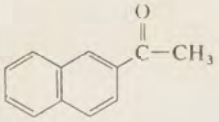
6. Firmenich & Co., French Patent 1,391,212, 1965.
7. **Friedel et al.,** *J. Agric. Food Chem.*, 19, 530, 1971.
8. **Parliment et al.,** French Patent 2,062,168.

	Methyl-4-methylvalerate	Methyl myristate
Other names	Methyl isobutrylacetate Methyl isocaproate Methyl-4-methyl pentanoate	Methyl *n*-tetradecanoate
Empirical formula	$C_7H_{14}O_2$	$C_{15}H_{30}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid or white, waxy solid
Molecular weight	130.18	242.41
Melting point		18°C (22°C)
Boiling point	142–143°C	300°C (295°C)
Specific gravity		0.870 at 15.5°C
Refractive index		1.4875 at 20°C
Solubility	Insoluble in water; soluble in alcohol and oils	Insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Sweet, pineapple-like flavor	Honey and orris-like odor; corresponding flavor at trace levels
Synthesis	From isocapric acid and methanol at the boil in the presence of H_2SO_4[6]	By direct esterification of methanol with myristic acid in the presence of gaseous HCl
Natural occurrence	Reported found in pineapple fruits[7]	Reported found in violet roots[8]
Reported uses[1]	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 44 ppm Candy 33 ppm Baked goods 33 ppm	Non-alcoholic beverages 0.25–0.50 ppm Ice cream, ices, etc. 0.25–0.50 ppm Candy 2.4 ppm Baked goods 0.30–2.0 ppm Gelatins and puddings 0.24 ppm
Regulatory status	FDA 121.1164; FEMA No. 2721	FDA 121.1164; FEMA No. 2722

REFERENCES

For References 1–5, see end of Part III.

6. Kohlrausch et al., *Z. Phys. Chem.*, 22, 366, 1933.
7. Haagen-Smit et al., *J. Am. Chem. Soc.*, 67, 1647, 1945.
8. Tiemann and Krüger, *Ber. Dtsch. Chem. Ges.*, 26, 2677, 1893.

	1-Methylnaphthalene	Methyl β-naphthyl ketone
Other names	α-Methylnaphthalene	2'-Acetonaphthone 2-Acetylnaphthalene Methyl naphthyl ketone β-Naphthyl methyl ketone
Empirical formula	$C_{11}H_{10}$	$C_{12}H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	White or nearly white crystalline solid
Assay		99% min[2]
Molecular weight	142.20	170.21
Melting point		56°C (52–54°C)
Boiling point	244°C 110°C at 12 mm Hg 107.4°C at 10 mm Hg	300–301°C 153.0°C[2]
Congealing point	−22°C	
Flash point		129°C
Specific gravity	1.0202 at 20°C	
Refractive index	1.6170 at 20°C	
Solubility	Insoluble in water; soluble in benzene; very soluble in alcohol and ether	1 gm in 5 ml of 95% alcohol;[2] insoluble in water; soluble in most common organic solvents
Organoleptic characteristics		Odor suggestive of orange blossom; strawberry-like flavor
Synthesis	Generally obtained from coal tar and petroleum oils[6]	Prepared by Friedel-Crafts reaction of naphthalene, acetyl chloride and $AlCl_3$[7]
Natural occurrence		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Gelatins and puddings 1.0 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.75 ppm Candy 5.3 ppm Baked goods 2.0 ppm Gelatins and puddings 2.2–3.0 ppm Chewing gum 480–700 ppm
Regulatory status	FEMA No. 3193	FDA 121.1164; FEMA No. 2723

REFERENCES

For References 1–5, see end of Part III.

6. *Ullmanns Enzyklopädie der Technischen Chemie*, Vol. 2, Urban and Schwarzenberg, 1960, 588.
7. Leroy, *Bull. Soc. Chim. Fr. Ser. 3*, 7, 649, 1892.

	Methyl nonanoate	Methyl-2-nonenoate
Other names	Methyl pelargonate	"Neofolione"
Empirical formula	$C_{10}H_{20}O_2$	$C_{10}H_{18}O_2$
Structure	$CH_3-(CH_2)_7-\overset{\overset{O}{\|}}{C}-O-CH_3$	$CH_3-(CH_2)_5-CH=CH-\overset{\overset{O}{\|}}{C}-O-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless or light-yellow liquid
Assay	>96%	95%
Molecular weight	172.27	170.25
Melting point	−35°C	
Boiling point	213.5–214°C	
Specific gravity	0.8331 at 0°C; 0.877 at 18°C	0.893–0.898 at 25°C
Refractive index	1.4302 at 25°C	1.4400–1.4440 at 20°C
Solubility	Insoluble in water; soluble in alcohol and ether	1:4 in 70% alcohol; insoluble in water
Organoleptic characteristics	Wine and coconut-like odor; below 10 ppm sweet, coconut-like flavor	Characteristic violet-like odor
Synthesis	By heating pelargonic acid with methyl alcohol in the presence of concentrated sulfuric acid and subsequent rectification; or by hydrogenation of 1,5-octadien-carboxylic acid (?) methyl ester using palladium chloride in methanol solution	Obtained in quantitative yields by treating methyl β-chlorocaproate with sodium acetate, or by dehydrogenating the corresponding saturated ester[6]
Natural occurrence	Reported found in orris derivatives	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.9 ppm Ice cream, ices, etc. 3.6 ppm Candy 6.2 ppm Baked goods 7.1 ppm	Non-alcoholic beverages 3.2 ppm Ice cream, ices, etc. 12 ppm Candy 9.9 ppm Baked goods 13 ppm
Regulatory status	FDA 121.1164; FEMA No. 2724	FDA 121.1164; FEMA No. 2725

REFERENCES

For References 1–5, see end of Part III.

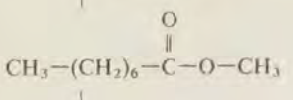
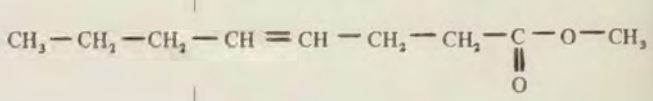
6. Melanetton, Brown and Henry, *J. Org. Chem.*, 28, 3261, 1963.

	Methyl 2-nonynoate	2-Methyloctanal
Other names	Methyl octine carbonate Methyl octyne carbonate	Methyl hexyl acetaldehyde
Empirical formula	$C_{10}H_{16}O_2$	$C_9H_{18}O$
Structure	$CH_3-(CH_2)_5-C\equiv C-\overset{\overset{O}{\|\|}}{C}-O-CH_3$	$CH_3-(CH_2)_5-\overset{\overset{CH_3}{\|}}{CH}-CHO$
Physical/chemical characteristics[3]		
Appearance	Colorless, oily liquid	Colorless, oily liquid
Molecular weight	168.24	142.24
Boiling point	232°C; 122°C at 20 mm Hg; 220°C	82–83°C at 20 mm Hg
Specific gravity	0.916–0.918 at 20°C; 0.932 at 15.5°C	0.8411 at 0°C
Refractive index	1.448–1.450 at 20°C (1.4515)	1.42335 at 14°C
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Characteristic violet-like odor; sweet taste reminiscent of fresh peach, unripe banana, and cucumber peel	Delicate, floral odor (rose or lily-like)
Synthesis	From 2-octene by way of 1-octyne and octyne carboxylic acid	By heating methoxymethyl hexyl carbinol with oxalic acid[6,7] or with anhydrous formic acid.[8,9] Also from hexanal and propionic aldehyde. Darzen's synthesis of reacting methyl hexyl ketone and ethyl chloroacetate with sodium ethylate; the resulting ester is then hydrolyzed to the acid and this heated under vacuum
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.69 ppm Ice cream, ices, etc. 0.28 ppm Candy 0.61 ppm Baked goods 2.2 ppm Gelatins and puddings 0.02–0.12 ppm Condiments 10 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2726	FDA 121.1164; FEMA No. 2727

REFERENCES

For References 1–5, see end of Part III.

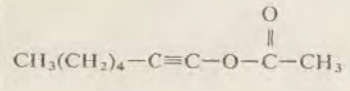
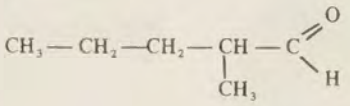
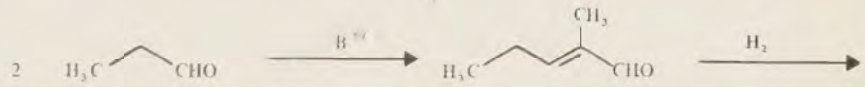
6. **Behal and Sommelet,** *Compt. Rend.*, 138, 92, 1904.
7. **Behal and Sommelet,** *Chem. Zentralbl.*, 2, 1791, 1906.
8. **Sommelet,** *Ann. Chem. Paris,* 8(9), 557, 1906.
9. **Sommelet,** *Bull. Soc. Chem. Fr.*, 4(1), 407, 1907.

	Methyl octanoate	Methyl-*cis*-4-octenoate
Other names	Methyl caprylate Methyl octoate Methyl octylate	
Empirical formula	$C_9H_{18}O_2$	$C_9H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	
Molecular weight	158.24	156.22
Boiling point	200°C (194–195°C)	90°C at 11 mm Hg
Specific gravity	0.887 at 15.5°C; 0.8784 at 20°C	
Refractive index	1.4180 (1.4170) at 20°C	
Solubility	Insoluble in water; soluble in alcohol	Soluble in ether
Organoleptic characteristics	Powerful, winey, fruity, and orange-like odor; oily, somewhat orange taste	
Synthesis	From coconut fatty acids by alcoholysis in the presence of gaseous HCl[6]	From *cis*-4-octenoic acid ethyl ester and methanol in the presence of sodium catalyst[9]
Natural occurrence	Reported found in orris essential oil[7] in the fruits of *Ananas sativus* Lindl.,[8] in strawberry, pineapple, and pear	Reported found in pineapple[10]
Reported uses[3]	Non-alcoholic beverages 0.02–1.0 ppm Ice cream, ices, etc. 1.0–10 ppm Candy 13 ppm Baked goods 1.0–40 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 4.0 ppm Baked goods 4.0 ppm Gelatins and puddings 2.0 ppm Preserves 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2728	FEMA No. 3367

REFERENCES

For References 1–5, see end of Part III.

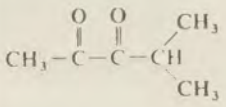
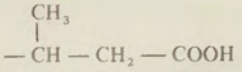
6. Haller and Youssoufian, *Compt. Rend.*, 143, 805, 1906.
7. Naves, *Helv. Chim. Acta*, 32, 2306, 1949.
8. Haagen-Smit et al., *J. Am. Chem. Soc.*, 67, 1647, 1945.
9. Näf-Muller and Willhalm, *Helv. Chim. Acta*, 54(7), 1880, 1971.
10. Creveling, Silverstein and Jennings, *J. Food Sci.*, 33(3), 284, 1968.

	Methyl-2-octynoate	2-Methyl pentanal
Other names	Methyl heptine carbonate Methyl heptyne carbonate Methyl-*n*-hept-1-yne-1-carboxylate	2-Methyl valeraldehyde
Empirical formula	$C_9H_{14}O_2$	$C_6H_{12}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow liquid	
Assay	96% min[2] (98%)	
Molecular weight	154.21	100.15
Melting point	215°C (217°C)	
Boiling point		116°C at 760 mm Hg
Flash point	Approx 89°C (95°C)	
Specific gravity	0.919–0.924 at 25°/25°C;[2] 0.9275–0.9375 at 15°/15°C	
Refractive index	1.4460–1.4490[2] (1.4460–1.4475) at 20°C	1.4120 at 20°C
Acid value	Not more than 1[2] (0.3)	
Solubility	1:5 and more in 70% alcohol;[2] 1:2 in 80% alcohol; insoluble in water	
Organoleptic characteristics	Odor similar to violets on dilution; if concentrated, powerful and unpleasant odor; wine-berry flavor (muscatel)	
Synthesis	From heptaldehyde via heptyne and heptyne carboxylic acid; the acid is subsequently esterified	From 2-methylpentanol by catalytic oxidation[6]
		
Natural occurrence	Not reported found in nature	A volatile component in onion,[7] garlic, milk, meat, and roasted peanuts[8]
Reported uses[3]	Non-alcoholic beverages 0.15 ppm Ice cream, ices, etc. 0.30 ppm Candy 1.4 ppm Baked goods 1.4 ppm Gelatins and puddings 1.7 ppm Chewing gum 13–20 ppm Jellies 0.23 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm Gelatins and puddings 2.0 ppm Chewing gum 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2729	FEMA No. 3413

REFERENCES

For References 1–5, see end of Part III.

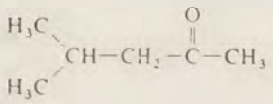
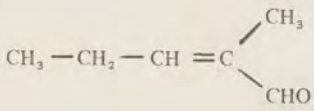
6. **Komarewsky et al.,** *J. Am. Chem. Soc.*, 66, 1117, 1944.
7. **Boelens et al.,** *J. Agric. Food Chem.*, 19, 984, 1971.
8. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Centraal Instituut voor Voedingsonderzoek, Zeist, Netherlands.

	4-Methyl-2,3-pentanedione	3-Methylpentanoic acid
Other names	Acetyl isobutyryl	3-Methylvaleric acid
Empirical formula	$C_6H_{10}O_2$	$C_6H_{12}O_2$
Structure		
Physical/chemical characteristics[4]		
Appearance	Yellow oil	
Molecular weight	114.15	116.16
Melting point	−2.4°C	
Boiling point	116°C	*d*-, 110°C at 30 mm Hg *d*-, 92–93°C at 10 mm Hg *l*-, 196–197°C *l*-, 105°C at 30 mm Hg *d,l*-, 197.2–197.8°C *d, l*-, 91–92°C at 10 mm Hg *d, l*-, 41°C
Specific gravity	0.9215 at 11°C	*d*-, 0.9276 at 20.5°C *l*-, 0.9230 at 25°C *d, l*-, 0.9262 at 20°C
Refractive index		*d*-, 1.4158 at 20.5°C *l*-, 1.4152 at 25°C *d, l*-, 1.4159 at 20°C
Optical rotation		*d*-, +8.5° at 20°C in ethanol *l*-, −8.9° at 20°C in ethanol
Organoleptic characteristics	Characteristic pungent odor	Sour, herbaceous, slightly green odor
Synthesis	Prepared from isonitroso methyl isobutyl ketone by treatment with concentrated H_2SO_4.[6] Other methods employ mesityl oxide as the starting material.[7,8]	From the diethylester of *sec*-butyl-malonic acid[9]
Natural occurrence	In coffee and beer	In the oil from tobacco leaves (*d*-form);[10-12] in cheese[13]
Reported uses[3]	Non-alcoholic beverages 7.6 ppm Ice cream, ices, etc. 5.6 ppm Candy 6.2 ppm Baked goods 8.3 ppm Gelatins and puddings 1.2–18 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2730	FEMA No. 3437

REFERENCES

For References 1–5, see end of Part III.

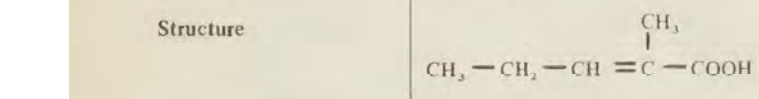
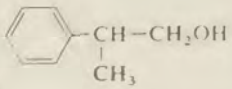
6. Otto and Peckmann, *Ber. Dtsch. Chem. Ges.*, 22, 2121, 1889.
7. Pauly, *Ber. Dtsch. Chem. Ges.*, 33, 503, 1900.
8. Dufraisse and Moureau, *C. R. Séances Acad. Sci. Paris*, 184, 99, 1927.
9. Vliet et al., *Org. Synth.*, 11, 76, 1931.
10. Sabetay et al., *C. R. Hebd. Séances Acad. Sci.*, 225, 887, 1947.
11. Onishi et al., *Bull. Agric. Chem. Soc. Jap.*, 20, 68, 1956; 21, 82, 1957.
12. Onishi et al., *Koryo*, 55, 9, 1960; *Chem. Abstr.*, 55, 12778, 1961.
13. Panouse et al., *Ind. Aliment. Agric.* p. 133, 1972.

	4-Methyl-2-pentanone	2-Methyl-2-pentenal
Other names	Methyl isobutyl ketone	3-Ethyl-2-methylacraldehyde 2-Propylidene propionaldehyde Methyl ethyl acrolein 2,4-Dimethyl crotonaldehyde Homotiglic aldehyde Isohexenal
Empirical formula	$C_6H_{12}O$	$C_6H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless mobile liquid
Molecular weight	100.16	98.15
Melting point	−83.5°C; −80.4°C	
Boiling point	117°C; 115.8°C	134–136°C at 745 mm Hg 77–78.5°C at 100 mm Hg 38–39°C at 18 mm Hg
Specific gravity	0.8062 at 20°C	0.8581 at 20°C
Refractive index	1.3959 at 20°C	1.4488 at 20°C
Solubility	Insoluble in water; slightly miscible with alcohol, ether, and benzene	Insoluble in water; soluble in alcohol, ether, benzene, and methanol
Organoleptic characteristics	Pleasant odor	Powerful grassy-green, slightly fruity odor
Synthesis	By hydrogenation of mesityl oxide over Ni at 160–190°C;[7] also by oxidation of methyl isobutyl carbinol	By aldolic condensation of propionaldehyde[6]
Natural occurrence	In orange and grape; in vinegar	Reported found as a volatile component in onion
Reported uses[4]	Non-alcoholic beverages 6.3 ppm Ice cream, ices, etc. 6.3 ppm Candy 6.3 ppm Baked goods 6.3 ppm	Non-alcoholic beverages 80.0 ppm Ice cream, ices, etc. 80.0 ppm Candy 80.0 ppm Baked goods 80.0 ppm Gelatins and puddings 80.0 ppm Chewing gum 80.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2731	FEMA No. 3194

REFERENCES

For References 1–5, see end of Part III.

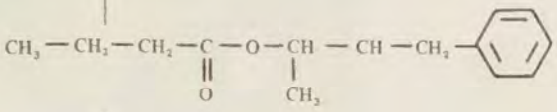
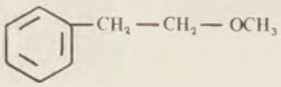
6. Rodd, *Chemistry of Carbon Compounds*, 2nd ed., Vol. 1, American Elsevier, New York, 1965, 59.
7. Darzens, *C. R. Séances Acad. Sci. Paris*, 140, 152, 1905.

	2-Methyl-2-pentenoic acid	β-Methyl phenethyl alcohol
Other names	3-Ethyl-2-methylacrylic acid β-Amylene-β-carboxylic acid 2-Pentene-2-carboxylic acid 2-Propylidenepropionic acid	Hydratropyl alcohol Hydrotropic alcohol 2-Phenylpropan-1-ol β-Phenylpropyl alcohol
Empirical formula	$C_6H_{10}O_2$	$C_9H_{12}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Prismatic crystals (*trans*-form)	Viscous liquid
Molecular weight	114.04	136.19
Melting point	24.4°C	
Boiling point	*trans*-, 112°C at 12 mm Hg *trans*-, 213°C at 750 mm Hg *trans*-, 106°C at 10 mm Hg *trans*-, 123–125°C at 29.5 mm Hg *cis*-, 94°C at 10 mm Hg *cis*-, -42°C	113–114°C at 14 mm Hg
Specific gravity	0.9812 at 25°C	1.015 at 15.5°C
Refractive index	1.4578 at 25°C (1.4488 at 25°C)	1.5270 at 20°C *d*-, +15.25°; *l*-, −15.16°
Solubility	Soluble in ether, chloroform, and carbon disulfide; slightly soluble in water.	
Organoleptic characteristics		Faint, aromatic odor reminiscent of hyacinth
Synthesis	By distillation of 2-hydroxy-2-methylvaleric acid (*cis*-form)[6]	By reduction of the corresponding aldehyde with zinc and acetic acid and subsequent saponification of the sodium salt. Two optically active isomers (*d*- and *l*-) are known.
Natural occurrence		
Reported uses[3,4]	Candy 1.0 ppm Baked goods 1.0 ppm Condiments 1.0 ppm Meat, meat sauces, soups 1.0 ppm	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 0.42 ppm Candy 1.2 ppm Baked goods 0.92 ppm
Regulatory status	FEMA No. 3195	FDA 121.1164; FEMA No. 2732

REFERENCES

For References 1–5, see end of Part III.

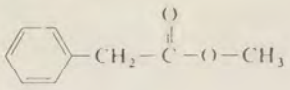
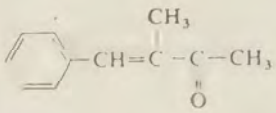
6. Lucas and Prater, *J. Am. Chem. Soc.*, 59, 1684, 1937.

	α-Methylphenethyl butyrate		Methylphenethyl ether	
Other names	1-Phenyl-2-propyl butyrate		Phenylethyl methyl ether Methyl phenylethyl ether	
Empirical formula	$C_{13}H_{18}O_2$		$C_9H_{12}O$	
Structure				
Physical/chemical characteristics[5]				
Appearance			Colorless mobile oil	
Molecular weight	206.27		136.20	
Boiling point			185–187°C 100–104°C at 25 mm Hg	
Solubility			Almost insoluble in water; soluble in alcohol and oils	
Organoleptic characteristics			Powerful diffusive and penetrating odor with a warm, floral note; "grassy" and pungent on dilution[9]	
Synthesis			By catalytic reduction of phenylacetaldehyde dimethyl acetal;[6] from phenylethyl alcohol and methanol[7]	
Natural occurrence	Reported not found in nature		Reported as occurring in *Pandanus odoratissimus*[7] and in the oil of *Tagetes signata*[8]	
Reported uses[3]	Non-alcoholic beverages Ice cream, ices, etc. Candy Gelatins and puddings	0.60 ppm 3.0 ppm 6.0 ppm 3.0 ppm	Non-alcoholic beverages	20.0 ppm
Regulatory status	FEMA No. 3197		FEMA No. 3198	

REFERENCES

For References 1–5, see end of Part III.

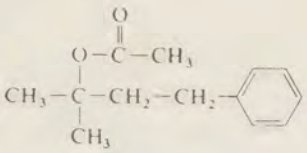
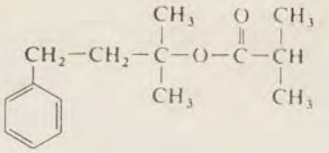
6. **Arctander,** *Perfume and Flavor Materials of Natural Origin,* 1961, 504.
7. **Deshapande,** *J. Indian Chem. Soc.,* 15, 509, 1938.
8. **Chopra, Nigam, Kapoor and Manda,** *Soap Perfum. Cosmet.,* 36, 686, 1963.
9. **Chopra et al.,** *Perfum. Rec.,* 54, 238, 1963.

	Methyl phenylacetate	3-Methyl-4-phenyl-3-butene-2-one
Other names	Methyl α-toluate	3-Benzylidene-butan-2-one Benzylidene methyl acetone
Empirical formula	$C_9H_{10}O_2$	$C_{11}H_{12}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless or nearly colorless liquid	Crystalline solid
Assay	98% min[2]	
Molecular weight	150.18	160.22
		38–40°C
Boiling point	215°C	124–125°C at 10 mm Hg
Flash point	89°C	
Specific gravity	1.061–1.067 at 25°/25°C;[2] 1.0633 at 16°C	1.0072 at 40.2°C
Refractive index	1.5050–1.5090 at 20°C;[2] 1.5091 at 16°C	1.5720 at 40.2°C
Acid value	1 max[2]	
Solubility	1:6 in 60% alcohol;[2] 1:2 in 70% alcohol; insoluble in water; soluble in most organic solvents	
Organoleptic characteristics	Intense odor suggestive of honey and jasmine; sweet, honey-like flavor	Camphor-like odor
Synthesis	By methanolic esterification of the corresponding acid or nitrile; by reacting HCl over a solution of benzyl nitrile in methanol[6]	By condensation of benzaldehyde with butanone in the presence of dry, gaseous HCl at low temperature[7,8]
Natural occurrence	In cocoa, coffee, and strawberry	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.9 ppm Ice cream, ices, etc. 2.5 ppm Candy 13 ppm Baked goods 12 ppm Gelatins and puddings 0.10 ppm Chewing gum 11 ppm Syrups 37 ppm	Non-alcoholic beverages 0.59 ppm Ice cream, ices, etc. 2.0 ppm Candy 2.8 ppm Baked goods 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2733	FDA 121.1164; FEMA No. 2734

REFERENCES

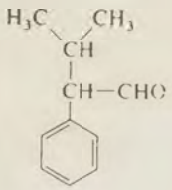
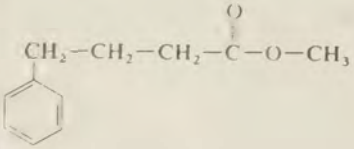
For References 1–5, see end of Part III.

6. Rising and Sieglitz, *J. Am. Chem. Soc.*, 40, 725, 1918.
7. Rateb and Soliman, *J. Chem. Soc.*, p. 1426, 1960.
8. Stiles et al., *J. Am. Chem. Soc.*, 81, 628, 1959.

	2-Methyl-4-phenyl-2-butyl acetate	2-Methyl-4-phenyl-2-butyl isobutyrate
Other names	Dimethyl phenylethyl carbinyl acetate 1,1-Dimethyl-3-phenylpropan-1-yl acetate	Dimethyl phenylethyl carbinyl isobutyrate Phenylethyl dimethylcarbinyl isobutyrate
Empirical formula	$C_{13}H_{18}O_2$	$C_{15}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless liquid
Assay	97.5%	
Molecular weight	206.28	234.34
Melting point		
Boiling point	275 C	250 C
Flash point	101°C	
Specific gravity	0.9865–0.9900 at 15 C; 0.990 at 15.5°C	
Refractive index	1.4880–1.4900 at 20 C	
Acid value	0.2 max	
Solubility	1:5–6 in 70% alcohol; insoluble in water	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Jasmine and hyacinth-like odor with a slightly rose undertone	Herbaceous, tea-like, sweet odor; fruit-juice flavor
Synthesis		By esterification of dimethyl phenylethyl carbinol with isobutyric acid or anhydride
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 1.8 ppm Ice cream, ices, etc. 0.5 ppm Candy 0.50–10 ppm Baked goods 0.50–10 ppm	Non-alcoholic beverages 0.50–11 ppm Ice cream, ices, etc. 1.0–44 ppm Candy 11 ppm Baked goods 2.0–30 ppm
Regulatory status	FDA 121.1164; FEMA No. 2735	FDA 121.1164; FEMA No. 2736

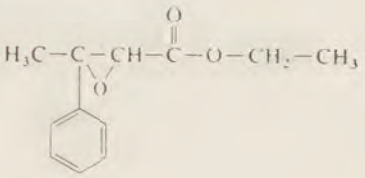
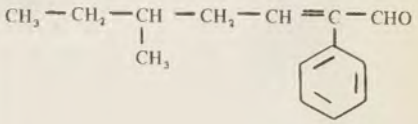
REFERENCES

For References 1–5, see end of Part III.

	3-Methyl-2-phenylbutyraldehyde	Methyl-4-phenylbutyrate
Other names	α-Isopropyl phenylacetaldehyde α-Phenyl isovaleraldehyde	γ-Phenylbutyric acid, methyl ester
Empirical formula	$C_{11}H_{14}O$	$C_{11}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Molecular weight	162.23	178.23
Boiling point	238°C	
Solubility	Insoluble in water; soluble in alcohol	Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Green, fruity odor when dilute. Below 5 ppm flavor is fruity; above 20 flavor is bitter.	Powerful, sweet, fruity, floral odor; extremely sweet, fruity flavor below 10 ppm
Synthesis	From phenyl isopropylglycidic acid; by rearrangement of 2-phenylpentane-1,2-diol	By direct esterification of γ-butyric acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.10 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.32–0.50 ppm	Non-alcoholic beverages 0.56 ppm Ice cream, ices, etc. 0.52 ppm Candy 1.6 ppm Baked goods 1.4 ppm
Regulatory status	FDA 121.1164; FEMA No. 2738	FDA 121.1164; FEMA No. 2739

REFERENCES

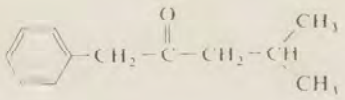
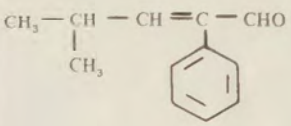
For References 1–5, see end of Part III.

	3-Methyl-3-phenyl glycidic acid ethyl ester	5-Methyl-2-phenyl-2-hexenal
Other names	Aldehyde C-16 Ethyl α,β-epoxy-β-methyl-hydrocinnamate Ethyl α,β-epoxy-β-methylphenyl propionate Ethyl 2,3-epoxy-3-phenyl-butanoate Ethyl methyl-phenyl-glycidate "Strawberry aldehyde"	
Empirical formula	$C_{12}H_{14}O_3$	$C_{14}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to pale-yellow liquid	
Assay	98% min[2] (99%)	
Molecular weight	206.24	202.28
Boiling point	150–153°C at 8 mm Hg	96–100°C at 0.7 mm Hg
Flash point	134°C	
Specific gravity	1.088–1.112 at 25°/25°C;[2] 1.0965–1.0985 at 15°/15°C	
Refractive index	1.5040–1.5130[2] (1.5050–1.5075) at 20°C	
Acid value	Not more than 2[2] (0.9)	
Ketone content	1% max (as C_8H_8O)	
Solubility	1:3 and more in 70% alcohol;[2] 1:2 in 80% alcohol; insoluble in water; soluble in most organic solvents	
Organoleptic characteristics	On dilution, strong, fruity odor suggestive of strawberry; characteristic, slightly acid taste reminiscent of strawberry	Cocoa aroma; often used in chocolate and cocoa-type flavors[8]
Synthesis	By reaction of acetophenone and the ethyl ester of monochloroacetic acid in the presence of an alkaline condensing agent[2]	From phenyl acetaldehyde and isopropyl acetaldehyde by aldolic condensation[6]
Natural occurrence	Not reported found in nature	Reported found in the neutral volatile fraction of roasted peanuts[7]
Reported uses[3]	Non-alcoholic beverages 5.6 ppm Ice cream, ices, etc. 6.7 ppm Candy 21 ppm Baked goods 18 ppm Gelatins and puddings 13 ppm Chewing gum 470 ppm	Non-alcoholic beverages 25.0 ppm Ice cream, ices, etc. 25.0 ppm Candy 25.0 ppm Baked goods 25.0 ppm Gelatins and puddings 25.0 ppm Chewing gum 25.0 ppm
Regulatory status	FDA GRAS; FEMA No. 2444	FEMA No. 3199

REFERENCES

For References 1–5, see end of Part III.

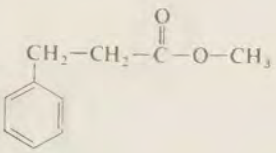
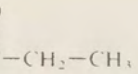
6. **Van Praag and Stein,** German Patent 1,921,560, assigned to International Flavors and Fragrances Inc., 1969.
7. **Van Praag and Stein,** German Patent 1,921,560, 1969.
8. **Van Praag and Stein,** German Patent 1,921,560, 1969.

	4-Methyl-1-phenyl-2-pentanone	4-Methyl-2-phenyl-2-pentenal
Other names	Benzyl isobutyl ketone Isobutyl benzyl ketone	
Empirical formula	$C_{12}H_{16}O$	$C_{12}H_{14}O$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless, oily liquid	
Molecular weight	176.26	174.23
Boiling point	250–251 C	82–87°C at 0.7 mm Hg
Specific gravity	0.969 at 0 C	
Solubility	Very slightly soluble in water; poorly soluble in propylene glycol; soluble in alcohol and oils	
Organoleptic characteristics	Sweet, woody, spicy odor; at low levels sweet and tart, fruity flavor	Cocoa aroma; often used in chocolate and cocoa-type flavors[9]
Synthesis	By passing phenylacetic acid and isovaleric acid over ThO_2 catalyst at 450–470 C[6,7,8]	By aldolic condensation of the corresponding aldehydes in the presence of a basic catalyst[10]
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 0.06–5.0 ppm Baked goods 5.0 ppm	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 1.5 ppm Candy 1.5 ppm Baked goods 1.5 ppm Gelatins and puddings 1.5 ppm Chewing gum 1.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2740	FEMA No. 3200

REFERENCES

For References 1–5, see end of Part III.

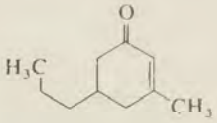
6. **Senderens,** *Compt. Rend.*, 150, 1338, 1910.
7. **Senderens,** *Bull. Soc. Chim. Fr.*, 4(7), 648, 1910.
8. **Senderens,** *Ann. Chim. Paris*, 8(28), 322, 1913.
9. **Van Praag and Stein,** German Patent 1,921,560 assigned to International Flavors and Fragrances Inc., 1969.
10. **Van Praag and Stein,** German Patent 1,921,560, 1969.

	Methyl-3-phenylpropionate	Methyl propionate
Other names	Methyl dihydrocinnamate Methyl hydrocinnamate Methyl phenyl propionate	Methyl propanoate
Empirical formula	$C_{10}H_{12}O_2$	$C_4H_8O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	98% min	
Molecular weight	164.21	88.11
Boiling point	238–239 C	79 C (80 C)
Flash point	>100 C	−2 C
Specific gravity	1.037–1.042 at 25 C; 1.0473 at 0 C	0.915 at 15.5 C; 0.9148 at 20 C
Refractive index	1.4990–1.5030 at 20 C	1.3750 at 20 C; 1.37767 at 18.5 C
Acid value	1 max	
Solubility	1:3 in 70% alcohol; almost insoluble in water	Slightly soluble in water (6.5%); completely miscible with alcohol, ether, and propylene glycol
Organoleptic characteristics	Strong floral-fruity odor	Fruity odor reminiscent of rum; sweet flavor suggestive of black currant
Synthesis	By reduction of methyl cinnamate in methanol solution[8] with hydrogen and Ni under pressure	By direct esterification of the acid with methanol in the presence of concentrated H_2SO_4[6]
Natural occurrence	Not reported found in nature	Probably occurring in California orange (var. Valencia) juice[7] and honey
Reported uses[3]	Non-alcoholic beverages 0.46 ppm Ice cream, ices, etc. 0.56 ppm Candy 1.7 ppm Baked goods 0.70–4.0 ppm	Non-alcoholic beverages 20 ppm Ice cream, ices, etc. 29 ppm Candy 96 ppm Baked goods 130 ppm
Regulatory status	FDA 121.1164; FEMA No. 2741	FDA 121.1164; FEMA No. 2742

REFERENCES

For References 1–5, see end of Part III.

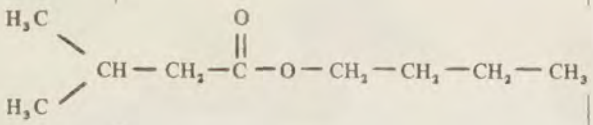
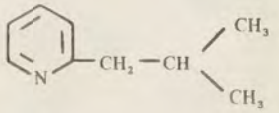
6. **Vogel,** *J. Chem. Soc.*, p. 629, 1948.
7. **Schultz et al.,** *J. Food Sci.*, 29, 790, 1964.
8. **Brochet and Bauer,** *Compt. Rend.*, 159, 191, 1914.

	3-Methyl-5-propyl-2-cyclohexen-1-one	Methyl propyl disulfide
Other names	"Celery ketone" 3-Methyl-5-propyl-2-cyclohexenone 1-Methyl-5-*n*-propyl-1-cyclohexen-3-one	
Empirical formula	$C_{10}H_{16}O$	$C_4H_{10}S_2$
Structure		$CH_3-S-S-CH_2-CH_2-CH_3$
Physical/chemical characteristics		
Appearance	Pale-yellow to colorless liquid	Pale-yellow, mobile liquid
Molecular weight	152.23	122.26
Boiling point	242–244°C; 122–123°C at 12 mm Hg	40–41°C at 9 mm Hg
Specific gravity	0.9267 at 22.3°C	
Refractive index		n_D^{20} 1.5075
Solubility	Insoluble in water; soluble in ether, alcohol, and oils	Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Warm, spicy, woody odor; similar flavor at low levels.	Odor and taste reminiscent of cooked onion
Synthesis	By condensation of butyric aldehyde with ethyl acetoacetate in the presence of diethylamine and subsequent saponification with a 10% KOH solution; or by condensation in the presence of piperidine in ethanol solution[14]	From Bunte salt and the corresponding thiol[6]
Natural occurrence	Not reported found in nature	Reported found in onion oil[7,8] and in *Allium* species[9–13]
Reported uses[3]		Baked goods 1.0 ppm Condiments, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm
Regulatory status	FDA 121.1164	FEMA No. 3201

REFERENCES

For References 1–5, see end of Part III.

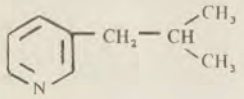
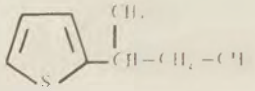
6. Milligan and Swan, *J. Chem. Soc.*, p. 6008, 1963.
7. Jacobs, *Am. Perfum.*, 70(5), 53, 1957.
8. Carson and Wong, *Am. Chem. Soc. Div. Pet. Chem. Prepr.*, 2(4), D115, 1957.
9. Bernhard, *Qual. Plant. Mater. Veg.*, 18(1–3), 72, 1969.
10. Wahlroos and Virtanen, *Acta Chem. Scand.*, 19(6), 1327, 1965.
11. Saghir, Mann and Yamaguchi, *Plant Physiol.*, 40(4), 681, 1965.
12. Saghir, Mann, Bernhard and Jacobson, *Proc. Am. Soc. Hortic. Sci.*, 84, 386, 1964.
13. Jacobsen et al., *Arch. Biochem. Biophys.*, 104(3), 473, 1964.
14. Whitmore and Roberts, *J. Org. Chem.*, 13, 31, 11948.

	2-Methylpropyl-3-methyl butyrate	2-(2-Methylpropyl)-pyridine
Other names	Isobutyl isovalerate	2-Isobutyl pyridine
Empirical formula	$C_9H_{18}O_2$	$C_9H_{13}N$
Structure		
Physical/chemical characteristics[5]		
Molecular weight	158.24	135.20
Boiling point	171.4°C 60–62°C at 12 mm Hg	181°C 110–111°C at 55 mm Hg
Specific gravity	0.8736 at 20°C	0.8973 at 20°C
Refractive index	1.4057 at 20°C	1.4831 at 20°C
Solubility	Insoluble in water; very soluble in acetone: soluble in alcohol and ether in all proportions	
Organoleptic characteristics	Aroma reminiscent of apple/raspberry	
Synthesis	By oxidation of the corresponding ketone[6]	From 2-pycolyllithium and isopropyl bromide;[6] from 2-methyl pyridine and isopropyl bromide in liquid ammonia in the presence of potassium metal and ferric nitrate[7]
Natural occurrence	Reported found in the oil from fruits of *Xanthoxylum piperitum*[7] and in the oil of *Elsholtzia ciliata*[8]	
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 8.0 ppm Baked goods 8.0 ppm Gelatins and puddings 5.0 ppm Preserves and spreads 5.0 ppm	Condiments, pickles 0.5 ppm Meat, meat sauces, soups 0.2 ppm
Regulatory status	FEMA No. 3369	FEMA No. 3370

REFERENCES

For References 1–5, see end of Part III.

6. Emmons and Lucas, *J. Am. Chem. Soc.*, 77, 2287, 1955.
7. Sakai, Yoshihara and Hirose, *Bull. Chem. Soc. Jap.*, 41(8), 1945, 1968.
8. Fujita, Tanaka and Iwamura, *Nippon Kagaku Zasshi*, 88(7), 763, 1967.
9. Osuch and Levine, *J. Am. Chem. Soc.*, 78, 1723, 1956.
10. Pines and Notari, *J. Am. Chem. Soc.*, 82, 2209, 1960.

	3-(2-Methylpropyl)-pyridine		2-(1-Methylpropyl)thiazole	
Other names	3-Isobutyl pyridine		2-*sec*-Butyl thiazole	
Empirical formula	$C_9H_{13}N$		$C_7H_{11}NS$	
Structure				
Physical/chemical characteristics[5]				
Molecular weight	135.19		141.23	
Boiling point	68–68.5°C at 8 mm Hg			
Refractive index	1.4912 at 20°C			
Synthesis	From β-picoline with $NaNH_2$ and alkyl chloride or bromide[6]			
Reported uses[5]	Non-alcoholic beverages	0.1 ppm	Ice cream, ices, etc.	0.1 ppm
	Ice cream, ices, etc.	0.2 ppm	Candy	0.5 ppm
	Candy	0.5 ppm	Baked goods	0.5 ppm
	Baked goods	1.0 ppm	Gelatins and puddings	0.1 ppm
	Gelatins and puddings	0.3 ppm	Condiments, pickles	0.5 ppm
	Cereals	1.0 ppm	Meat, meat sauces, soups	0.2 ppm
Regulatory status	FEMA No. 3371		FEMA No. 3372	

REFERENCES

For References 1–5, see end of Part III.

6. Wibaut and Hoogzand, *Chem. Weekbl.*, 52, 357, 1956.

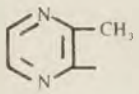
	Methyl propyl trisulfide
Other names	Propyl methyl trisulfide
Empirical formula	$C_4H_{10}S_3$
Structure	$CH_3-S-S-S-CH_2-CH_2-CH_3$
Physical/chemical characteristics	
Appearance	Pale-yellow, mobile liquid
Molecular weight	154.32
Boiling point	52°C at 1.2 mm Hg
Refractive index	N_d^{21} 1.5578
Organoleptic characteristics	Powerful, penetrating warm-herbaceous odor somewhat reminiscent of onion
Synthesis	By an adaptation of Westlake's procedure[6]
Natural occurrence	Reported found in cocoa;[7] also in the volatile portion of fresh onion oil
Reported uses[3]	Baked goods 2.0 ppm Condiments, pickles 2.0 ppm Meat, meat sauces, soups 2.0 ppm
Regulatory status	FEMA No. 3308

REFERENCES

For References 1–5, see end of Part III.

6. Westlake et al., *J. Am. Chem. Soc.*, 72, 436, 1950; *Chem. Abstr.*, 44, 4739a, 1950.
7. Marion, et al., *Helv. Chim. Acta*, 50(6), 1509, 1967.

2-Methylpyrazine

Other names	2-Methyl-1,4-diazine Methylpyrazine
Empirical formula	$C_5H_6N_2$
Structure	
Physical/chemical characteristics	
Assay	C: 63.81%; H: 6.43%; N: 29.76%
Molecular weight	94.12
Boiling point	136–137°C
Specific gravity	1.0290 at 20°C
Refractive index	1.5067 at 18.7°C
Mass spectra[10]	39 (21), 40 (18), 52 (7), 53 (17), 66 (3), 67 (55), 79 (1), 94 (100), 95 (5)
IR spectra[10]	S (6.8, 6.9, 7.1, 8.6, 9.5, 9.8, 12.0) M (3.3, 6.3, 6.5, 7.7, 8.0, 8.5, 10.2) W (5.2, 5.7)
UV spectra[10]	(2.66.0, 272.0 nm)
Solubility	Soluble in water, alcohol, and ether in all proportions; soluble in acetone
Organoleptic characteristics	Odor threshold: 105,000 ppb in water,[9] 60,000 ppb in water[11]
Synthesis	From the corresponding carboxylic acid;[6] by catalytic dehydrogenation of 2-methylpiperazine;[7] by condensation of methylglyoxal with ethylenediamine[12]
Natural occurrence	Reported to be present in the following foods: bakery products, roasted barley, cocoa products, coffee, dairy products, meat, peanuts, filberts, pecans, popcorn, potato products, rum and whisky, soy products;[8] a volatile flavor component in roasted filberts;[13] also in toasted off-flavors[14]

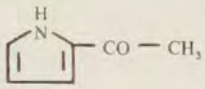
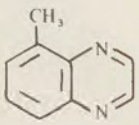
Reported uses[3]				
Non-alcoholic beverages	10.0 ppm	Gelatins and puddings	10.0 ppm
Ice cream, ices, etc.	10.0 ppm	Meat, meat sauces, soups	10.0 ppm
Candy	10.0 ppm	Milk, dairy products	10.0 ppm
Baked goods	10.0 ppm	Cereals	10.0 ppm

Regulatory status	FEMA No. 3309

REFERENCES

For References 1–5, see end of Part III.

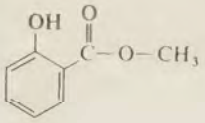
6. Stoehr, *J. Fr. Chim.*, 51(2), 449, 1895.
7. Kitchen and Hanson, *J. Am. Chem. Soc.*, 73, 1838, 1951.
8. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
9. Koehler et al., *J. Food Sci.*, 36, 816, 1971.
10. Bondarovich et al., *J. Agric. Food Chem.*, 15, 1093, 1967.
11. Guadagni et al., *J. Sci. Food Agric.*, 23, 1435, 1972.
12. Ishiguro and Matsumura, *Yakugaku Zasshi*, 78, 229, 1958.
13. Sheldon et al., *J. Food Sci.*, 37(2), 313, 1972.
14. Sapers et al., *J. Food Sci.*, 36(1), 93, 1971.

	Methyl-2-pyrrolyl ketone		5-Methylquinoxaline	
Other names	2-Acetyl pyrrole 2-Acetopyrrole			
Empirical formula	C_6H_7NO		$C_9H_8N_2$	
Structure				
Physical/chemical characteristics[5]				
Appearance	Crystals (from water)			
Molecular weight	109.13		144.19	
Melting point	90°C		20–21°C	
Boiling point	220°C		120°C at 15 mm Hg	
Solubility	Soluble in water, alcohol and ether			
Synthesis	From pyrryl magnesium iodide and acetyl chloride;[6] a volatile flavor component in roasted filberts[8]			
Natural occurrences	Reported found in the essential oils of tobacco leaves and tea[7]		Reported found in coffee[6]	
Reported uses[3]	Non-alcoholic beverages	50.0 ppm	Non-alcoholic beverages	10.0 ppm
	Ice cream, ices, etc.	50.0 ppm	Ice cream, ices, etc.	10.0 ppm
	Candy	50.0 ppm	Candy	10.0 ppm
	Gelatins and puddings	50.0 ppm	Gelatins and puddings	10.0 ppm
Regulatory status	FEMA No. 3202		FEMA No. 3203	

REFERENCES

For References 1–5, see end of Part III.

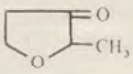
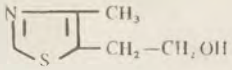
6. Oddo, *Berichte*, 43, 1014, 1910.
7. Onishi and Yamamoto, *Bull. Agric. Chem. Soc.*, 21, 90, 1957.
8. Sheldon et al., *J. Food Sci.*, 37(2), 313, 1972.
9. Stoll et al., *Helv. Chim. Acta*, 50(2), 628, 1967.

	Methyl salicylate	Methyl sulfide
Other names	Methyl *o*-hydroxybenzoate	Dimethyl sulfide
Empirical formula	$C_8H_8O_3$	C_2H_6S
Structure		$H_3C-S-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	152.14	62.04
Melting point	−8.3°C (−8.6°C)	−83.2°C
Boiling point	222.2°C (223.3°C)	37.3–37.5°C
Flash point	96°C	
Specific gravity	1.180–1.185 at 25°C	0.8449 at 20°C
Refractive index	1.5350–1.5380 at 20°C	
Solubility	1:7 in 70% alcohol; almost insoluble in water; soluble in most common organic solvents and glacial acetic acid	Insoluble in water; soluble in alcohol and ether
Organoleptic characteristics	Characteristic wintergreen-like odor	Unpleasant odor of wild radish, cabbage-like; can be tolerated as a green-vegetable note only at very low levels (0.1–3.0 ppm)
Synthesis	By extraction from natural sources; or by esterification of salicylic acid with methanol	By reaction of potassium sulfide with methyl chloride in methanol solution;[7] from potassium methyl sulfate and potassium sulfide
Natural occurrence	Reported found in the oil of wintergreen (*Gaultheria procumbens*);[6] subsequently found also in birch, tuberose, *Dianthus caryophyllus* L., *Acacia cavenia* Hook. and Arn., ylang-ylang, and several fruit juices—cherry, apple, raspberry, and others	Reported found in American peppermint oil,[8] the oil of Algerian geranium,[9] and butter[10]
Reported uses[3]	Non-alcoholic beverages 59 ppm Ice cream, ices, etc. 27 ppm Candy 840 ppm Baked goods 54 ppm Chewing gum 8,400 ppm Syrups 200 ppm	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 0.30 ppm Candy 1.4 ppm Baked goods 1.6 ppm Gelatins and puddings 0.13 ppm Syrups 0.50 ppm
Regulatory status	Status not fully defined by FDA; FEMA No. 2745	FDA 121.1164; FEMA No. 2746

REFERENCES

For References 1–5, see end of Part III.

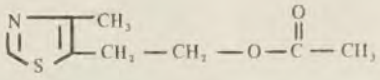
6. Cahours, *Annalen*, 48, 60, 1843.
7. Regnault, *Annalen*, 34, 24, 1840.
8. *Schimmel Ber.*, p. 61, October 1896.
9. *Schimmel Ber.*, p. 50, April 1909.
10. Ruys, *Fr. Ses Parfums*, 47(9), 34, 1966.

	2-Methyltetrahydrofuran-3-one		4-Methyl-5-thiazoleethanol	
Other names			4-Methyl-5-(β-hydroxyethyl)-thiazole 5-Hydroxyethyl-4-methylthiazole 5-(2-Hydroxyethyl)-4-methylthiazole	
Empirical formula	$C_5H_8O_2$		C_6H_9NOS	
Structure				
Physical/chemical characteristics[5]				
Appearance			Viscous oily liquid	
Molecular weight	100.11		143.21	
Boiling point	139°C		135°C at 7 mm Hg 103°C at 1 mm Hg	
Specific gravity			1.196 at 24°C	
Refractive index	1.4291 at 20°C			
Solubility			Very soluble in water; soluble in alcohol, ether, benzene, and chloroform	
Organoleptic characteristics			Characteristic disagreeable odor of thiazole compounds; somewhat pleasant, nut-like on extreme dilution	
Synthesis	By hydrolytic decarboxylation of 2-methyl-4-carbomethoxytetrahydrofuran-3-one;[6] by acid-catalyzed ring closure of β-alkoxydiazoketones[7]		By reduction of ethyl-4-methylthiazole-5-acetate using $LiAlH_4$;[10] by condensation of thioformamide with bromoacetopropanol[11] or with γ,γ-dichloro-γ,γ-diacetodipropyl ether[12,13]	
Natural occurrence	Reported found as a constituent in coffee aroma;[8] also as a volatile flavor component in roasted filbert nuts[9]			
Reported uses[3]	Non-alcoholic beverages	10.0 ppm	Non-alcoholic beverages	55.0 ppm
	Ice cream, ices, etc.	10.0 ppm	Ice cream, ices, etc.	55.0 ppm
	Candy	10.0 ppm	Candy	55.0 ppm
	Baked goods	10.0 ppm	Baked goods	55.0 ppm
	Gelatins and puddings	10.0 ppm	Gelatins and puddings	55.0 ppm
	Chewing gum	10.0 ppm	Chewing gum	55.0 ppm
	Condiments, pickles	10.0 ppm	Condiments	55.0 ppm
	Meat, meat sauces, soups	10.0 ppm	Meat, meat sauces, soups	55.0 ppm
	Milk, dairy products	10.0 ppm	Milk, dairy products	55.0 ppm
	Cereals	10.0 ppm	Cereals	55.0 ppm
Regulatory status	FEMA No. 3373		FEMA No. 3204	

REFERENCES

For References 1–5, see end of Part III.

6. **Gianturco, Giammarino and Friedel,** *Tetrahedron Lett.*, 20, 1763, 1964.
7. **Wynberg,** *Angew. Chem.*, p. 453, 1963.
8. **Stoll et al.,** *Helv. Chim. Acta,* 50(2), 628, 1967.
9. **Sheldon et al.,** *J. Food Sci.*, 37(2), 313, 1972.
10. **Eusebi, Brown and Cerecedo,** *J. Am. Chem. Soc.*, 71, 2931, 1949.
11. **Buchman,** *J. Am. Chem. Soc.*, 58, 1803, 1936.
12. **Stein and Stevens,** French Patent 945,198, British Patent 641,426, assigned to Merck & Co. Inc.
13. **Londergau and Schmitz,** U.S. Patent 2,654,760, assigned to E. I. du Pont de Nemours & Co., 1953.

	4-Methyl-5-thiazoleethanol acetate	2-Methyl thioacetaldehyde
Other names	4-Methyl-5-(2-acetoxyethyl)-thiazole	C_3H_6OS
Empirical formula	$C_8H_{11}O_2NS$	
Structure		CH_3-S-CH_2-CHO
Physical/chemical characteristics		
Molecular weight	185.24	90.14
Boiling point	105–108°C at 4 mm Hg	
Synthesis	From 2-methylthio-4-methyl-5-(2-acetoxyethyl)-thiazole and AlHg;[6] by dehydrogenation with sulfur at 130°C of the β-acetyl derivative of 4-methyl-5-(β-hydroxyethyl)-3-thiazoline[7]	By hydrolysis of the diethyl acetal of 2-methyl thioacetaldehyde with diluted HCl; the diethyl acetal is prepared from diethylbromoacetal treated with sodium methyl mercaptide[8]
Reported uses[3]	Non-alcoholic beverages 55.0 ppm Ice cream, ices, etc. 55.0 ppm Candy 55.0 ppm Baked goods 55.0 ppm Gelatins and puddings 55.0 ppm Chewing gum 55.0 ppm Condiments 55.0 ppm Meat, meat sauces, soups 55.0 ppm Milk, dairy products 55.0 ppm Cereals 55.0 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50 ppm Baked goods 0.50 ppm Gelatins and puddings 0.50 ppm Chewing gum 0.50 ppm Condiments 0.50 ppm Meat, meat sauces, soups 0.50 ppm Milk, dairy products 0.50 ppm Cereals 0.50 ppm
Regulatory status	FEMA No. 3205	FEMA No. 3206

REFERENCES

For References 1–5, see end of Part III.

6. *Chem. Abstr.*, 50, 5634c, 1956.
7. **Thiel, Asinger and Stengler,** *Annalen.*, p. 161, 1958.
8. **Cope, Kovacic and Burg,** *J. Am. Chem. Soc.*, 71, 3658, 1949.

	4-(Methylthio)butanal		1-(Methylthio)-2-butanone	
Other names	4-(Methylmercapto)butanal			
Empirical formula	$C_5H_{10}S$		$C_5H_{10}SO$	
Structure	$CH_3-S-CH_2-CH_2-CH_2-CHO$		$CH_3-S-CH_2-CO-CH_2-CH_3$	
Physical/chemical characteristics				
Appearance			Colorless liquid	
Molecular weight	106.18		118.20	
Boiling point			52–53°C at 8 mm Hg	
Specific gravity			0.9970 at 22°C	
Refractive index			1.4700 at 20°C	
Organoleptic characteristics			Odor reminiscent of mushroom, with a characteristic garlic undertone	
Synthesis			From chloro-1-butan-2-one[6]	
Natural occurrence			Reported found as a constituent in coffee aroma[6]	
Reported uses[3]	Non-alcoholic beverages	0.5 ppm	Condiments	1.0 ppm
	Ice cream, ices, etc.	0.5 ppm	Soups	1.0 ppm
	Candy	1.0 ppm	Sauces	1.0 ppm
	Baked goods	1.0 ppm		
	Meat, meat sauces, soups	5.0 ppm		
	Vegetables	5.0 ppm		
Regulatory status	FEMA No. 3414		FEMA No. 3207	

REFERENCES

For References 1–5, see end of Part III.

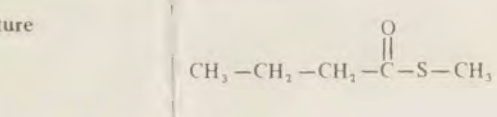
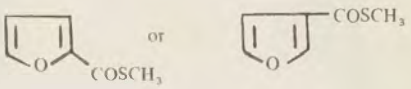
6. **Stoll et al.**, *Helv. Chim. Acta*, 50, 628, 1967.

	4-Methylthio-2-butanone	3-Methylthiobutyraldehyde
Other names	3-Methylmercapto-2-butanone	3-Methylthiobutanal
Empirical formula	$C_5H_{10}OS$	$C_5H_{10}OS$
Structure	$CH_3-S-CH_2-CH_2-\underset{\underset{O}{\|\|}}{C}-CH_3$	$CH_3-S-\underset{\underset{CH_3}{\|}}{CH}-CH_2-CHO$
Physical/chemical characteristics		
Molecular weight	118.19	118.19
Boiling point	106°C at 55 mm Hg 77–78°C at 20 mm Hg	63°C at 10 mm Hg 80–92°C at 14 mm Hg
Specific gravity		0.997 at 20°C
Refractive index	1.4711 at 25°C	1.5078 at 20°C
Organoleptic characteristics	Flavor like arrowhead	
Synthesis	From methylvinyl ketone and methylmercaptan;[6] from methylvinyl ketone and methyl-bis (methylthio)aluminum[7]	By addition of methanethiol to the corresponding unsaturated aldehyde (previously cooled to –20°C), using piperidine or copper acetate as catalyst;[8,10] by a patented oxo process[11]
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm Gelatins and puddings 1.0 ppm Meat, meat sauces, soups 1.0 ppm	Condiments, pickles 2.0 ppm Vegetables 2.0 ppm
Regulatory status	FEMA No. 3375	FEMA No. 3374

REFERENCES

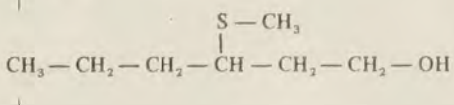
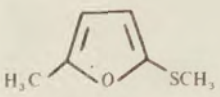
For References 1–5, see end of Part III.

6. Reimer, *J. Am. Chem. Soc.*, 78, 2132, 1956.
7. Lalancette and Cole, *Can. J. Chem.*, 49, 2983, 1971.
8. Bonstany, *J. Chem. U.A.R.*, 9(3), 317, 1966.
9. Bateman, Cunneen and Ford, *J. Chem. Soc.*, p. 3056, 1956.
10. Reisner, *J. Am. Chem. Soc.*, 78, 2132, 1956.
11. Badische Aniline und Soda Fabrik, British Patent 683,267.

	Methyl thiobutyrate		Methyl thiofuroate	
Other names	Thiobutyric acid, methyl ester Methanethiol *n*-butyrate		Thiofuroic acid, methylester	
Empirical formula	$C_5H_{10}OS$		$C_6H_6O_2S$	
Structure				
Physical/chemical characteristics				
Molecular weight	118.10		142.12	
Boiling point			92–93°C at 11 mm Hg	
Reported uses[3]	Non-alcoholic beverages	0.0005 ppm	Non-alcoholic beverages	3.0 ppm
	Ice cream, ices, etc.	0.05 ppm	Ice cream, ices, etc.	3.0 ppm
	Candy	0.5 ppm	Candy	3.0 ppm
	Baked goods	7.0 ppm	Baked goods	5.0 ppm
	Gelatins and puddings	0.06 ppm	Condiments	3.0 ppm
	Protein foods	5.0 ppm	Meat, soups	3.0 ppm
Regulatory status	FEMA No. 3310		FEMA No. 3311	

REFERENCES

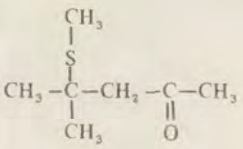
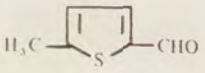
For References 1–5, see end of Part III.

	3-Methylthio-1-hexanol		2-Methyl-5-thiomethylfuran	
Other names	3-Methylmercapto-1-hexanol		2-Methyl-4-(methylthio)furan	
Empirical formula	$C_7H_{16}OS$		C_6H_8OS	
Structure				
Physical/chemical characteristics				
Appearance			Pale-yellow liquid	
Molecular weight	148.26		128.19	
Boiling point			80°C at 45–50 mm Hg 66–67°C at 23 mm Hg	
Specific gravity			1.0574 at 20°C	
Refractive index			1.5170 at 20°C	
Organoleptic characteristics			Very strong sulfurated odor	
Synthesis			From 2-methylfuran with CH_3SCl;[6] from 2-methylfuran with an organolithium compound[7]	
Natural occurrence			Constituent of coffee[8]	
Reported uses[3]	Non-alcoholic beverages	3.0 ppm	Baked goods	1.5 ppm
	Ice cream, ices, etc.	5.0 ppm	Meat, meat sauces, soups	1.5 ppm
	Baked goods	6.0 ppm		
	Gelatins and puddings	4.0 ppm		
	Condiments	4.0 ppm		
	Confections	5.0 ppm		
Regulatory status	FEMA No. 3438		FEMA No. 3366	

REFERENCES

For References 1–5, see end of Part III.

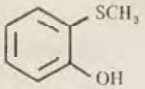
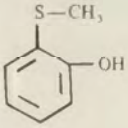
6. **Stoll et al.,** *Helv. Chim. Acta,* 50, 687, 1967.
7. **Goldfarb et al.,** *Dokl. Akad. Nauk SSSR,* 151(2), 2231, 1963; *Chem. Abstr.,* 59, 8681d, 1963.
8. **Stoll et al.,** *Helv. Chim. Acta,* 50, 687, 1967.

	4-Methylthio-4-methyl-2-pentanone		5-Methyl-2-thiophenecarboxaldehyde	
Other names			5-Methyl-2-thenaldehyde	
Empirical formula	$C_7H_{14}OS$		C_6H_6OS	
Structure				
Physical/chemical characteristics				
Molecular weight	146.25		126.17	
Boiling point	84°C at 12 mm Hg 78°C at 15 mm Hg		52.5°C at 0.7 mm Hg 113–114°C at 25 mm Hg	
Refractive index	1.4750 at 13°C		1.5742 at 20°C	
Synthesis	From mesityl oxide by addition of methyl sulfide;[6] from acetone and methylbis(methylthio) aluminum[7]		From thiophene (or its derivatives) and formamide in the presence of $POCl_3$;[8] from N-(2-thenyl)formaldimines[9]	
Natural occurrence			Reported as occurring in roasted peanuts[10]	
Reported uses[3]	Non-alcoholic beverages	1.0 ppm	Non-alcoholic beverages	0.50 ppm
	Ice cream, ices, etc.	1.0 ppm	Ice cream, ices, etc.	0.50 ppm
	Candy	2.0 ppm	Candy	0.50 ppm
	Baked goods	2.0 ppm	Baked goods	0.50 ppm
	Gelatins and puddings	1.0 ppm	Gelatins and puddings	0.50 ppm
	Meat, meat sauces, soups	1.0 ppm	Chewing gum	0.50 ppm
			Condiments	0.50 ppm
			Meat, meat sauces, soups	0.50 ppm
			Milk, dairy products	0.50 ppm
			Cereals	0.50 ppm
Regulatory status	FEMA No. 3376		FEMA No. 3209	

REFERENCES

For References 1–5, see end of Part III.

6. **Bravo et al.**, *Gazz. Chim. Ital.*, 98, 1046, 1968.
7. **Lalancette et al.**, *Can. J. Chem.*, 49, 2983, 1971.
8. Abbott Laboratories, German Patent 953,082, 1956.
9. **Harbough and Dickert**, *J. Am. Chem. Soc.*, 71, 3922, 1949.
10. **Walradt et al.**, *J. Agric. Food Chem.*, 19(5), 972, 1971.

	2-Methylthiophenol	*o*-(Methylthio)phenol
Other names	Erroneously called *o*-toluenethiol	2-Hydroxy-2-methylmercaptobenzene 2-Methylmercapto phenol Methyl-(2-hydroxyphenol)sulfide 1-Thioguaiacol
Empirical formula	C_7H_8OS	C_7H_8OS
Structure		
Physical/chemical characteristics		
Appearance		Liquid
Molecular weight	140.19	140.20
Boiling point	105°C at 22 mm Hg	218–219°C 105°C at 22 mm Hg
Specific gravity	1.168 at 25°C	1.168 at 25°C
Synthesis	By diazotization of methyl-(2-aminophenyl)-sulfide and decomposition by boiling[6]	From the diazonium salt of methyl-(2-aminofuryl)-sulfide[9]
Natural occurrence	In coffee[7,8]	Reported found as a constituent in coffee aroma[10]
Reported uses[3]	Baked goods 0.20 ppm Soups, sauces 0.20 ppm	Non-alcoholic beverages 0.20 ppm Ice cream, ices, etc. 0.20 ppm Candy 0.20 ppm Gelatins and puddings 0.20 ppm
Regulatory status	FEMA No. 3240	FEMA No. 3210

REFERENCES

For References 1–5, see end of Part III.

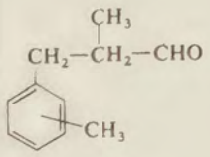
6. Holt et al., *J. Am. Chem. Soc.*, 46, 2335, 1924.
7. Goldmann, *Helv. Chim. Acta*, 50, 628, 1967.
8. Wolter et al., *Z. Ernährungswiss.*, 9, 123, 1969.
9. Holt and Reid, *J. Am. Chem. Soc.*, 46, 2335, 1924.
10. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.

	3-(Methylthio)propanol	3-Methylthiopropionaldehyde
Other names	Methionol 3-Methylthiol propyl alcohol γ-Hydroxypropyl methyl sulfide γ-Methyl mercaptopropyl alcohol Methyl-3-hydroxypropyl sulfide	Methional β-Methiopropionaldehyde (true name) Methyl-β-mercaptopropionaldehyde 3-Methylthiopropanol
Empirical formula	$C_4H_{10}OS$	C_4H_8OS
Structure	$CH_3-S-CH_2-CH_2-CH_2OH$	$CH_3-S-CH_2-CH_2-C(=O)H$
Physical/chemical characteristics		
Appearance	Pale-yellowish, mobile liquid	Pale-yellow, mobile liquid
Molecular weight	106.19	104.10
Boiling point	195°C 93–94°C at 17 mm Hg	165°C
Specific gravity	1.03	1.04
Refractive index	1.4832 at 20°C	
Solubility	Slightly soluble in water; soluble in alcohol, propylene glycol, and oils	Almost insoluble in water; soluble in alcohol and propylene glycol
Organoleptic characteristics	Powerful sweet soup or meat-like odor and flavor in high dilution	Powerful onion, meat-like odor; pleasant, warm, meat and soup-like flavor at low levels
Synthesis	From propylene chlorhydrin and sodium hydrosulfide[6]	By transamination and decarboxylation of various amino acids; by oxidation of the alcohol
	$H_3C-SH + CH_2OH \rightarrow S-CH_2OH$	
Natural occurrence	Identified in the volatile portion of soy sauce,[7–9] and in tomatoes and wine[10,11]	In potato and potato chips
Reported uses[3]	Non-alcoholic beverages 0.05 ppm Candy 0.1 ppm	Non-alcoholic beverages 0.35 ppm Ice cream, ices, etc. 0.01–1.0 ppm Candy 0.01–1.0 ppm Baked goods 0.66 ppm Condiments 0.62 ppm Meats 1.9 ppm
Regulatory status	FEMA No. 3415	FDA GRAS; FEMA No. 2747

REFERENCES

For References 1–5, see end of Part III.

6. Kisner, *J. Am. Chem. Soc.*, 50, 2352, 1928.
7. Akabori et al., *Proc. Imp. Acad. Tokyo*, 12, 136, 1936.
8. Buttery et al., *J. Food Chem.*, 19, 524, 1971.
9. Johnson et al., *Chem. Ind.*, (London), p. 1212, 1971.
10. Weurman Report, 3rd ed.
11. Müller et al., *Am. J. Enol. Vitic.*, 22, 156, 1971.

	3-Methylthiopropyl isothiocyanate	2-Methyl-3-tolyl propionaldehyde (mixed *o-*, *m-*, *p-*)
Other names	3-Methylmercaptopropyl isothiocyanate Ibervirin[6]	
Empirical formula	$C_5H_9NS_2$	$C_{11}H_{14}O$
Structure	$H_3C-S-CH_2-CH_2-CH_2-NCS$	
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless, oily liquid
Assay		Commercial product mainly *para*-isomer with some *ortho*- and only traces of *meta*-isomer
Molecular weight	147.26	162.23
Boiling point	116°C at 9 mm Hg	
Solubility		Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic radish odor	Extremely sweet, fruity odor; somewhat balsamic with bitter-almond notes
Synthesis	From 3-methylthiopropylamine and $CSCl_2$[6]	Commercially available as a mixture of the three isomers; from tolyl aldehyde (*o-*, *m-*, *p-* mixture) by condensation with propionaldehyde followed by hydrogenation
Natural occurrence	Reported found in the hydrolysates of crucifer seeds and *Lesquerella* seed meal,[8] and in *Iberis sempervirens* seeds[9]	Not reported found in nature
Reported uses[3]	Gelatins and puddings 4.0 ppm Frozen pies 4.0 ppm	Non-alcoholic beverages 0.05 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm
Regulatory status	FEMA No. 3312	FDA 121.1164; FEMA No. 2748

REFERENCES

For References 1–5, see end of Part III.

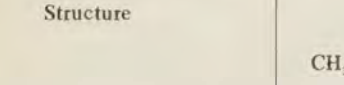
6. Kjaer, Gruelin and Larsen, *Acta Chem. Scand.*, 9, 1143, 1955; *Chem. Abstr.*, 49, 12782f, 1955.
7. Daxenbichler, VanEtten, Brown, and Jones, *J. Agric. Food Chem.*, 12(2), 127, 1964.
8. Daxenbichler, VanEtten, Zobel, and Wolff, *J. Am. Oil Chem. Soc.*, 39, 244, 1962.
9. Kjaer, Gruelin, and Larsen, *Acta Chem. Scand.*, 9, 1143, 1955; *Chem. Abstr.*, 49, 12782f, 1955.

	2-Methyl undecanal	Methyl 9-undecenoate
Other names	"Aldehyde C-12, M.N.A." 2-Methylhendecanal Methyl nonyl acetaldehyde	Methyl 9-hendecenoate Methyl 9-undecylenate
Empirical formula	$C_{12}H_{24}O$	$C_{12}H_{22}O_2$
Structure	$CH_3-(CH_2)_8-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-CHO$	$CH_3-CH=CH-(CH_2)_7-\overset{\displaystyle O}{\overset{\Vert}{C}}-O-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow liquid	Colorless to pale straw-yellow, oily liquid
Assay	94% min[2]	
Molecular weight	184.32	198.31
Melting point		−27.5°C
Boiling point	114°C (232°C) at 10 mm Hg	247–248°C; 142°C at 26 mm Hg
Flash point	69°C	
Specific gravity	0.822–0.830 at 25°/25°C[2]	0.8861 at 20°C
Refractive index	1.4310–1.4360 at 20°C[2]	1.4388 at 20°C
Acid value	10 max[2]	
Solubility	Soluble in alcohol and most organic solvents; insoluble in water; 1:4 in 80% alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic fatty odor assuming a floral note on dilution; acrid, fatty unpleasant flavor at high levels; at low levels the flavor is honey- and nut-like	Sweet, persistent, light, fatty, green odor reminiscent of wine and iron; oily, brandy-like flavor at low concentrations; unpleasant at high levels
Synthesis	By cracking the corresponding glycidic acid;[2] from α-nonyl acrolein; from methyl nonyl ketone and ethyl monochloroacetate in the presence of sodium ethylate	By direct esterification of the acid with methanol and concentrated H_2SO_4[6] or HCl;[7] by thermal decomposition of methyl ricinoleate[8]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.31 ppm Ice cream, ices, etc. 0.11 ppm Candy 0.94 ppm Baked goods 1.3 ppm Gelatins and puddings 0.50–2.5 ppm Chewing gum 0.20 ppm Jellies 0.33 ppm	Non-alcoholic beverages 3.7 ppm Ice cream, ices, etc. 6.7 ppm Candy 22 ppm Baked goods 22 ppm
Regulatory status	FDA 121.1164; FEMA No. 2749	FDA 121.1164; FEMA No. 2750

REFERENCES

For References 1–5, see end of Part III.

6. **Komppa,** *Ber. Dtsch. Chem. Ges.*, 34, 897, 1901.
7. **Bornwater,** *Recl. Trav. Chim. Pays-Bas*, 2g, 410, 1907.
8. **Grün and Wirth,** *Ber. Dtsch. Chem. Ges.*, 55, 2208, 1922; *Chem. Zentralbl.*, 2, 747, 1928.

	Methyl undecyl ketone	Methyl 2-undecynoate
Other names	Hendecyl methyl ketone 2-Tridecanone	Methyl decine carbonate Methyl decyne carbonate
Empirical formula	$C_{13}H_{26}O$	$C_{12}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White wax or colorless crystalline platelets	Colorless, oily liquid
Molecular weight	198.34	196.29
Melting point	28–29°C	
Boiling point	263°C 195°C at 110 mm Hg	121°C at 5 mm Hg; 230°C at 760 mm Hg
Specific gravity	0.82168 at 30°C	0.9177 at 20°C; 0.940 at 15.5°C
Refractive index	1.43175 at 30°C	1.4465 (1.4530) at 20°C
Solubility	Insoluble in water; very soluble in alcohol, ether, acetone, and benzene	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Warm-oily, herbaceous odor reminiscent of nut	Powerful, waxy, green, floral odor; sweet flavor reminiscent of violet
Synthesis	By heating a mixture of lauric acid and acetic acid over thorium oxide at 450°C[6]	By methylation of the corresponding acid at the boil in the presence of HCl[7] or at room temperature in the presence of H_2SO_4.[8] The acid can be prepared from methyl nonyl ketone by reaction with phosphorous pentachloride, which yields the acetylenic compound. Treatment of this with potassium carbonate yields undecyne, which is then converted to the acid by treatment with Na and methyl chlorocarbonate.
Natural occurrences	Reported found in coconut and palm oils; also in the oil of *Schizandra nigra* Max. (Matsubusa)	Not reported found in nature
Reported uses[3]	Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Baked goods 5.0 ppm Gelatins and puddings 3.0 ppm Margarine 3.0 ppm	Non-alcoholic beverages 0.10–5.0 ppm Ice cream, ices, etc. 20 ppm Candy 15 ppm Baked goods 15 ppm
Regulatory status	FEMA No. 3388	FDA 121.1164; FEMA No. 2751

REFERENCES

For References 1–5, see end of Part III.

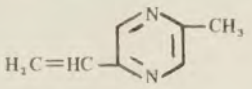
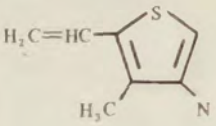
6. Dreger et al., *Ind. Eng. Chem.*, 36, 610, 1944.
7. Osskerko, *Chem. Ber.*, 70, 56, 1937.
8. Jeffery and Vogel, *J. Chem. Soc.*, p. 678, 1948.

	Methyl valerate	2-Methylvaleric acid
Other names	Methyl pentanoate Methyl-*n*-valerate Methyl valerianate	2-Methylpentanoic-1-acid Methyl propyl acetic acid α-Methyl valeric acid Pentane-2-carboxylic acid
Empirical formula	$C_6H_{12}O_2$	$C_6H_{12}O_2$
Structure	$CH_3-O-\overset{\overset{O}{\|\|}}{C}-(CH_2)_3-CH_3$	$CH_3-CH_2-CH_2-\underset{\underset{CH_3}{\|}}{CH}-\overset{\overset{O}{\|\|}}{C}-OH$
Physical/chemical characteristics[5]		
Appearance	Colorless, mobile liquid	Solidifies at room temperature in a mass similar to ice; otherwise a colorless liquid
Molecular weight	116.16	116.16
Boiling point	126–127°C	195–196°C (194°C)
Specific gravity	0.8895 at 20°C	0.9230 at 20°C
Refractive index	1.3969 at 20°C	1.4136 at 20°C
Optical rotation		*d*-, +18.5° at 16°C, undiluted; *l*-, −18.4° at 25°C, undiluted
Solubility	Very slightly soluble in water; soluble in propylene glycol, alcohol, and oils	Soluble in water; miscible with alcohol and some essential oils
Organoleptic characteristics	Pungent, green-fruity odor, apple and pineapple-like; corresponding flavor at 10–50 ppm	Powerful, pungent, acrid odor; below 10 ppm agreeable, sour, oily flavor; at higher concentrations, too acidic
Synthesis	By direct esterification of valeric acid with methanol in the presence of concentrated H_2SO_4.[6] *Note:* this ester hydrolyzes readily.	By catalytic oxidation of 2-methyl pentanealdehyde; from 2-chloropentane with sodium and CO_2 under pressure; by decarboxylation of methyl propyl malonic acid. Two optically active isomers are known
Natural occurrence	Reported found in small amounts in the essential oil from the fruits of *Ananas sativus* Schult.[7]	In coffee, wine, and cheese
Reported uses[3]	Non-alcoholic beverages 9.1 ppm Ice cream, ices, etc. 25 ppm Candy 28 ppm Baked goods 39 ppm	Candy 0.80 ppm
Regulatory status	FDA 121.1164; FEMA No. 2752	FDA 121.1164; FEMA No. 2754

REFERENCES

For References 1–5, see end of Part III.

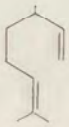
6. **Vogel,** *J. Chem. Soc.*, p. 630, 1948.
7. **Haagen-Smit et al.,** *J. Am. Chem. Soc.*, 67, 1647, 1945.

	2-Methyl-5-vinylpyrazine	4-Methyl-5-vinylthiazole
Empirical formula	$C_7H_8N_2$	C_6H_7NS
Structure		
Physical/chemical characteristics		
Assay	C: 69.97%; H: 6.71%; N: 23.31%	
Molecular weight	120.16	125.19
Boiling point	65–66°C at 12 mm Hg	78–82°C at 18–20 mm Hg
Mass spectra[5]	39 (16), 40 (7), 52 (60), 54 (29), 66 (3), 67 (2), 79 (10), 80 (1), 93 (12), 94 (9), 119 (17), 120 (100)	
IR spectra[5]	S (6.7, 8.6, 9.7, 10.1, 10.7) M (3.3, 7.1, 7.2, 7.4, 7.6, 10.8, 11.1) W (5.3, 6.1, 6.5, 7.8, 7.9, 8.2, 9.2, 11.4)	
UV spectra[5]	(233.3, 290.5, 297.0 nm)	
Solubility		Soluble in alcohol
Synthesis	By methylation of the Mannich base obtained by reacting formaldehyde and dimethylamine with dimethyl-2,5-pyrazine, followed by the Hoffman degradation[6]	By a patented process[6]
Natural occurrence	Reported to be present in the following foods: coffee, dairy products, peanuts, filberts, potato products[7]	Compound of cocoa aroma;[7] compound of yellow passion fruit aroma[8]
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Gelatins and puddings 10.0 ppm	Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Baked goods 8.0 ppm Gelatins and puddings 8.0 ppm Meat, meat sauces, soups 6.0 ppm
Regulatory status	FEMA No. 3211	FEMA No. 3313

REFERENCES

For References 1–5, see end of Part III.

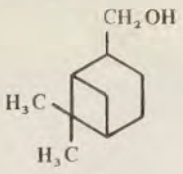
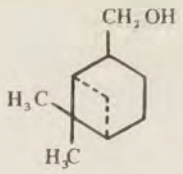
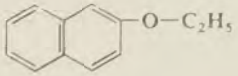
6. Kamal et al., *J. Org. Chem.*, 27, 1355, 1962.
7. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
8. Bondarovich et al., *J. Agric. Food Chem.*, 15, 1093, 1967.
9. U.S.S.R. Patent 164, 878, 1964.
10. Stoll, Dietrich, Sunolt and Winter, *Helv. Chim. Acta*, 50(7), 2065, 1967; *Chem. Abstr.*, 61, 13809b, 1964; *Chem. Abstr.*, 66, 9499f, 1967.
11. Winter and Kloti, *Helv. Chim. Acta*, 55(6), 1916, 1972.

	Myrcene	Myristaldehyde
Other names	7-Methyl-3-methylene-1,6-octadiene	Aldehyde C-14 (true) Myristic aldehyde Tetradecanal *n*-Tetradecyl aldehyde Tetradecyl aldehyde
Empirical formula	$C_{10}H_{16}$	$C_{14}H_{28}O$
Structure		$CH_3-(CH_2)_{12}-CHO$
Physical/chemical characteristics[5]		
Appearance	Oily liquid	Colorless to slightly yellow liquid; polymerizes readily to a white mass, melting at 65°C
Assay		85–92%
Molecular weight	136.23	212.36
Melting point		20.5°C (23°C)
Boiling point	65–66°C (166–168°C) at 20 mm Hg	155°C (260°C) at 10 mm Hg
Specific gravity	0.8013 at 15°C	0.825–0.835 at 25°C
Refractive index	1.4650 at 20°C	1.4380–1.4450 at 20°C
Solubility	Insoluble in water; soluble in alcohol, chloroform, and ether	1:1 in 80% alcohol; insoluble in water and most common organic solvents
Organoleptic characteristics	Pleasant odor	Strong, fatty, orris-like odor; sweet, fatty, "citrus-peel" flavor (diluted)
Synthesis	From linalool.[6] For structure identification see references 7 and 8.	Industrially prepared from the corresponding myristic acid
Natural occurrence	Reported found in *Mircia acris* D.C.; in the distillates from leaves of *Rhus cotinus* and *Barosma venustum* (52% and 43%, respectively); in lemon grass, cypress, artemisia, orange, and lemon; in the fruits of *Phellodendron amurense* (92%) and *Phellodendron japonicum*; in the oils of *Picea balsamea*, *Tsuga canadensis*, *Abies balsamea*, clary sage, and others.	Reported found in the essential oils of *Ocotea usambarensis* Engl., *Pinus sabiniana* Dougl., and probably others
Reported uses[3]	Non-alcoholic beverages 4.4 ppm Ice cream, ices, etc. 6.4 ppm Candy 0.50–13 ppm Baked goods 4.9 ppm	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 0.06–8.0 ppm Candy 1.9 ppm Baked goods 0.08–24 ppm Gelatins and puddings 0.15 ppm
Regulatory status	FDA 121.1164; FEMA No. 2762	FDA 121.1164; FEMA No. 2763

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For References 1–5, see end of Part III.

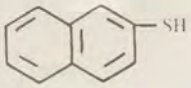
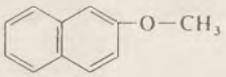
6. **Arbusow and Abramow,** *Ber. Dtsch. Chem. Ges.*, 67, 1942, 1934.
7. **Ruzička and Stoll,** *Helv. Chim. Acta*, 7, 272, 1924.
8. **Power and Kleber,** *Pharm. Rundsch.*, 13, 60, 1895.

	Myrtenol	β-Naphthyl ethyl ether
Other names	6,6-Dimethyl-2-oxymethlybicyclo[1.1.3]-hept-2-ene 10-Hydroxy-2-pinene 2-Pinen-10-ol	"Bromelia" 2-Ethoxynaphthalene Ethyl-2-naphthyl ether Ethyl-β-naphthyl ether β-Naphthol ethyl ether Nerolin II Nerolin bromelia
Empirical formula	$C_{10}H_{16}O$	$C_{12}H_{12}O$
Structure	 *l*-form  *d*-form	
Physical/chemical characteristics[5]		
Appearance		White, crystalline solid
Molecular weight	152.24	172.23
Melting point		37°C
Boiling point	218°C at 771 mm Hg	282°C
Congealing point	103–104°C at 11 mm Hg	>35.0°C[2]
Specific gravity	0.9763 at 20°C	1.064 at 36°C
Refractive index	1.4967 at 20°C	1.597 at 36°C
Optical rotation	+45, 45°	
Solubility		1:5 in 95% alcohol;[2] insoluble in water; poorly soluble in propylene glycol
Organoleptic characteristics		Odor suggestive of orange blossom with faint, fruity undertone; corresponding sweet taste suggestive of strawberry (on extreme dilution only)
Synthesis	Can be obtained in *d,l*-form from α-pinene with SeO_2 in ethanol[6,7]	By esterification of β-naphthol with ethyl alcohol and sulfuric acid;[1,3] from β-naphtholsodium and diethylsulfate in weak aqueous base; from β-naphtholsodium and ethyl bromide
Natural occurrence	In cranberry and bilberry,[8] mint,[9] and hop oil[10-12]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 10 ppm Candy 10 ppm Gelatins and puddings 10 ppm Milk, dairy products 10 ppm	Non-alcoholic beverages 0.65 ppm Ice cream, ices, etc. 0.74 ppm Candy 2.8 ppm Baked goods 3.6 ppm Gelatins and puddings 0.12 ppm
Regulatory status	FEMA No. 3439	Status not fully defined by FDA; FEMA No. 2768

REFERENCES

For References 1–5, see end of Part III.

6. DuPont et al., *Bull. Soc. Chim. Fr.*, 50, 536, 1935.
7. Schmidt, *Chem. Abstr.*, 37, 4715, 1943.
8. von Sydow et al., *Lebensm. Wiss. Technol.*, 2, 78, 1969.
9. Canova, 5th International Congress on Essential Oils, Sao Paulo, 1971.
10. Lammens et al., *J. Inst. Brew.*, 74, 341, 1968.
11. Drawert et al., *Brauwinenschaft*, 22, 169, 1969.
12. Naya et al., *Bull. Chem. Soc. Jap.*, 45, 2887, 1972.
13. *Ullmanns Enzyklopädie der Technischen Chemie*, 3rd ed., Vol. 12, Urban and Schwarzenberg, 1960, 605.

	2-Naphthyl mercaptan	β-Naphthyl methyl ether
Other names	2-Naphthalenethiol 2-Mercaptonaphthalene 2-Thionaphthol β-Thionaphthol	2-Methoxynaphthalene Methyl-2-naphthyl ether Methyl-β-naphthyl ether β-Naphthol methyl ether Nerolin I Nerolin yara-yara "Yara-yara"
Empirical formula	$C_{10}H_8S$	$C_{11}H_{10}O$
Structure		
Physical/chemical characteristics		
Appearance	Crystals (from ethanol)	White, crystalline solid
Molecular weight	160.24	158.20
Melting point	81°C	72°C (71.5–73.5°C)
Boiling point	285°C (decomposes) 210.5°C at 100 mm Hg 189°C at 50°C 162°C at 20°C	274°C (sublimes when heated)
Congealing point		71.5–73.0°C[2]
Specific gravity	1.1607 at 20°C	
Refractive index	1.6802 at 20°C	
Solubility	Slightly soluble in water and diluted alkalis; very soluble in alcohol and ether	1 gm in 25 ml of 95% alcohol;[2] soluble in ether, chloroform, and benzene
Organoleptic characteristics	Disagreeable mercaptan-like odor	Intensely sweet, floral odor suggestive of orange blossoms; free from naphthol by-odor; sweet, strawberry taste
Synthesis	By catalytic hydrogenation of a sulfonic acid derivative of naphthalene;[6] by reduction of naphthalenesulfonyl chloride with zinc[7]	From potassium β-naphthol and methyl chloride at 300°C; by methylation of β-naphthol with dimethyl sulfate or by direct esterification with methyl alcohol[8]
Natural occurrence		Not reported found in nature
Reported uses[3]	Baked goods 0.5 ppm Meat, meat sauces, soups 0.5 ppm Cereals 0.5 ppm	
Regulatory status	FEMA No. 3314	Status not fully defined by FDA

REFERENCES

For References 1–5, see end of Part III.

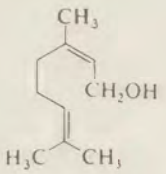
6. **Lazier and Signaigo,** U.S. Patent 2,402,641; *Chem. Abstr.,* 40, 5768, 1946.
7. **Holt,** U.S. Patent 2,216,840, assigned to E. I. duPont de Nemours & Co., 1940.
8. **Gattermann,** *Chem. Ann.,* 244, 72, 1888.

	d-Neomenthol
Other names	*d*-β-Pulegomenthol
Empirical formula	$C_{10}H_{20}O$
Structure	Stereoisomer of menthol (see Menthol)
Physical/chemical characteristics[5]	
Appearance	Liquid
Molecular weight	156.27
Melting point	−22°C
Boiling point	211.5–212.5°C at 755–760 mm Hg; 107–108°C at 20 mm Hg; 98°C at 16 mm Hg; 87°C at 8 mm Hg
Specific gravity	0.903 at 15°/15°C; 0.8995 at 20°C; 0.8970 at 22°C
Refractive index	1.4617 at 17°C; 1.4594–1.4603 at 20–22°C
Optical rotation	+17°48′ at 16°C; +19°42′ at 18°C; +20° 0′ at 20°C
Solubility	Insoluble in water; soluble in alcohol and acetone
Organoleptic characteristics	Menthol-like odor; used in mixtures of menthols as a substitute for *l*-menthol
Synthesis	See References 6 and 7
Natural occurrence	Small quantities found in *Mentha arvensis*
Reported uses[3]	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 31 ppm Candy 50 ppm Baked goods 48 ppm
Regulatory status	FDA 121.1164; FEMA No. 2666

REFERENCES

For References 1–5, see end of Part III.

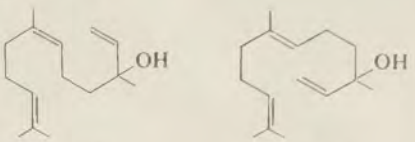
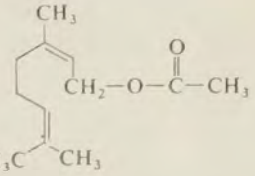
6. *Beilstein's Encyclopedia of Organic Chemistry*, B6[3], Springer Verlag, p. 139.
7. Guenther, *The Essential Oils*, Vol. 2, D. Van Nostrand Co., 1949, 220.

	Nerol
Other names	2-*cis*-3,7-Dimethyl-2,6-octadien-1-ol *Note*: see Geraniol for *trans*-form.
Empirical formula	$C_{10}H_{18}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid
Assay	95% min[10]
Molecular weight	154.24
Boiling point	225–226°C[9]
Specific gravity	0.8771–0.8788 at 15°C[9] 0.877–0.879 at 20/4°C[10]
Refractive index	1.462 at 20°C;[9] 1.475–1.478 at 20°C[10]
Solubility	1:5 in 50% alcohol; insoluble in water; soluble in most common organic solvents
Organoleptic characteristics	Fresh, sweet, rose-like odor; bitter flavor
Synthesis	From pinene.[6] For selective synthesis of stereoisomers, see reference 7; for gas chromatographic analysis of geraniol and nerol, see reference 8.
Natural occurrence	Reported found in neroli oil (with geraniol) and in the essential oils of: lemon grass, Ceylon citronella, ylang-ylang, champaca, cajenne bois-de-rose, and bergamot; also in lemon, sweet orange, and petitgrain bergamot; in clary sage, lavandin, lavender, Mexican linaloe, myrrh, jasmine, Paraguay petitgrain. Also reported among the volatile constituerts of currant aroma. *Helicrysum angustifolium* contains up to 30–50% nerol.
Reported uses[3]	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 3.9 ppm Candy 16 ppm Baked goods 19 ppm Gelatins and puddings 1.0–1.3 ppm Chewing gum 0.80 ppm
Regulatory status	FDA 121.1164; FEMA No. 2770

REFERENCES

For References 1–5, see end of Part III.

6. **Bedoukian**, *Perfumery and Flavoring Synthetics*, 2nd ed., American Elsevier, 1967.
7. **Yukawa, Hanafusa and Fujita**, *Bull. Chem. Soc. Jap.*, 2(37), 158, 1964.
8. **Naves and Odermatt**, *Bull. Soc. Chim. Fr.*, p. 377, 1958.
9. **Blumann and Zeitschell**, *Ber. Dtsch. Chem. Ges.*, 44, 2590, 1911.
10. The Givaudan Index, *Givaudan-Delawanna*, Inc., 1949.

	Nerolidol	Neryl acetate
Other names	3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol	2-*cis*-3,7-Dimethyl-2,6-octadien-1-yl acetate
Empirical formula	$C_{15}H_{26}O$	$C_{12}H_{20}O_2$
Structure	 *cis-* *trans-*	
Physical/chemical characteristics[5]		
Appearance	Colorless to straw-yellow liquid	Colorless to slightly yellow, oily liquid
Assay	90% min	95% min
Molecular weight	222.36	196.29
Boiling point	89–100 C at 0.3 mm Hg; 145°C at 12 mm Hg	134°C (231°C) at 25 mm Hg
Specific gravity	0.870–0.880 at 25°/25°C;[2] 0.8788 at 16°C	0.903–0.906 at 15°C; 0.907–0.913 at 25 C
Refractive index	1.4789–1.4830 at 20°C;[2] 1.4801 at 16°C	1.4510–1.4540 (1.4600–1.4650) at 20 C
Optical rotation	Natural: −11° to +14°; synthetic: optically inactive	
Ester content	Not more than 0.5% (as nerolidyl acetate)	
Solubility	1:4 in 70% alcohol[2]	1:5.6 in 70% alcohol; soluble in the essential oils and most common organic solvents
Organoleptic characteristics	Faint, floral odor similar to rose and apple; unusually sweet, fresh, tenacious odor	Very sweet, floral, orange-blossom and rose-like odor; initially fresh and pungent, and then a honey-like flavor with a raspberry undertone
Synthesis	The natural product can be *dextro-* or *laevo*-rotatory, whereas the synthetic product is optically inactive. The double bond at positions 6–7 accounts for the *cis-* and *trans-* forms. For synthesis see references 6, 7, and 8.	By esterification of nerol with acetic acid; also prepared from myrcene by hydrobromination and esterification[11]
Natural occurrence	Reported found in over 25 natural sources, including the essential oils of neroli, ylang-ylang, Peru balsam; in currant aroma; also reported in *Dalbergia sissoo* (60%, *dl-*),[9] vervain, the distillation waters of petitgrain bigarade, *Helicrysum italicum*,[10] *Myrocarpus frondosus* and *Myrocarpus fastigiatus* (80%, *d-*), Tolu balsam, *Acacia farnesiana*, orange-flower water, Paraguay petitgrain, jasmine, *Melaleuca smithii*, and *Melaleuca viridiflora*	Reported found in the essential oils of lemon, neroli, and petitgrain bigarade
Reported uses[3]	Non-alcoholic beverages 0.91 ppm Ice cream, ices, etc. 0.92 ppm Candy 3.5 ppm Baked goods 2.0–8.0 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 1.6 ppm Candy 5.1 ppm Baked goods 15 ppm
Regulatory status	FDA 121.1164; FEMA No. 2772	FDA 121.1164; FEMA No. 2773

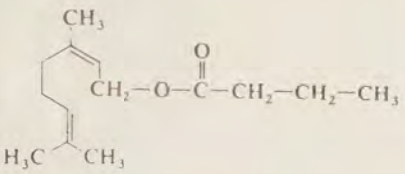
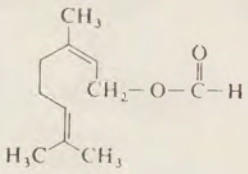
REFERENCES

For References 1–5, see end of Part III.

6. Ružička, *Helv. Chim. Acta*, 6, 488, 1923.
7. Ružička and Capato, *Helv. Chim. Acta*, 8, 259, 1925.
8. Ofrier et al., *Helv. Chim. Acta*, 42, 2577, 1959.
9. Kathpalia and Dutt, *Indian Soap J.*, 18, 213, 1953.
10. Rovesti, *Riv. Ital. EPPOS*, 17, 19, 1935.
11. *Schimmel Ber.*, p. 200, 1955.

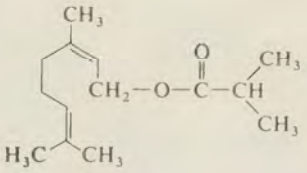
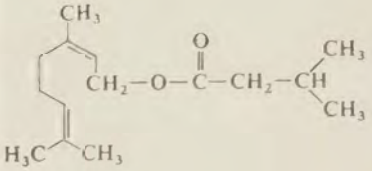
For further information on nerolidol see the following:

A. Vlad and Sančck, *Collect. Czech. Chem. Commun.*, 27(7), 1726, 1962.
B. Naves, *Bull. Soc. Chim. Fr.*, 18, 505, 1951; *Helv. Chim. Acta*, 30, 279, 1947.
C. Naves and Odermatt, *Bull. Soc. Chim. Fr.*, p. 377, 1958.
D. Lebedewa et al., *J. Gen. Chem. USSR*, 21, 1183, 1951.
E. Gildemeister and Hoffman, *Die Aetherischen Oele*, Vol. 3b, Akademie Verlag, 1962, 239.

	Neryl butyrate	Neryl formate
Other names	2-*cis*-3,7-Dimethyl-2,6-octadien-1-yl butyrate Neryl-*n*-butyrate	2-*cis*-3,7-Dimethyl-2,6-octadien-1-yl formate
Empirical formula	$C_{14}H_{24}O_2$	$C_{11}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay		91% min
Molecular weight	224.44	182.26
Boiling point	239°–240°C	215°C (225°C)
Specific gravity	0.8968–0.8986 at 15°/15°C; 0.895 at 15.5°C	0.9163–0.9169 at 15°C; 0.920 at 15.5°C
Refractive index	1.4539–1.4556 (1.4590) at 20°C	1.4558–1.4578 (1.4565) at 20°C
Solubility	1:6 in 80% alcohol; insoluble in water	1:10 in 70% alcohol; almost insoluble in water
Organoleptic characteristics	Very sweet, leafy, floral, neroli-like odor; sweet taste similar to cocoa	Sweet, herbaceous, green, penetrating odor suggestive of neroli and rose; sweet, tart, and fruity flavor
Synthesis	By azeotropic esterification of nerol with butyric acid or conventionally using butyric anhydride	By direct esterification of nerol. The pure ester tends to decompose readily.
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 6.2 ppm Ice cream, ices, etc. 22 ppm Candy 16 ppm Baked goods 25 ppm	Non-alcoholic beverages 5.3 ppm Ice cream, ices, etc. 23 ppm Candy 17 ppm Baked goods 22 ppm
Regulatory status	FDA 121.1164; FEMA No. 2774	FDA 121.1164; FEMA No. 2776

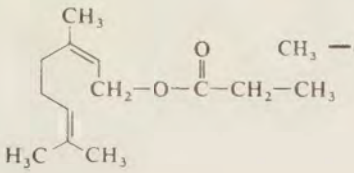
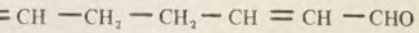
REFERENCES

For References 1–5, see end of Part III.

	Neryl isobutyrate	Neryl isovalerate
Other names	2-*cis*-3,7-Dimethyl-2,6-octadien-1-yl isobutyrate	2-*cis*-3,7-Dimethyl-2,6-octadien-1-yl isovalerate Neryl-β-methylbutyrate
Empirical formula	$C_{14}H_{24}O_2$	$C_{15}H_{26}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	224.34	238.38
Boiling point	130°C (232°C) at 3 mm Hg	252°C
Specific gravity	0.8915–0.8936 at 15°C	0.8898 at 15°C
Refractive index	1.4508–1.4527 at 20°C	1.4531 at 20°C
Solubility	1:5 in 80% alcohol; almost insoluble in water	1:8 in 80% alcohol; insoluble in water
Organoleptic characteristics	Delicate, sweet, rose-like fragrance with a slightly fruity undertone; sweet, strawberry taste	Strong, rich, fruity odor reminiscent of bergamot, clary sage, and petitgrain; bitter taste; below 10 ppm flavor is berry-like, somewhat similar to black currant and apple.
Synthesis	By esterification of nerol using isobutyric acid or the anhydride	By esterification of nerol with isovaleric acid
Natural occurrence	In oil of hop	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 1.8 ppm Candy 3.3 ppm Baked goods 5.4 ppm	Non-alcoholic beverages 0.97 ppm Ice cream, ices, etc. 1.6 ppm Candy 4.0 ppm Baked goods 5.7 ppm
Regulatory status	FDA 121.1164; FEMA No. 2775	FDA 121.1164; FEMA No. 2778

REFERENCES

For References 1–5, see end of Part III.

	Neryl propionate	Nona-2-*trans*,-6-*cis*-dienal
Empirical formula	$C_{13}H_{22}O_2$	$C_9H_{14}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless to pale yellow oil
Molecular weight	210.31	138.21
Boiling point	233°C	187°C 85–87°C at 11 mm Hg 80°C at 4 mm Hg
Specific gravity	0.9044 at 15°/15°C	0.8678 at 20°C
Refractive index	1.4550 at 20°C	1.4460 at 20°C
Solubility	Very slightly soluble in water; soluble in alcohol; 1:15 in 70% alcohol	Almost insoluble in water; soluble in alcohol, propylene glycol, and oils
Organoleptic characteristics	Ether-like, sweet and intense fruity odor reminiscent of jasmine and rose; "jam-like" aroma of fruit preserves; sweet taste suggestive of plum	Odor reminiscent of green cucumber; the organoleptic character is attributed almost entirely to olfactory sensations
Synthesis	By esterification of nerol with propionic acid	From natural hexenol;[6-8] from steam distillation of fresh cucumber[9]
Natural occurrence	In oil of hop	Reported as naturally occuring in violet leaves and flowers, and in cucumber juice[10]
Reported uses[3]	Non-alcoholic beverages 6.3 ppm Ice cream, ices, etc. 23 ppm Candy 21 ppm Baked goods 21 ppm	Condiments 1.0 ppm Preserves and spreads 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2777	FEMA No. 3377

REFERENCES

For References 1–5, see end of Part III.

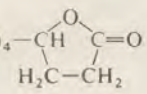
6. Ružička, Schinz and Susz, *Helv. Chim. Acta*, 27, 1561, 1944.
7. Jutz, *Chem. Ber.*, 92, 1983, 1959.
8. Sondheimer, *J. Am. Chem. Soc.*, 74, 4040, 1952.
9. Takei et al., *J. Agric. Chem. Soc. Jap.*, 15, 193, 1939; *Chem Abstr.*, 33, 6524, 1939.
10. Takei and Ono, *J. Agric. Chem. Soc. Jap.*, 15, 193, 1939.

	2,4-Nonadienal	2,6-Nonadienal diethyl acetal
Empirical formula	$C_9H_{14}O$	$C_{13}H_{24}O_2$
Structure	$CH_3-(CH_2)_3-CH=CH-CH=CH-CHO$	$CH_3-CH_2-CH=CH-CH_2-CH_2-CH=CH-CH(OCH_2CH_3)(OCH_2CH_3)$
Physical/chemical characteristics[5]		
Appearance		Colorless oily liquid
Molecular weight	138.20	212.34
Boiling point	72–74°C at 3 mm Hg 97–99°C at 10 mm Hg	67–70°C at 0.2 mm Hg
Specific gravity	0.862 at 25°C	
Refractive index	1.5184 at 27°C	1.4439 at 18°C
Solubility		Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics		Odor reminiscent of green cucumber
Synthesis	By the method of Marshall and Whiting;[6] by reduction with $LiAlH_4$ of dienoic acid prepared by the Doebner synthesis, followed by oxidation of the resulting dienol with MnO_2 to the corresponding 2,4-dienol[7]	By direct hydrogenation of the corresponding acetylenic acetal, using a palladium/calcium carbonate catalyst (2-*cis*,6-*cis*-form)[6]
Natural occurrence	Reported found in the oxidized flavor of skim milk;[8] in peas by enzymatic formation from lipids;[9] in salmon oil;[10] in sunflower oil (*cis*-, *trans*-, and *trans*, *trans*-form);[11] in the autooxidation of lard;[12] in frozen peas;[13] in tomatoes;[14] and as a volatile component in fish products[15]	
Reported uses[3]	Baked goods 0.20 ppm Condiments 0.20 ppm Meat, meat sauces, soups 0.20 ppm Milk, dairy products 0.20 ppm Cereals 0.20 ppm	Ice cream, ices, etc. 0.1 ppm Candy 0.1 ppm Condiments, pickles 0.1 ppm Meat, meat sauces, soups 0.1 ppm
Regulatory status	FEMA No. 3212	FEMA No. 3378

REFERENCES

For References 1–5, see end of Part III

6. Pippen and Nonaka, *J. Org. Chem.*, 23, 1580, 1958.
7. Forss and Hancox, *Aust. J. Chem.*, 9, 420, 1956.
8. Forss, Pont and Stark, *J. Dairy Res.*, 22, 345, 1955.
9. Grosch, *Z. Lebensm. Unters. Forsch.*, 135(2), 75, 1967; *Chem. Abstr.*, 68, 58612w, 1968.
10. Wyatt and Day, *J. Food Sci.*, 28, 305, 1963.
11. Swoboda and Lee, *J. Sci. Food Agric.*, 16(11), 680, 1965.
12. Gaddis, Ellis and Curie, *J. Am. Oil Chem. Soc.*, 43(3), 147, 1966.
13. Whitfield and Shipton, *J. Food Sci.*, 31(3), 328, 1966.
14. Buttery et al., *J. Agric. Food Chem.*, 19(3), 524, 1971.
15. *J. Chromatogr.*, 61(1), 133, 1971.
16. Sandheimer, *J. Am. Chem. Soc.*, 74, 4040, 1952.

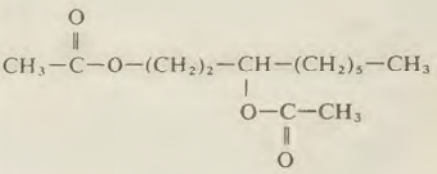
	2,6-Nonadien-1-ol	γ-Nonalactone
Other names	"Cucumber alcohol" Nonadienol *trans*-2-*cis*-6-Nonadienol (natural) *trans*-2-*trans*-6-Nonadienol (synthetic) "Violet leaf alcohol"	Aldehyde C-18 (so called) γ-Amyl butyrolactone Coconut aldehyde 4-Hydroxynonanoic acid, γ-lactone Nonanolide-1,4 Prunolide[10]*
Empirical formula	$C_9H_{16}O$	$C_9H_{16}O_6$
Structure	$CH_3-CH_2-CH=CH-(CH_2)_2-CH=CH-CH_2OH$	
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless to very pale, straw-yellow liquid
Assay		97% min[2] (98%)
Molecular weight	140.23	156.23
Boiling point	96–98°C (196°C) at 12 mm Hg	243°C
Flash point		>100°C (132°C)
Specific gravity	0.87	0.958–0.966 at 25°/25°C;[2] 0.969–0.971 at 15°/15°C
Refractive index		1.4460–1.4500[2] (1.4465–1.4480) at 20°C
Acid value		Not more than 5[2]
Solubility	Very slightly soluble in water; soluble in alcohol, propylene glycol, and essential oils	1:5 in 50% alcohol;[2] 1:2 in 60% alcohol; insoluble in water; soluble in most common organic solvents
Organoleptic characteristics		Strong odor reminiscent of coconut; fatty, peculiar taste
Synthesis	Prepared from naturally occurring 3-hexen-1-ol (leaf alcohol)[6] to yield the natural *trans*-2-*cis* form, or from synthetic hexenol to yield the *trans*-2-*trans* form	By reacting methylacrylate and hexanol in the presence of ditertiarybutyl peroxide; by condensation of undecylenic acid and malonic acid; by lactonization of nonenoic acid
Natural occurrence	Originally isolated in the oils of violet leaf[7] and violet flowers[8] (hence, the name "violet leaf alcohol"). Its structure has been studied by L. Ružička.[9] It has been isolated also in cucumber.[10]	Reported found in nature—peaches and apricots,[11] roasted barley,[12] rum,[13] and tomato[14]
Reported uses[3]	Non-alcoholic beverages 0.01 ppm Alcoholic beverages 0.01 ppm Ice cream, ices, etc. 0.05 ppm Candy 0.05–0.50 ppm Baked goods 0.01 ppm	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 14 ppm Candy 33 ppm Baked goods 55 ppm Gelatins and puddings 28 ppm Chewing gum 15 ppm Icings 25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2780	FDA 121.1164; FEMA No. 2781

* Givaudan-Delawanna, Inc., 330 W. 42nd St., New York, N.Y.

REFERENCES

For References 1–5, see end of Part III.

6. Takei et al., *Chem. Zentralbl.*, 2, 3396, 1938.
7. Ružička and Schinz, *Helv. Chim. Acta*, 18, 381, 1935.
8. Ružička, *Chem. Zentralbl.*, 2, 3170, 1938.
9. Ružička et al., *Helv. Chim. Acta*, 27, 1561, 1944.
10. Takei et al., *Chem. Zentralbl.*, 2, 3705, 1939.
11. Ruys, *Fr. Ses Parfums*, 9(47), 34, 1966.
12. Wang et al., *J. Agric. Biol. Chem.*, 34(4), 561, 1970.
13. Liebich et al., *J. Chromatogr.*, 8, 527, 1970.
14. Buttery et al., *J. Agric. Food Chem.*, 19(13), 524, 1971.

	n-Nonanal	1,3-Nonanediol acetate, mixed esters
Other names	Aldehyde C-9 Nonanoic aldehyde *n*-Nonyl aldehyde α-Oxononane Pelargonic aldehyde	Hexylene glycol diacetate 3-Hexyl-1,3-propanediol acetate, mixed esters Nonanediol-1,3-acetate "Octylcrotonyl acetate" *Also:* diacetate; diasmol; diasmylacetate; drago-jasimia; jasmelia; jasmonyl; jersemal; nonane; tepylacetate; ysminia
Empirical formula	$C_9H_{18}O$	$C_{13}H_{24}O_4$
Structure	$CH_3-(CH_2)_7-CHO$	
Physical/chemical characteristics[5]		
Appearance	Colorless to light-yellow liquid	Colorless to slightly yellow liquid
Assay	92% min[2]	
Molecular weight	142.24	244.34
Boiling point	91–92°C (191°C) at 22 mm Hg	
Flash point		>100°C
Specific gravity	0.820–0.830 at 25°/25°C;[2] 0.8280 at 16°C	0.964–0.970 (0.960–0.970) at 25°/25°C
Refractive index	1.4220–1.4290 at 20°C;[2] 1.4274 at 18°C	1.4410–1.4450 (1.4400–1.4500) at 20°C
Saponification value		280–320 (300–330)
Acid value	Not more than 10[2]	1 max
Solubility	Soluble in alcohol and most common organic solvents; 1:3 in 70% alcohol; insoluble in water	1:4 in 60% alcohol; 1:2 in 70% alcohol; slightly soluble in water
Organoleptic characteristics	Strong, fatty odor developing an orange and rose note on dilution; fatty, citrus-like flavor	Intense floral odor reminiscent of jasmine
Synthesis	By catalytic oxidation of the corresponding alcohol (*n*-nonanol) or reduction of the corresponding acid	The commercial product is a mixture of the two possible isomers; the starting material is usually 1-octene
Natural occurrence	Reported as a constituent in the oils of sweet and bitter orange, mandarin, lemon, lime, orris, Ceylon cinnamon, ginger, *Xanthoxylum rhetsa*, rose,[6] and clary sage;[7] in the turpentines from *Pinus jeffreyi* Grev. and Balf., *Pinus sabiniana* Dangl., and others	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 1.3 ppm Candy 4.1 ppm Baked goods 2.3 ppm Gelatins and puddings 6.0 ppm Chewing gum 0.20–38 ppm	Non-alcoholic beverages 0.30–1.0 ppm Ice cream, ices, etc. 0.50–1.0 ppm Candy 1.5–6.0 ppm Baked goods 1.5–4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2782	FDA 121.1164; FEMA No. 2783

REFERENCES

For References 1–5, see end of Part III.

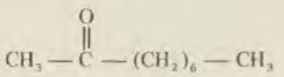
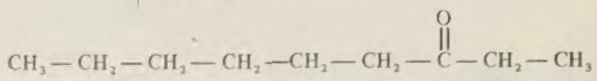
6. Calvarano, *Essenze Deriv. Agrum.*, 28, 157, 1958.
7. Tesseire, *Recherches*, 9, 10, 1959.

	Nonanoic acid	2-Nonanol
Other names	Nonoic acid *n*-Nonylic acid Octane-1-carboxylic acid Pelargonic acid	Methyl *n*-heptyl carbinol
Empirical formula	$C_9H_{18}O_2$	$C_9H_{20}O$
Structure	$CH_3-(CH_2)_7-COOH$	$CH_3-(CH_2)_6-\underset{\displaystyle OH}{\underset{\vert}{CH}}-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Assay	>98%	
Molecular weight	158.24	144.26
Melting point	9°C	
Boiling point	255.6°C	*d*-, 105°C at 19 mm Hg *dl*-, 193–194°C *dl*-, 91°C at 12 mm Hg
Congealing point	>12.24°C	-35°C
Specific gravity	0.90552 at 20°C	*d*-, 0.8230 at 20°C *dl*-, 0.8471 at 20°C
Refractive index	1.4379 at 20°C	*d*-, 1.4299 at 20°C
Optical rotation		+8.98° at 19°C
Solubility	1:8 in 50% alcohol; 1:3 in 60% alcohol; insoluble in water; soluble in most organic solvents	Insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Fatty, characteristic odor; corresponding unpleasant taste	Powerful fruity-green odor
Synthesis	By oxidation of methylnonyl ketone; by oxidation of oleic acid; or from heptyl iodide via malonic ester synthesis	From nonene[10]
Natural occurrence	Reported found in several essential oils, either free or esterified: rose, geranium, orris, *Litsea cubeba*, *Artemisia arborescens* L., hops, *Chamaecyparis pisifera* Endl.,[6] *Eremocitrus glauca* L.,[7] French lavender,[8] and in oak musk[9]	Reported found in *Ruta pinnata* leaf oil[11] and in coconut oil[12]
Reported uses[3]	Non-alcoholic beverages 1.8 ppm Ice cream, ices, etc. 7.8 ppm Candy 6.6 ppm Baked goods 13 ppm Shortening 10 ppm	Baked goods 15.0 ppm Condiments, pickles 80.0 ppm Dips, spreads 12.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2784	FEMA No. 3315

REFERENCES

For References 1–5, see end of Part III.

6. Uchida, *Chem. Zentralbl.*, 2, 1577, 2198, 1928.
7. Hitchcock and Jones, *Chem. Zentralbl.*, 1, 2281, 1937.
8. Seidel et al., *Helv. Chim. Acta*, 27, 663, 1944.
9. Stoll and Scherrer, *Chem. Zentralbl.*, 2, 2512, 1938.
10. Kulesza et al., *Riechst. Aromen Koerperpflegem.*, 19(1), 8, 1969.
11. Estevez-Reyes and Gonzalez-Gonzalez, *An. Quim.*, 66(2), 167, 1970; 73:48483, 1970.
12. Jasperson and Jones, *J. Soc. Chem. Ind.*, 66, 15, 1967.

	2-Nonanone	3-Nonanone
Other names	Methyl heptyl ketone	Ethyl hexyl ketone 3-Oxononanone
Empirical formula	$C_9H_{18}O$	$C_9H_{18}O$
Structure		
Physical/chemical characteristics		
Appearance	Colorless, oily liquid; solidifies when cold	
Molecular weight	142.24	142
Melting point	-15°C	
Boiling point	194–196°C	190°C 80°C at 20 mm Hg
Congealing point		-8°C
Specific gravity	0.8317 at 20°C	0.825 at 20°C
Refractive index	1.4175 at 20°C	1.4208 at 20°C
Solubility	Insoluble in water; soluble in alcohol	
Organoleptic characteristics	Characteristic rue odor; rose and tea-like flavor	
Synthesis	By dry distillation of barium caprylate and barium acetate at 0.5–2 mm Hg;[6] or by oxidation of methyl heptyl carbinol at room temperature using chromic acid.[7] It can be isolated also from natural products by fractional distillation	By prolonged boiling of *o*-propionic acid triethyl ester with excess hexylmagnesium bromide in ether under a nitrogen atmosphere[12]
Natural occurrence	Reported found in the essential oil of rue (*Ruta angustifolia* Pers., *R. Bracteosa, R. montana* L., and *R. gravelolens*). Also identified in the oil of carnation,[8] in coconut oil,[9] and in the distillate from leaves of a variety of *Boronia ledifolia*.[10] Reported found in mixture with methyl nonyl ketone in the essential oil of *Ruta chalepensis*.[11]	In banana,[13] passion fruit,[14] and cooked beef[15]
Reported uses[3]	Non-alcoholic beverages 0.55 ppm Ice cream, ices, etc. 0.10–1.0 ppm Candy 0.40–4.0 ppm Baked goods 0.40–4.0 ppm	Non-alcoholic beverages 20 ppm Alcoholic beverages 20 ppm Candy 20 ppm Baked goods 20 ppm Gelatins and puddings 20 ppm Chewing gum 20 ppm Milk, dairy products 20 ppm Cereals 20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2785	FEMA No. 3440

REFERENCES

For References 1–5, see end of Part III.

6. Morgan and Holmes, *J. Chem. Ind.*, 44, 109T; *Chem. Zentralbl.*, 1, 2215, 1925.
7. Van Gysegem, *Chem. Zentralbl.*, 1, 530, 1907.
8. Schimmel and Co., *Chem. Zentralbl.*, 1, 1086, 1903.
9. Haller et al., *Chem. Zentralbl.*, 2, 28, 1910.
10. Penfold and Morrison, *Chem. Abstr.*, 43, 3148, 1949.
11. Costa and do Vale, *Chem. Abstr.*, 48, 11732, 1954.
12. Barré, *Can. J. Res.*, 27, 65, 1949.
13. Tressl et al., *Z. Naturforsch.*, Teil B, 24, 781, 1969.
14. Winter et al., *Helv. Chim. Acta*, 55, 1916, 1972.
15. Chang, Proceedings, 3rd Nordic Aroma Symposium, Hameenlinna, Finland, 1972, 203.

	3-Nonanon-l-yl acetate	2-Nonenal
Other names	"Compound 1051" 1-Hydroxy-3-nonanone acetate "Ketone alcohol ester" Methylol methyl hexyl ketone acetate 3-Oxononanyl acetate	3-Hexylacrolein β-Hexylacrolein Iris aldehyde® α-Nonenyl aldehyde Heptylidene aldehyde
Empirical formula	$C_{11}H_{20}O_3$	$C_9H_{16}O$
Structure	$CH_3(CH_2)_5-\overset{\overset{O}{\|}}{C}-CH_2-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_3$	$CH_3-(CH_2)_6-CH=CH-CHO$
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Almost colorless or pale straw-colored oily liquid; readily oxidizes to noneoic acid on exposure to air
Molecular weight	200.28	140.23
Boiling point		189°C 56–58°C at 0.1 mm Hg
Specific gravity		0.8418 at 25°C
Refractive index		1.4502 at 25°C
Solubility	Very slightly soluble in water; soluble in alcohol, propylene glycol, and oils	Insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Herbaceous, fruity odor	Very powerful, penetrating fatty odor in concentrated form; orris-like, waxy, and quite pleasant on dilution; odor reminiscent of dried orange peels
Synthesis	By condensation of methyl hexyl ketone with formaldehyde under mild alkaline conditions to yield β-ketol, which is subsequently acetylated	By oxidation of 9,10,12-trihydroxystearic acid (Criegee reaction)[6]
Natural occurrence	Not reported found in nature	Reported found in orris oil
Reported uses[3]	Non-alcoholic beverages 0.30 ppm Ice cream, ices, etc. 0.30 ppm Candy 0.80–5.0 ppm Baked goods 1.0 ppm Condiments 10 ppm	Baked goods 0.20 ppm Condiments 0.20 ppm Meat, meat sauces, soups 0.20 ppm Milk, dairy products 0.20 ppm Cereals 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2786 3-Nonanon-l-yl acetate has been found actually to consist of a mixture of three related compounds. In view of this, it is being dropped from the GRAS list pending possible future review by an expert panel.[7]	FEMA No. 3213

REFERENCES

For References 1–5, see end of Part III.

6. Scaulan and Swern, *J. Am. Chem. Soc.*, 62, 2309, 1940.
7. Hall and Oser, *Food Technol.*, 24, 533, 1970.

	trans-2-Nonen-1-ol	Nonyl acetate
Other names		Acetate C-9 Nonanol acetate *n*-Nonyl acetate Pelargonyl acetate
Empirical formula	$C_9H_{18}O$	$C_{11}H_{22}O_2$
Structure	$CH_3-(CH_2)_5-CH=CH-CH_2OH$	$CH_3(CH_2)_8-O-\overset{\overset{O}{\|}}{C}-CH_3$
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Assay		97% min
Molecular weight	142.23	186.30
Boiling point	108–110°C at 17 mm Hg	212°C
Specific gravity	0.845 at 15°C	0.864–0.868 at 25°C; 0.8785 at 15°C
Refractive index	1.4476 at 15°C	1.4220–1.4260 (1.4328) at 20°C
Solubility		1:1 in 80% alcohol; 1:6 in 70% alcohol
Organoleptic characteristics		Floral, fruity (mushroom-gardenia) odor; corresponding flavor on dilution; bitter taste when concentrated
Synthesis	By hydrolysis of the corresponding acetate; the acetate is prepared from 1-bromo-2-nonene and acetic anhydride in acetic acid solution[6]	By direct esterification of *n*-nonyl alcohol with acetic acid
Natural occurrence	Reported found as a volatile component in Cucurbitaceae (cucumber, squash, pumpkin, etc.)[7,8]	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 0.15 ppm Ice cream, ices, etc. 0.15 ppm Candy 0.2 ppm Baked goods 0.2 ppm Gelatins and puddings 0.15 ppm Meat, meat sauces, soups 0.15 ppm	Non-alcoholic beverages 0.81 ppm Ice cream, ices, etc. 0.81 ppm Candy 1.9 ppm Baked goods 3.1 ppm
Regulatory status	FEMA No. 3379	FDA 121.1164; FEMA No. 2788

REFERENCES

For References 1–5, see end of Part III.

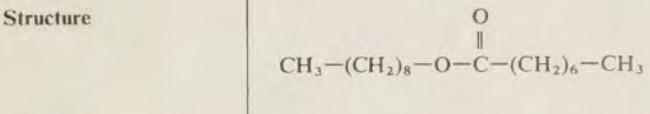
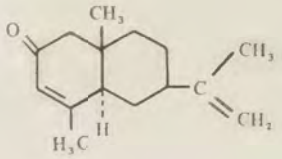
6. Delaby and Guillot-Allègre, *Bull. Soc. Chim. Fr.*, [4] 53, 307, 1933.
7. Kemp, Stoltz and Knavel, *J. Agric. Food Chem.*, 20, 196, 1972.
8. Kemp, Knavel and Stoltz, *Phytochemistry*, 10(8), 1925, 1971.

	Nonyl alcohol	Nonyl isovalerate
Other names	Alcohol C-9 Nonanol-1 1-Nonanol Octyl carbinol Pelargonic alcohol	Nonanol isopentanoate
Empirical formula	$C_9H_{20}O$	$C_{14}H_{28}O_2$
Structure	$CH_3-(CH_2)_7-CH_2OH$	$CH_3(CH_2)_8-O-\overset{\overset{O}{\|}}{C}-CH_2-\underset{\underset{CH_3}{\diagdown}}{\overset{\overset{CH_3}{\diagup}}{CH}}$
Physical/chemical characteristics[5]		
Appearance	Colorless, mobile liquid	Colorless liquid
Assay	97% min	
Molecular weight	144.26	228.37
Melting point	−5°C	
Boiling point	213.5–215°C	264°C
Flash point	82°C	
Specific gravity	0.824–0.830 at 25°C; 0.8274 at 20°C	
Refractive index	1.4310–1.4350 (1.43347) at 20°C	
Solubility	Very slightly soluble in water; soluble in most common organic solvents; 1:3 in 60% alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic rose-orange odor; slightly fatty, bitter taste reminiscent of orange	Heavy fruit odor (apple-hazelnut with citrus notes); sweet, warm, floral taste
Synthesis	By reduction of ethyl pelargonate; from heptaldehyde via heptanol and heptylmagnesium bromide with ethylene oxide	By esterification of *n*-nonanol with isovaleric acid
Natural occurrence	Reported as occurring frequently in nature, free or esterified; in the essential oils of grapefruit, Guinea sweet orange, Italian and Israeli sweet orange, bitter orange;[6] in oak musk concrete and others. It has been identified also in cheese.	In rue (*Ruta graveolens* L.)
Reported uses[3]	Non-alcoholic beverages 0.70 ppm Ice cream, ices, etc. 0.61 ppm Candy 2.0 ppm Baked goods 1.9 ppm Chewing gum 18 ppm	Non-alcoholic beverages 0.50–1.0 ppm Ice cream, ices, etc. 0.50 ppm Candy 1.0–2.0 ppm Baked goods 1.4 ppm
Regulatory status	FDA 121.1164; FEMA No. 2789	FDA 121.1164; FEMA No. 2791

REFERENCES

For References 1–5, see end of Part III.

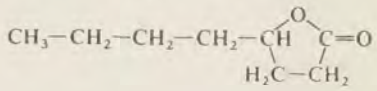
6. **Mehlitz and Minas,** *Ind. Obst Gemueseverwert.*, 50, 861, 1965.

	Nonyl octanoate	Nootkatone
Other names	Nonyl caprylate *n*-Nonyl octoate Nonyl octylate	4,4a,5,6,7,8-Hexahydro-6-isopropenyl-4,4a-dimethyl-2(3H)-naphthalenone 4a,5-Dimethyl-1,2,3,4,4a,5,6,7-keto-3-isopropenyl-naphthalene 5,6-Dimethyl-8-isopropenylbicyclo-(4,4,0)-dec-1-en-3-one
Empirical formula	$C_{17}H_{34}O_2$	$C_{15}H_{22}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Crystals (from light petroleum fractions)
Molecular weight	270.46	218.34
Melting point		36 - 37°C
Boiling point	315°C	
Specific gravity	0.86	
Optical rotation		195.5° (c = 1.5 in chloroform)
Solubility	Insoluble in water; soluble in alcohol	Practically insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Sweet, rose odor with a mushroom note; very powerful flavor	Pleasant taste
Synthesis	By esterification of *n*-nonanol with *n*-octanoic acid	By oxidation of valencene (a sesquiterpene) with tertiary butyl chromate[6]
Natural occurrence	This ester is found in bitter orange oil	Reported found in grapefruit oil and juice; traces are also reported found in the oils of bergamot, lemon, lime, orange, and tangerine;[7] also reported formed in canned orange juice on storage[8]
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Baked goods 0.06 ppm	Non-alcoholic beverages 10.0 ppm Candy 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2790	FEMA No. 3166

REFERENCES

For References 1–5, see end of Part III.

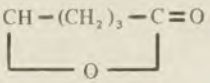
6. *J. Food Sci.*, 30, 876, 1965.
7. *J. Food Sci.*, 29, 565, 1964.
8. *Dfsh. Lebensm. Rundsch.*, 68(6), 173, 1972.

	9,12-Octadecadienoic acid (48%) plus 9,12,15-octadecatrienoic acid (52%)	γ-Octalactone
Other names	Methyl linoleate (48%) and methyl linolenate (52%) mixture	γ-*n*-Butyl-γ-butyrolactone 4-Hydroxyoctanoic acid, γ-lactone *n*-Octalactone Octanolide-1,4
Empirical formula	$C_{19}H_{34}O_2$ (48%) $C_{19}H_{32}O_2$ (52%)	$C_8H_{14}O_2$
Structure	$CH_3(CH_2)_4CH=CHCH_2CH=CH-(CH_2)_7-COOCH_3$ [48%] $CH_3CH_2CH=CHCH_2CH=CHCH_2CH=CH-(CH_2)_7-COOCH_3$ [52%]	
Physical/chemical characteristics[5]		
Appearance	Colorless oil	Slightly yellow liquid
Assay		95% min
Molecular weight	294.46 (48%) 292.44 (52%)	142.20
Boiling point		132–133°C at 20 mm Hg; 83–86°C at 1 mm Hg (234°C)
Flash point		>100°C
Specific gravity		0.970–0.980 at 25°/25°C
Refractive index		1.443–1.447 at 20°C; 1.4610 at 15°C
Acid value		8 max
Solubility	Miscible in fats, oil, and most organic solvents	1:3 in 50% alcohol; 1:2 in 60% alcohol; 1:3 in 70% alcohol; slightly soluble in water; somewhat soluble in propylene glycol
Organoleptic characteristics		Strong, fruity odor reminiscent of coconut; very sweet taste
Synthesis	Prepared from safflower seed oil[6]	Prepared synthetically from epoxy-1,2-hexane and sodio-malonic ester. After saponification the oxyacid is extracted with ether and is lactonized.
Natural occurrence	In safflower seed[6]	Reported found in apricots and peaches[7]
Reported uses[3]	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 10 ppm Candy 10 ppm Baked goods 10 ppm Gelatins and puddings 10 ppm Condiments 10 ppm Jellies, preserves, spreads 10 ppm	Non-alcoholic beverages 4.8 ppm Ice cream, ices, etc. 16 ppm Candy 16 ppm Baked goods 17 ppm Gelatins and puddings 15 ppm Syrups 57 ppm
Regulatory status	FEMA No. 3411	FDA 121.1164; FEMA No. 2796

REFERENCES

For References 1–5, see end of Part III.

6. **Parker et al.,** *Biochem. Prep.*, 4, 88, (1955).
7. **Ruys,** *Fr. Ses Parfums*, 47(9), 34, 1966.

	Δ-Octalactone
Other names	Tetrahydro-6-propyl-5-hydroxy-2H-pyran-2-one Octanoic acid, Δ-lactone
Empirical formula	$C_8H_{14}O_2$
Structure	
Physical/chemical characteristics[5]	
Molecular weight	142.20
Boiling point	115–117°C at 12 mm Hg 104°C at 3 mm Hg
Specific gravity	0.972 at 25°C
Refractive index	1.4480 at 25°C
Synthesis	From 5-hydroxyoctanoic acid by reduction with $NaBH_4$ in water;[6] by microbiological reduction of the corresponding keto acid;[7,8] from 5-hydroxyoctanoic methyl amide by alkaline saponification, using $Ba(OH)_2$.[9]
Natural occurrence	Reported found as a volatile flavor component in coconut oil,[10] in butterfat,[11] in milk fat,[12,13] in the essence of the Blenheim variety of apricot,[14] and in pineapple;[15] also reported found in yellow passion fruit[16]
Reported uses[3]	Non-alcoholic beverages 20.0 ppm Ice cream, ices, etc. 20.0 ppm Candy 20.0 ppm Baked goods 20.0 ppm Gelatins and puddings 20.0 ppm Margarine 20.0 ppm Salad oil 20.0 ppm Shortening 20.0 ppm
Regulatory status	FEMA No. 3214

REFERENCES

For References 1–5, see end of Part III.

6. Stetter and Dierichs, *Chem. Abstr.*, 46, 7520d, 1952.
7. U.S. Patent 3,076,750, assigned to Lever Brothers Co.; *Chem. Abstr.*, 58, P11928e, 1963.
8. Muys, van der Ven and de Jouge, *Appl. Microbiol.*, 11(5), 389, 1963.
9. Lukěs and Cerný, *Collect. Czech. Chem. Commun.*, 24, 2722, 1959.
10. Allen, *Chem. Ind.* (London), 36, 1560, 1965.
11. van Beers and van der Zijden, *Rev. Fr. Corps Gras*, 13(7), 463, 1966; *Chem. Abstr.*, 65, 6194a, 1967.
12. Khatsi, Libbey and Day, *J. Agric. Food Chem.*, 14(5), 465, 1966.
13. Wyatt, Pereira and Day, *Lipids*, 2(3), 208, 1967.
14. Tang and Jennings, *J. Agric. Food Chem.*, 16(2), 252, 1968.
15. Naf-Müller and Willhalm, *Helv. Chim. Acta*, 54(7), 1880, 1971.
16. Winter and Klöty, *Helv. Chim. Acta*, 55(6), 1916, 1972.

	n-Octanal	Octanal dimethyl acetal
Other names	Aldehyde C-8 Caprylaldehyde Caprylic aldehyde *n*-Octaldehyde *n*-Octylaldehyde	Aldehyde C-8 dimethyl acetal Caprylaldehyde dimethyl acetal 1,1-Dimethoxy octane Octaldehyde dimethyl acetal
Empirical formula	$C_8H_{16}O$	$C_{10}H_{22}O_2$
Structure	$CH_3-(CH_2)_6-CHO$	$CH_3-(CH_2)_6-CH(O-CH_3)_2$
Physical/chemical characteristics[5]		
Appearance	Colorless to light-yellow liquid	Colorless liquid
Assay	92% min[2]	
Molecular weight	128.22	174.29
Boiling point	171–173°C	185°C
Flash point	54°C	
Specific gravity	0.818–0.830 at 25/25°C;[2] 0.8211 at 20°C	0.86
Refractive index	1.4170–1.4250[2] (1.42167) at 20°C	1.4153 at 22.5°C
Acid value	Not more than 10[2]	
Solubility	Soluble in alcohol and most common organic solvents; 1:2 in 70% alcohol; insoluble in water	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Sharp, fatty, fruity odor; characteristic pungent, fatty flavor	Characteristic woody aroma reminiscent of cognac
Synthesis	By oxidation of the corresponding alcohol or reduction of the corresponding acid; also from coconut fatty acids via methyl-*n*-octoate	By condensation of octaldehyde with methanol using dry HCl as a dehydrating agent
Natural occurrence	Reported found in the essential oils of: sweet orange, bitter orange, mandarin, tangerine, grapefruit, Mexican lime, lemon, Taiwan citronella, rose, lemongrass, *Pinus sabiniana*, *Pinus jeffreyi*, *Xanthoxylum rhetsa*,[6] lime petitgrain,[7] clary sage,[8] lavandin, and others	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 1.6 ppm Candy 3.4 ppm Baked goods 4.4 ppm Gelatins and puddings 3.0–6.1 ppm Chewing gum 0.10 ppm	Non-alcoholic beverages 0.74 ppm Alcoholic beverages 3.0 ppm Ice cream, ices, etc. 0.78 ppm Candy 2.8 ppm Baked goods 2.8 ppm
Regulatory status	FDA 121.1164; FEMA No. 2797	FDA 121.1164; FEMA No. 2798

REFERENCES

For References 1–5, see end of Part III.

6. **Naves**, *Chem. Abstr.*, 45, 4889, 1951.
7. **Peyron**, *Fr. Ses Parfums*, 6(1), 17, 1958.
8. **Tesseire**, *Recherches*, 9, 10, 1959.

	Octanoic acid	1-Octanol
Other names	Caprylic acid C-8 acid *n*-Octoic acid *n*-Octylic acid	Alcohol C-8 *n*-Caprylic alcohol Heptyl carbinol Octyl alcohol
Empirical formula	$C_8H_{16}O_2$	$C_8H_{18}O$
Structure	$CH_3-(CH_2)_6-COOH$	$CH_3-(CH_2)_6-CH_2OH$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid; solidifies to leafy crystals when cold	Colorless liquid
Assay		98% min[2]
Molecular weight	144.21	130.23
Melting point	16.3°C (17°C)	−15.4 to −16.3°C
Boiling point	239.7°C	194–195.2°C
Flash point		>84.5°C
Specific gravity	0.90884 at 20°C	0.822–0.830 at 25/25°C;[2] 0.8246–0.8270 at 20°C
Refractive index	1.4335 (1.4327) at 20°C	1.4280–1.4310[2] (1.42920) at 20°C
Acid value		Not more than 1[2]
Solubility	Almost insoluble in cold water; 1:400 in hot water; soluble in alcohol, ether, chloroform, and others	1:5 in 50% alcohol;[2] 1:3 in 60% alcohol; 0.05% in water; soluble in propylene glycol
Organoleptic characteristics	Faint, fruity-acid odor; slightly sour taste	Fresh, orange-rose odor, quite sweet; oily, sweet, slightly herbaceous taste
Synthesis	By fermentation and fractional distillation of the volatile fatty acids present in coconut oil	By reduction of some caprylic esters such as methyl caprylate with sodium ethoxide
Natural occurrence	Reported as frequently occurring naturally in the essential oils of: *Cupressus torulosa*, *Cryptomeria japonica*, *Andropogon iwarancusa*, *Cymbopogon javanensis*, camphor, nutmeg, lemon grass, lime, tobacco (flowers), *Artemisia herba-alba*, camomile, hops, and others; also reported in apple aroma, coconut oil as glyceride, and wine as an ester. It has been identified (free and esterified) among the constituents of petitgrain lemon oil.[6]	Reported as frequently occurring in essential oils as an ester. The free alcohol has been reported found in the essential oils of: green tea, grapefruit, California orange, *Andropogon intermedius*, *Heracleum villosum*, violet leaves, *Anethum graveolens*, and bitter orange[6]
Reported uses[3]	Non-alcoholic beverages 2.9 ppm Ice cream, ices, etc. 2.0 ppm Candy 13 ppm Baked goods 18 ppm Condiments 12 ppm	Non-alcoholic beverages 2.9 ppm Ice cream, ices, etc. 0.91 ppm Candy 2.8 ppm Baked goods 3.0 ppm Gelatins and puddings 1.5 ppm Chewing gum 16–57 ppm
Regulatory status	FDA 121.1164; FEMA No. 2799	FDA 121.1164; FEMA No. 2800

REFERENCES

For References 1–5, see end of Part III.

6. Peyron, *Riv. Ital. EPPOS*, 8, 413, 1965.
7. Mehlitz and Minas, *Ind. Obst Gemueseverwert.*, 50, 861, 1965.

	2-Octanol	3-Octanol
Other names	*sec*-Capryl alcohol Methyl hexyl carbinol Hexyl methyl carbinol *sec-n*-Octyl alcohol	Amyl ethyl carbinol Ethyl *n*-amyl carbinol *d-n*-Octanol
Empirical formula	$C_8H_{18}O$	$C_8H_{18}O$
Structure	$CH_3-(CH_2)_5-\underset{\displaystyle OH}{\underset{\vert}{CH}}-CH_3$	$CH_3-CH_2-\underset{\displaystyle OH}{\underset{\vert}{CH}}-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Molecular weight	130.23	130.23
Melting point	−38.6°C	
Boiling point	*dl*-, 180°C; *l*-, 80°C at 11 mm Hg	178.5–179.5°C
Specific gravity	0.8193 at 20°C; *d*-, 0.8170 at 25°C	0.8247 at 20°C
Refractive index	1.42444 at 20°C; *l*-, 1.4256; *d*-, 1.4256	1.4252 at 20°C
Optical rotation	*l*-, −9.84°; *d*-, −9.79	+11.3° at 20°C; 0.9791 gm in 20 cc alcohol +10.20° at 20°C; 1.0196 gm in 20 cc benzene
Solubility	Soluble in most common organic solvents	Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic disagreeable but aromatic odor	Sweet, nutty, warm, herbaceous odor
Synthesis	By distilling sodium ricinoleate with an excess of sodium hydroxide[6-10]	Can be prepared in the racemic form by reduction of ethyl-*n*-amyl ketone with sodium in ether solution[12]
Natural occurrence	Two optically active isomers of the alcohol have been found. Reported in the oil of Reunion geranium;[11] also identified in a few species of mint and lavender	It has been identified (free and esterified) in a variety of mint;[13] also reported in lavender[14] and the essential oils of *Mentha arvensis* var. *piperascens*[15] and *Mentha spicata*[16]
Reported uses[3]	Ice cream, ices, etc 0.60 ppm Candy 3.0 ppm Baked goods 4.0 ppm Gelatins and puddings 2.0 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2801	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.

6. Bouis, *Annalen*, 80, 303, 1851; 92, 395, 1854; 97, 34, 1855.
7. Moschnin, *Annalen*, 87, 111, 1853.
8. Schorlemmer, *Annalen*, 147, 222, 1868.
9. Neison, *J. Chem. Soc.* (London), 27, 507, 837, 1874.
10. Freund and Schonfeld, *Ber. Dtsch. Chem. Ges.*, 24, 3352, 1891.
11. Bohnsack, *Ber. Dtsch. Chem. Ges.*, 75, 502, 1942.
12. Pickard and Kenyon, *J. Chem. Soc. Fr.*, 103, 1923, 1913.
13. Naves, *Helv. Chim. Acta*, 26, 1034, 1943.
14. Benezet, *Chem. Abstr.*, 40, 6757, 1946.
15. Carnero, Benezet and Igolen, *Chem. Abstr.*, 43, 4427, 1949.
16. Bryan, Burnett and Wearn, *J. Am. Chem. Soc.*, 73, 1848, 1951.

	2-Octanone	3-Octanone
Other names	*n*-Hexyl methyl ketone Methyl hexyl ketone	Amyl ethyl ketone E.A.K. Ethyl amyl ketone Ethyl-*n*-amyl ketone
Empirical formula	$C_8H_{16}O$	$C_8H_{16}O$
Structure	$CH_3-\overset{\overset{O}{\|}}{C}-C_6H_{13}$	$CH_3-CH_2-\overset{\overset{O}{\|}}{C}-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, mobile liquid
Assay	98% min	98% min
Molecular weight	128.21	128.21
Boiling point	175°C (172–173°C) 16°C	169–170°C (172°C)
Flash point	61°C	Approx 50°C
Specific gravity	0.8225–0.8255 at 15°C; 0.8185 at 20°C	0.817–0.821 at 23°C; 0.8254 at 15°C
Refractive index	1.4150–1.4165 at 20°C; 1.41613 at 20°C	1.4130–1.4170 (1.41536) at 20°C
Acid value	0.9 max	
Solubility	1:9–12 in 50% alcohol; 1:1–1.7 in 70% alcohol. Forms azeotropes with: *d*-limonene (57%), phenol (32%), phenethyl alcohol (5%), *o*-cresol (12%), ethylene glycol (76%), and cineol (55%)	1:7 in 60% alcohol; 1:3 in 70% alcohol; soluble in most common organic solvents; almost insoluble in water
Organoleptic characteristics	Floral and bitter, green, fruity (unripe apple) odor; bitter, camphoraceous taste	Strong, penetrating, fruity odor reminiscent of lavender
Synthesis	By oxidation of methyl hexyl carbinol with $K_2Cr_2O_7$ and sulfuric acid;[11] also by oxidation of 2-octanol over zinc oxide at 330–340°C[12]	It can be prepared by passing a mixture of vapors of caproic acid and acetic acid over ThO_2 at 400°C,[6] or by oxidation of *d*-ethyl *n*-amyl carbinol with chromates. Another synthetic route is reported.[7]
Natural occurrence	Reported found in small quantities in the essential oil of *Ruta montana* L.[13] and in a few varieties of banana and citrus fruits	Reported identified in the low-boiling fraction of the essential oil of lavender;[8] also reported found in the essential oils of *Lavandula vera* (10%)[9] and French lavender[10]
Reported uses[3]	Non-alcoholic beverages 0.10–1.0 ppm Ice cream, ices, etc. 0.20–1.0 ppm Candy 0.40–4.0 ppm Baked goods 0.40–4.0 ppm	Non-alcoholic beverages 3.3 ppm Ice cream, ices, etc. 10 ppm Candy 11 ppm Baked goods 11 ppm
Regulatory status	FDA 121.1164; FEMA No. 2802	FDA 121.1164; FEMA No. 2803

REFERENCES

For References 1–5, see end of Part III.

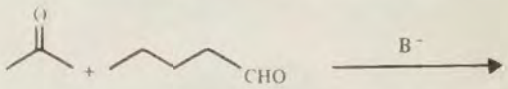
6. Pickard et al., *J. Chem. Soc.* (London), p. 103, 1944.
7. Behal, *Bull. Soc. Chim. Fr. 2*, 50, 359, 1888.
8. Schimmel and Co., *Chem. Zentralbl.*, 1, 1086, 1903; 2, 1124, 1903.
9. Williams et al., *Chem. Zentralbl.*, 2, 3852, 1936.
10. Crabalona, *Chem. Zentralbl.*, 1, 306, 1940.
11. Schorlemmer, *Annalen*, 147, 224, 1868.
12. Ottensooser, *Bull. Soc. Chim. Fr. 4*, 41, 324, 1927.
13. St. Pfau, *Helv. Chim. Acta*, 22, 382, 1939.

	3-Octanon-1-ol	2-Octenal
Other names	Caproyl ethanol Compound 1010 Hexanoyl etharol γ-Ketoctanol "Ketone alcohol" Methylol methyl amyl ketone 3-Oxooctanol	2-Pentyl acrolein α-Amyl acrolein
Empirical formula	$C_8H_{16}O_2$	$C_8H_{14}O$
Structure	$CH_3-(CH_2)_4-\overset{\overset{O}{\|\|}}{C}-CH_2-CH_2OH$	$CH_2=\overset{\overset{CHO}{\|}}{C}-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular point	144.21	126.20
Boiling point	94.6°C at 8–9 mm Hg	174°C 81°C at 48 mm Hg 72°C at 30 mm Hg
Specific gravity Refractive index		0.8562 at 14°C 1.4373 at 20°C
Solubility	Very slightly soluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Fruity, herbaceous, spicy odor; slightly bitter above 20 ppm; otherwise, warm and fruity	Peculiar green-leafy odor, less fatty than octanal; orange, honey-like, cognac-like aroma
Synthesis	By partial hydrogenation of the corresponding di-ketone at 100 C over Raney Ni in methanol solution; also by condensation of methyl amyl ketone with formaldehyde under mildly alkaline conditions	By prolonged heating of a solution of heptanal and formaldehyde in the presence of dimethylamino hydrochloride;[6] by boiling 4,5-diketo-3-pentyltetrahydrofuran under a nitrogen blanket[7]
Natural occurrence	Not reported found in nature	A volatile flavor component in potato chips[8]
Reported uses[3]	Non-alcoholic beverages 0.20 ppm Ice cream, ices, etc. 0.30 ppm Candy 0.80 ppm Baked goods 0.60–0.80 ppm Condiments 1.0 ppm	Candy 1.0 ppm Baked goods 1.0 ppm Condiments 1.0 ppm Meat, meat sauces, soups 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2804	FEMA No. 3215

REFERENCES

For References 1–5, see end of Part III.

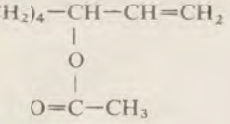
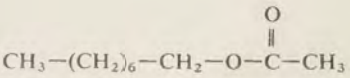
6. Marvel, Myers and Saunders, *J. Am. Chem. Soc.*, 70, 1698, 1948.
7. Hinder, Schinz and Seidel, *Helv. Chim. Acta*, 30, 1500, 1947.
8. Deck, Pokorny, and Chang, *J. Food Sci.*, 38(2), 345, 1973.

	1-Octen-3-ol	3-Octen-2-one
Other names	Amyl vinyl carbinol Matsutake alcohol 3-Octenol *n*-Pentyl vinyl carbinol	
Empirical formula	$C_8H_{16}O$	$C_8H_{14}O$
Structure	$CH_3-(CH_2)_4-CH(OH)-CH=CH_2$	$CH_3-C(=O)-CH=CH-(CH_2)_3-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	
Molecular weight	128.21	126.19
Boiling point	175–175.2°C; 68–71°C at 12 mm Hg	
Specific gravity	0.84	
Optical rotation	−7°49′ (−13° to −18°) at 14°C	
Solubility	Insoluble in water; soluble in alcohol	
Organoleptic characteristics	Powerful, sweet, earthy odor with strong, herbaceous note reminiscent of lavender-lavandin, rose, and hay; sweet, herbaceous taste	
Synthesis	From magnesium amyl bromide and acrolein[6]	By bubbling air in a solution of an organoborane derivative of 1-butene and 1-butyn-2-one in tetrahydrofuran;[11] also 
Natural occurrence	Originally reported (Ito and Imai) found in the mushroom *Armillaria matsutake*, a parasite growing on the radical hairs of *Pinus densiflora* in the forests of Japan.[7] It has been isolated also in the essential oils of *Mentha pulegium* L.,[8] lavender,[9] and *Mentha timjia*.[10]	Reported found in roasted filberts[12]
Reported uses[3]	Non-alcoholic beverages 0.20 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 6.0 ppm Condiments 6.0 ppm Soups 6.0 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm Gelatins and puddings 2.0 ppm Condiments, pickles 0.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2805	FEMA No. 3416

REFERENCES

For References 1–5, see end of Part III.

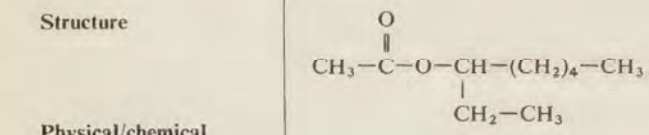
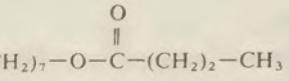
6. Levene and Walti, *J. Biol. Chem.*, 94, 593, 1931.
7. Murahashi, *Chem. Zentralbl.*, 1, 1958, 1937; 2, 1249, 1938.
8. Naves, *Helv. Chim. Acta*, 26, 1992, 1943.
9. Crabalona, *Bull. Soc. Chim. Fr.*, 11, 67, 1944.
10. Sficas, *Chem. Abstr.*, 48, 3934, 1954.
11. Suzuki et al., *Hokkaido Daigaku Kagakubu Kenkyu Hokoku*, 45, 1971; *Chem. Abstr.*, 75, 129860h, 1971.
12. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Centraal Instituut voor Voedingsonderzoek, Zeist, Netherlands.

	1-Octen-3-yl acetate	Octyl acetate
Other names	3-Acetoxy octene "Amyl crotonyl acetate" Amyl vinyl carbinyl acetate Octenyl acetate β-Octenyl acetate *n*-Pentyl vinyl carbinyl acetate	Acetate C-8 Capryl acetate *n*-Octyl acetate *Note*: Do not confuse with 2-ethyl hexyl acetate
Empirical formula	$C_{10}H_{18}O_2$	$C_{10}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay		98% min
Molecular weight	170.25	172.27
Boiling point	80°C (190 C) at 15 mm Hg	203–208°C
Flash point		88.5°C
Specific gravity	0.8775 (0.89) at 20°C	0.865–0.868 at 25°C; 0.8730–0.8740 at 15°C
Refractive index	1.4253 at 20°C	1.4180–1.4210 (1.4190–1.4207) at 20°C
Solubility	1:4 in 70% alcohol	1:4 in 70% alcohol; 1:15–20 in 60% alcohol; soluble in most common organic solvents
Organoleptic characteristics	Characteristic odor reminiscent of lavender and lavandin	Fruity odor reminiscent of neroli and jasmine; fruity, slightly bitter taste suggestive of peach
Synthesis	By acetylation of amyl vinyl carbinol	By acetylation of the corresponding alcohol
Natural occurrence		Reported found in the essential oils of green tea and *Heracleum giganteum* L.; also identified in the essential oil of bitter orange[6]
Reported uses[3]		Non-alcoholic beverages 1.6 ppm Ice cream, ices, etc. 0.87 ppm Candy 4.7 ppm Baked goods 6.0 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2806

REFERENCES

For References 1–5, see end of Part III.

6. **Mehlitz and Minas,** *Ind. Obst Gemueseverwert.*, 50, 861, 1965.

	3-Octyl acetate	Octyl butyrate
Other names		Octyl-*n*-butyrate
Empirical formula	$C_{10}H_{20}O_2$	$C_{12}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	172.27	200.32
Melting point		−56°C
Boiling point	191–191.5°C; 74°C at 10 mm Hg	244°C (245°C)
Specific gravity	0.8641 at 20°C	0.8549 at 30°C
Refractive index	1.4152 at 20°C	1.4210 at 20°C
Solubility		Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic, complex aroma with a rose and jasmine note and an apple-lemon undertone; sweet, peach-like flavor	Green, herbaceous odor remotely reminiscent of orange but more so of galbanum and parsley; sweet, melon-like flavor
Synthesis		From *n*-octanol and butyric acid in the presence of HCl[6]
Natural occurrence	Reported found in the essential oil of *Mentha pulegium* L.[9]	Reported found in the essential oil of *Heracleum villosum* Fisch.[7] and in the oil from fruits of *Pastinaca sativa*[8]
Reported uses[3]		Non-alcoholic beverages 0.53 ppm Ice cream, ices, etc. 1.3 ppm Candy 2.9 ppm Baked goods 2.9 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2807

REFERENCES

For References 1–5, see end of Part III.

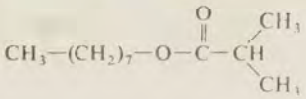
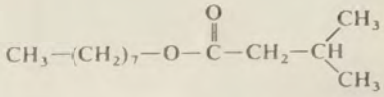
6. Biltery and Gisseleire, *Bull. Soc. Chim. Belg.*, 44, 569, 1935.
7. Rutowski and Vinogradowa, *Chem. Zentralbl.*, 2, 1311, 1927.
8. Renesse, *Chem. Ann.*, 166, 80, 1873.
9. Naves, *Helv. Chim. Acta*, 26, 1036, 1999, 1943.

	n-Octyl formate	Octyl heptanoate
Other names	Octyl formate Octyl methanoate	Octyl heptoate Octyl heptylate
Empirical formula	$C_9H_{18}O_2$	$C_{15}H_{30}O_2$
Structure	$CH_3-(CH_2)_7-O-\overset{\overset{O}{\|}}{C}-H$	$CH_3-(CH_2)_7-O-\overset{\overset{O}{\|}}{C}-(CH_2)_5-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	96% min[2]	
Molecular weight	158.24	242.41
Melting point		−21.5°C
Boiling point	198–199°C; 73°C at 10 mm Hg	290.8°C
Specific gravity	0.869–0.872 at 25°/25°C;[2] 0.8786 at 15°C	0.85200 at 20°C
Refractive index	1.4180–1.4200 at 20°C;[2] 1.41813 at 15°C	1.43488 at 20°C
Acid value	Not more than 1; may increase on storage[2]	
Solubility	1:5 and more in 70% alcohol;[2] insoluble in water; soluble in most common organic solvents	Soluble in most common organic solvents; insoluble in water
Organoleptic characteristics	Fruity odor with a rose-orange note; bitter flavor, refreshingly fruity-green at low concentrations	Characteristic fruity, slightly fatty odor; corresponding flavor
Synthesis	By esterification of *n*-octyl alcohol with formic acid; by boiling *n*-octyl chloride with formamide in the presence of small amounts of HCl[8]	By esterification of *n*-octyl alcohol with heptanoic acid in the presence of mineral acids[6,7]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.01–1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 5.0 ppm Baked goods 7.0 ppm	Non-alcoholic beverages 0.13–1.0 ppm Ice cream, ices, etc. 0.13–1.0 ppm Candy 0.13–2.0 ppm Baked goods 0.20–2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2809	FDA 121.1164; FEMA No. 2810

REFERENCES

For References 1–5, see end of Part III.

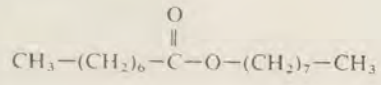
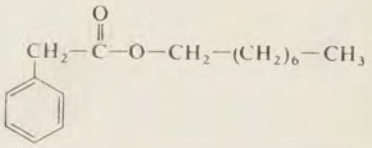
6. Gartenmeister, *Justus Liebigs Ann. Chem.*, 233, 284, 1886.
7. Bilterys and Gisseleire, *Bull. Soc. Chim. Belg.*, 44, 578, 1935.
8. E. I. du Pont de Nemours & Co., U.S. Patent 2,375,401, 1942.

	Octyl isobutyrate	*n*-Octyl isovalerate
Other names		*n*-Octyl-3-methylbutyrate
Empirical formula	$C_{12}H_{24}O_2$	$C_{13}H_{26}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	200.32	214.35
Boiling point	237°C	245°C
Specific gravity	0.87	0.86
Solubility	Almost insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Fruity, fatty fragrance with a soft and humid undertone reminiscent of parsley and fern root; sweet flavor suggestive of grape	Strong odor reminiscent of fatty aldehyde with an apple-pineapple undertone
Synthesis	Esterification of *n*-octanol with isobutyric acid	By esterification of *n*-octanol with isovaleric acid
Natural occurrence	Reported found among the volatile components of hop[7]	Reported found among the volatile constituents of the aroma of fresh Florida orange juice[6]
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.4 ppm Candy 3.5 ppm Baked goods 3.5 ppm Chewing gum 0.50 ppm	Non-alcoholic beverages 0.90 ppm Ice cream, ices, etc. 0.80–1.0 ppm Candy 1.0–4.0 ppm Baked goods 1.0–4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2808	FDA 121.1164; FEMA No. 2814

REFERENCES

For References 1–5, see end of Part III.

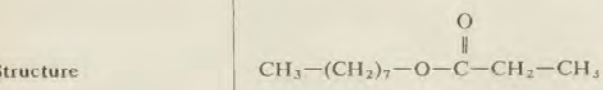
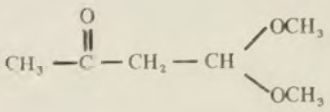
6. Wolford et al., *J. Food Sci.*, 28, 320, 1963.
7. Buttery et al., *Nature*, 202, 701, 1964.

	Octyl octanoate	*n*-Octyl phenylacetate
Other names	Octyl caprylate *n*-Octyl octoate Octyl octylate	Octyl-α-toluate *n*-Octyl-α-toluate
Empirical formula	$C_{16}H_{32}O_2$	$C_{16}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, viscous liquid
Molecular weight	256.44	248.37
Melting point	−18°C	315°C
Boiling point	306°C; 307°C; 192–193°C at 30 mm Hg	
Specific gravity	0.860 at 15.5°C; 0.8554 at 25°C	0.983 at 15.5°C
Refractive index	1.4925 (1.4352) at 20°C	
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Faint, fatty odor reminiscent of green tea; oily, fruity, sweet, mildly green taste	Pleasant, slightly fatty, citrus-like odor
Synthesis	By esterification of octanoic acid with octyl alcohol in the presence of HCl catalyst;[6] or by passing vapors of octanoic acid and hydrogen over a copper chromium oxide catalyst at high temperature (320°C)[7]	By esterification of *n*-octanol with phenylacetic acid
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.50–1.0 ppm Ice cream, ices, etc. 0.50–1.0 ppm Candy 0.50–2.0 ppm Baked goods 0.50–2.0 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 1.0 ppm Candy 0.20–4.0 ppm Baked goods 4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2811	FDA 121.1164; FEMA No. 2812

REFERENCES

For References 1–5, see end of Part III.

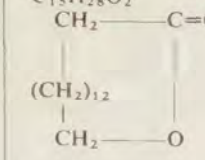
6. **Ruhoff and Reid,** *J. Am. Chem. Soc.*, 55, 3827, 1933.
7. Kessler Chemical Corp., U.S. Patent 1,997,172, 1934.

	Octyl propionate		3-Oxobutanal, dimethyl acetal	
Other names			3-Ketobutyraldehyde, dimethyl acetal Acetyl acetaldehyde, dimethyl acetal 1,1-Dimethoxy-3-butanone	
Empirical formula	$C_{11}H_{22}O_2$		$C_6H_{12}O_3$	
Structure				
Physical/chemical characteristics[5]				
Appearance	Colorless liquid			
Molecular weight	186.30		132.16	
Boiling point	228°C (225°C)			
Specific gravity	0.87044 at 15°C; 0.870 at 15°C			
Refractive index	1.4225 at 20°C			
Solubility	Insoluble in water; soluble in alcohol and propylene glycol			
Organoleptic characteristics	Complex, waxy odor reminiscent of myrtle berries with a pineapple undertone			
Synthesis	By esterification of *n*-octanol with propionic acid			
Natural occurrence	In oil of hop		Closely related materials (e.g., the diethyl-acetal) reported in roasted cocoa[6]	
Reported uses[3]	Non-alcoholic beverages	0.84 ppm	Ice cream, ices, etc.	80 ppm
	Ice cream, ices, etc.	0.57 ppm	Candy	80 ppm
	Candy	3.6 ppm	Baked goods	160 ppm
	Baked goods	2.0–4.0 ppm	Gélatins and puddings	80 ppm
			Condiments	500 ppm
			Meat, soups	2,000 ppm
Regulatory status	FDA 121.1164; FEMA No. 2813		FEMA No. 3381	

REFERENCES

For References 1–5, see end of Part III.

6. van der Wal et al., *J. Agric. Food Chem.*, 19(2), 276, 1971.

	ω-Pentadecalactone
Other names	Angelica lactone Exaltolide® 15-Hydroxypentadecanoic acid, ω-lactone Pentadecanolide "Thibetolide"
Empirical formula	$C_{15}H_{28}O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Plastic solid at room temperature; limpid and colorless when liquified
Assay	98% min
Molecular weight	240.39
Melting point	30–31°C to 36–37°C
Boiling point	150°C at 5 mm Hg (Muscolacton, Lactone M.C. 15) 176°C at 15 mm Hg
Congealing point	36°C min ("Thibetolide")
Specific gravity	0.9447 at 33°C
Refractive index	1.4669 at 33°C
Solubility	Insoluble in water; almost insoluble in glycerol; 1:6 in 80% alcohol; soluble in alcohol
Organoleptic characteristics	Extraordinarily persistent, musk-like odor
Synthesis	Commercially available under a variety of Trade names: Exaltolide®, "Thibetolide," "Muscolacton," "Lactone M.C. 15," and others. For synthesis see References 6 through 21.
Natural occurrence	Originally reported found in the essential oil from angelica roots[22–25]
Reported uses[3]	Non-alcoholic beverages, 0.27 ppm; alcoholic beverages, 0.50 ppm; ice cream, ices, etc., 0.68 ppm; candy, 1.4 ppm; baked goods, 1.5 ppm; gelatins and puddings, 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2840

REFERENCES

For References 1–5, see end of Part III.

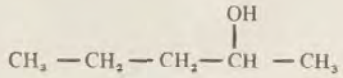
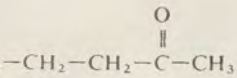
6. Ružička and Stoll, *Helv. Chim. Acta*, 11, 1159, 1928.
7. Stoll and Gardner, *Helv. Chim. Acta*, 17, 1609, 1934.
8. Stoll et al., *Helv. Chim. Acta*, 17, 1283, 1289, 1934.
9. Stoll et al., *Helv. Chim. Acta*, 18, 1087, 1935.
10. Stoll and Rouver, *Parfum. Mod.*, 29, 207, 1935.
11. Hunsdiecker and Erlbach, *Ber. Dtsch. Chem. Ges.*, 80, 129, 1947.
12. Hunsdiecker et al., Dutch Patent 53,032.
13. Haarman and Reimer, German Patent 449,217; *Chem. Zentralbl.*, 2, 2351, 1927.
14. Stoll, *Helv. Chim. Acta*, 30, 1393, 1947.
15. Polak and Schwarz, Dutch Patent 67,458.
16. Carothers et al., *J. Am. Chem. Soc.*, 51, 51, 1929; 69, 129, 1947.
17. Collaud, *Helv. Chim. Acta*, 25, 965, 1942; 26, 849, 1155, 1943.
18. Klouven and Koh, *Parfum. Kosmet. II*, 43, 35, 1962.
19. McCrae, *Tetrahedron*, 20(7), 1173, 1964.
20. Tesseire and Corbier, *Recherches*, 11, 27, 1961.
21. Roure-Bertrand and DuPont, French Patent 1,005,766, 1947.
22. Muller, *Ber. Dtsch. Chem. Ges.*, 14, 2576, 1881.
23. Beilstein and Wiegand, *Ber. Dtsch. Chem. Ges.*, 15, 1741, 1882.
24. Ciamician and Silber, *Ber. Dtsch. Chem. Ges.*, 29, 1811, 1896.
25. Kerschbaum, *Ber. Dtsch. Chem. Ges.*, 60, 902, 1927.

	2,4-Pentadienal	2,3-Pentanedione
Other names		Acetyl propionyl
Empirical formula	C_5H_6O	$C_5H_8O_2$
Structure	$CH_2=CH-CH=CH-CHO$	$CH_3-C(=O)-C(=O)-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance		Yellow liquid
Molecular weight	82.09	100.12
Melting point		−52°C
Boiling point	*cis*-, 29 30°C at 10 mm Hg *trans*-, 30°C at 10 mm Hg	110–112°C (180°C)
Specific gravity		0.955–0.959 at 15°C
Refractive index	*cis*-, 1.5115 at 19°C *trans*-, 1.5185–1.5190 at 19°C	1.4081 (1.40135) at 19°C
Solubility		Partially water soluble (1:15)
Organoleptic characteristics		Somewhat sweet odor similar to quinone
Synthesis	From 2-ethoxy-Δ^3-dihydropyrone and phosphoric acid;[6] the *cis*- and *trans*-isomers can be prepared from the corresponding penta-2,4-dien-1-ol (*cis*- or *trans*-form) in methylene chloride in the presence of manganese dioxide[7]	By oxidation of methyl propyl ketone with excess $NaNO_2$ and diluted HCl in the presence of hydroxylamine hydrochloride under nitrogen blanket
Natural occurrence		Identified in the essential oil of Finnish pine[8]
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm Gelatins and puddings 1.0 ppm Chewing gum 1.0 ppm Condiments 1.0 ppm Meat, meat sauces, soups 1.0 ppm Milk, dairy products 1.0 ppm Cereals 1.0 ppm	Non-alcoholic beverages, 0.60 ppm; ice cream, ices, etc., 3.3 ppm; candy, 5.9 ppm; baked goods, 9.6 ppm; gelatins and puddings, 0.28 ppm; toppings, 0.30 ppm
Regulatory status	FEMA No. 3217	FDA 121.1164; FEMA No. 2841

REFERENCES

For References 1–5, see end of Part III.

6. Woods and Sanders, *J. Am. Chem. Soc.*, 68, 2483, 1946.
7. Boehm and Whiting, *J. Chem. Soc.*, p. 2541, 1963.
8. Aschau, *Z. Angew. Chem.*, 20, 1815, 1907.

	2-Pentanol	2-Pentanone
Other names	Methyl *n*-propyl carbinol *sec-n*-Amyl alcohol	Ethyl acetone Methyl propyl ketone
Empirical formula	$C_5H_{12}O$	$C_5H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid at room temperature
Molecular weight	88.15	86.13
Melting point		77.75°C
Boiling point	118–119°C 62°C at 60 mm Hg	102°C
Specific gravity	*dl*-, 0.8053 at 25°C *d*-, 0.8101 at 20°C	0.810 at 15.5°C; 0.80435 at 25°C
Refractive index	*dl*-, 1.4063 at 15°C *d*-, 1.4056 at 20°C	1.3985 (1.38946) at 20°C
Optical rotation	*d*-, +13.9 at 20°C *l*-, −13.4 at 15°C	
Solubility	Very soluble in water; soluble in alcohol and ether	Slightly soluble in water; miscible with alcohol and ether
Organoleptic characteristics		Wine, acetone-like, characteristic odor
Synthesis	By catalytic reduction of methyl *n*-propyl ketone[1,0]	By dry distillation of a mixture consisting of calcium acetate and calcium butyrate;[6] also by oxidation of sodium or ammonium *n*-caproate with H_2O_2
Natural occurrence		Reported found in wood spirit;[7,8] also reported present in *Ananas sativus*,[9] a few banana species, grape vines, and some citrus fruits
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Baked goods 2.0 ppm Gelatins and puddings 2.0 ppm Condiments, pickles 2.0 ppm Meat, meat sauces, soups 2.0 ppm Cereals 2.0 ppm	Non-alcoholic beverages 13 ppm Ice cream, ices, etc. 34 ppm Candy 32 ppm Baked goods 32 ppm
Regulatory status	FEMA No. 3316	FDA 121.1164; FEMA No. 2842

REFERENCES

For References 1–5, see end of Part III.

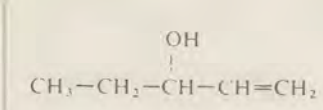
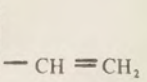
6. Friedel, *Annalen*, 108, 124, 1858.
7. Vladesco, *Ber. Dtsch. Chem. Ges.*, 23, 435, 1890.
8. Buisine, *Chem. Zentralbl.*, 1, 1020, 1899.
9. Haagen-Smit et al., *J. Am. Chem. Soc.*, 67, 1646, 1945.
10. Wilson, *J. Am. Chem. Soc.*, 70, 1313, 1948.

	2-Pentenal	4-Pentenoic acid
Other names	2-Ethylacrylic aldehyde	Allyl acetate Allyl acetic acid
Empirical formula	C_5H_8O	$C_5H_8O_2$
Structure	$CH_3-CH_2-CH=CH-CHO$	$CH_2=CH-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-OH$
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Molecular weight	84.11	100.12
Melting point		−22 to −23°C
Boiling point	124°C 56°C at 65 mm Hg	189°C (93°C at 20 mm Hg)
Specific gravity	0.8532 at 21°C	0.9809 at 20°C
Refractive index	1.4439 at 21°C	1.4281 at 20°C
Solubility		Slightly soluble in water; readily soluble in alcohol and ether
Organoleptic characteristics		Sour, caramellic flavor with sweet aftertaste; acrid flavor and odor at high levels
Synthesis	By treating β-phenoxyacrolein with secondary amines, Grignard reagent, and active methylene compounds;[6] by heating 1-ethoxy-1,3-pentadiene with H_3PO_4 at 80°C;[7] from *cis*- and *trans*-but-2-ene-1,4-diol and $SOCl_2$, followed by treatment of the chloroalcohol with methyl magnesium bromide and final oxidation with MnO_2[8]	By decarboxylation by heating allylmalonic acid; or from the corresponding ethyl ester prepared by boiling ethyl 4-chloro-*n*-valerate in quinoline
Natural occurrence	Reported found in aqueous orange essence (*trans*-form);[9] as a flavor component in cognac oil;[10] in *Chrysocoris stolli*;[11] in tomato aroma;[12] in the autooxidation of cod liver oil;[13] in peas;[14] as a flavoring component in reverted soy bean oil;[15,16] in salmon oil;[17] in strawberry;[18] in potato chips during storage;[19] in raspberry;[20] in butterfat fishy flavor[21]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Candy 10.0 ppm Gelatins and puddings 10.0 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Margarine 2.0 ppm
Regulatory status	FEMA No. 3218	FDA 121.1164; FEMA. No. 2843

REFERENCES

For References 1–5, see end of Part III.

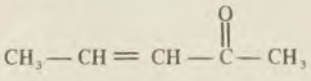
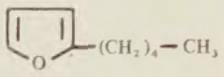
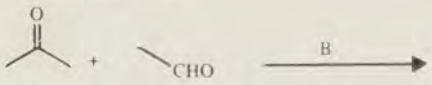
6. Gelin and Makula, *Bull. Soc. Chim. Fr.*, (3), 1129, 1968.
7. Nazarov et al., *Zh. Obshch. Khim.*, 29, 3692, 1959.
8. Thomas and Warburton, *J. Chem. Soc.*, p. 2988, 1965.
9. Moshonas and Shaw, *J. Food Sci.*, 38, 360, 1973.
10. Schaefer and Timmer, *J. Food Sci.*, 35(1), 10, 1970.
11. Choudhuri and Das, *Arch. Int. Physiol. Biochim.*, 77(4), 609, 1969.
12. Schormueller and Kochmann, *Z. Lebensm. Unters. Forsch.*, 141(1), 1, 1969.
13. Fisher et al., *Lipids*. 3(1), 88, 1968.
14. Grosch, *Z. Lebensm. Unters. Forsch.*, 135(2), 75, 1967.
15. Smouse and Chang, *J. Am. Oil Chem. Soc.*, 44(8), 509, 1967.
16. Iwata, Morita, and Ota, *Yukagaku*, 14(5), 241, 1965.
17. Wyatt and Day, *J. Food Sci.*, 28, 305, 1963.
18. Winter and Willhalm, *Helv. Chim. Acta*, 47(5), 1215, 1964.
19. Dornseifer and Powers, *Food Technol.*, 17(10), 118, 1963.
20. Winter and Sundt, *Helv. Chim. Acta*. 45, 2195, 1962.
21. Forss, Dunstone and Stark, *J. Dairy Res.*, 27, 211, 1960.

	1-Penten-3-ol	1-Penten-3-one
Other names	Ethyl vinyl carbinol	Ethyl vinyl ketone Propionyl ethylene
Empirical formula	$C_5H_{10}O$	C_5H_8O
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid; polymerizes readily with heat or in the presence of alkali
Molecular weight	86.13	84.04
Boiling point	114 C; 32 C at 15 mm Hg	68–70°C at 200 mm Hg 38°C at 60 mm Hg 31°C at 47 mm Hg
Specific gravity	0.8344 at 25 C	0.8468 at 20°C
Refractive index	1.4223 at 25 C	1.4192 at 20°C
Optical rotation	+10.5° (*d*, in ethanol); −7.1° (*l*, in ethanol)	
Solubility	Sparsely soluble in water; miscible with alcohol and ether	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics		Powerful, penetrating odor
Synthesis	By prolonged contact of 1-chloro-2-pentene with NaOH solution.[6] For the synthesis of the optically active forms, see references 7, 8, and 9.	By reacting ethylene with a mixture of propionyl chloride, aluminum trichloride and carbon disulfide[10]
Natural occurrence	In orange, strawberry, and tomato	A flavor component of orange essence[11]
Reported uses[3]		Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 8.0 ppm Baked goods 8.0 ppm Gelatins and puddings 5.0 ppm Condiments, pickles 0.01 ppm Milk, dairy products 0.005 ppm Preserves 5.0 ppm
Regulatory status	FDA 121.1164	FEMA No. 3382

REFERENCES

For References 1–5, see end of Part III.

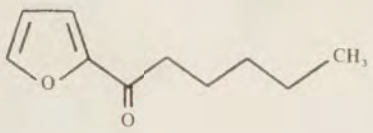
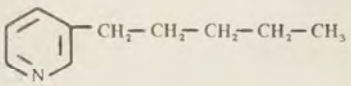
6. Meisenheimer and Link, *Chem. Ann.*, 479, 231, 1930.
7. Kohler, *J. Am. Chem. Soc.*, 38, 525, 1916.
8. Hurd and McNamee, *J. Am. Chem. Soc.*, 59, 104, 1937.
9. Bouis, *Ann. Chim. Paris*, 10(9), 497, 1928.
10. MacMahon et al., *J. Am. Chem. Soc.*, 70, 2971, 1948.
11. Moshonas and Shaw, *J. Food Sci.*, 38(2), 360, 1973.

	3-Penten-2-one	2-Pentyl furan
Other names	Ethylidene acetone Methyl propenyl ketone	
Empirical formula	C_5H_8O	$C_9H_{14}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	84.31	138.08
Boiling point	122°C	57–59°C at 10 mm Hg
Specific gravity	0.861 at 15°C 0.8624 at 20°C	0.8837 at 23°C
Refractive index	1.4350 at 20°C	1.4462
Organoleptic characteristics	Fruity odor becoming pungent on storage; used in tobacco flavors	Fruity odor
Synthesis	From 4-hydroxy-pentan-2-one refluxed with oxalic acid;[6] also 	From 2-furyl-1-pentene by catalytic reduction with Ni-Raney[9]
Natural occurrence	Reported found among the volatile components of roasted peanuts;[7] also in cranberry, bilberry, rum, cocoa, coffee, tea, roasted filberts, roasted peanuts, and potato chips[8]	Reported found as a constituent in coffee aroma;[10] a volatile flavor component in roasted filberts[11]
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 4.0 ppm Baked goods 4.0 ppm Gelatins and puddings 4.0 ppm Milk, dairy products 1.0 ppm Cereals 2.0 ppm	Non-alcoholic beverages 3.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm Meat, meat sauces, soups 3.0 ppm Milk, dairy products 3.0 ppm Cereals 3.0 ppm
Regulatory status	FEMA No. 3417	FEMA No. 3317

REFERENCES

For References 1–5, see end of Part III.

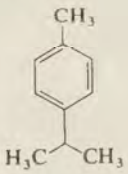
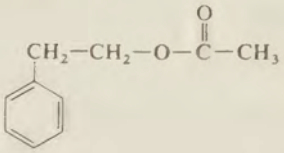
6. *Chem. Abstr.*, 70, 26505p, 1969.
7. Walradt et al., *J. Agric. Food Chem.*, 19, 972, 1971.
8. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Centraal Instituut voor Voedingsonderzoek, Zeist, Netherlands.
9. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.
10. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.
11. Sheldon et al., *J. Food Sci.*, 37(2), 313, 1972.

	Pentyl-2-furyl ketone		2-Pentyl pyridine	
Other names	2-Hexanoylfuran 1-(2-Furyl-1-hexanone)		2-Amyl pyridine	
Empirical formula	$C_{10}H_{14}O_2$		$C_{10}H_{15}N$	
Structure				
Physical/chemical characteristics				
Molecular weight	166		149.23	
Boiling point			82.5–84.5°C at 8–9 mm Hg 102–107°C	
Specific gravity			0.8881 at 20°C	
Refractive index			1.4834 at 20°C	
Synthesis			By alkylation of 2-pycollyl lithium;[6] by hydrogenation of 2-pentenyl pyridine[7]	
Natural occurrence			Reported as occurring in shallow-fried beef;[8] also as a steam-volatile component in roasted Spanish peanuts[9]	
Reported uses[3]	Non-alcoholic beverages	0.05 ppm	Ice cream, ices, etc.	0.1 ppm
	Ice cream, ices, etc.	0.05 ppm	Candy	0.5 ppm
	Baked goods	0.15 ppm	Baked goods	1.0 ppm
	Gelatins and puddings	0.10 ppm	Gelatins and puddings	0.1 ppm
	Chewing gum	0.15 ppm	Condiments, pickles	0.4 ppm
	Milk, dairy products	0.05 ppm	Meat, meat sauces, soups	0.5 ppm
Regulatory status	FEMA No. 3418		FEMA No. 3383	

REFERENCES

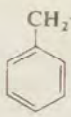
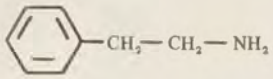
For References 1–5, see end of Part III.

6. **Osuch and Levine,** *J. Am. Chem. Soc.*, 78, 1723, 1956.
7. *Chem. Abstr.*, 71, 61162z, 1969.
8. **Watanabe et al.,** *J. Agric. Food Chem.* 19, 1017, 1971.
9. **Walradt et al.,** *J. Agric. Food Chem.*, 19, 972, 1971.

	α-Phellandrene	Phenethyl acetate
Other names	1-Isopropyl-4-methyl-2,4-cyclohexadiene 4-Isopropyl-1-methyl-1,5-cyclohexadiene 5-Isopropyl-2-methyl-1,3-cyclohexadiene *p*-Mentha-1,5-diene 1-Methyl-4-isopropyl-1,5-cyclohexadiene 2-Methyl-5-isopropyl-1,3-cyclohexadiene	Benzyl carbinyl acetate 2-Phenylethyl acetate
Empirical formula	$C_{10}H_{16}$	$C_{10}H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, mobile oil	Colorless liquid
Assay		98% min[2]
Molecular weight	136.23	164.21
Boiling point	*dl*-, 175–176°C; *d*-, 175–176°C at 754 mm Hg; *l*-, 173–175°C at 754 mm Hg	232°C
Flash point		105°C
Specific gravity	*dl*-, 0.841 at 22°C; *d*-, 0.8565 at 15°C; *l*-, 0.848 at 15°C	1.030–1.034 at 25°/25°C[2]
Refractive index	*dl*-, 1.4760 at 22°C; *d*-, 1.4732 at 19°C; *l*-, 1.47694 at 20°C	1.4970–1.5010 at 20°C[2]
Acid value		Not more than 1.0[2]
Optical rotation	*d*-, +40°40′; *l*-, −84°10′	
Solubility	Insoluble in water; soluble in ether	1:2 and more in 70% alcohol;[2] soluble in most common organic solvents
Organoleptic characteristics	Pleasant, fresh, citrus, peppery odor with a discrete mint note	Floral odor reminiscent of rose with a honey-like undertone; sweet, fruit-like taste reminiscent of raspberry
Synthesis	The *l*-form by isolation from *Eucalyptus numerosa* and similar oils; also from the manufacture of synthetic menthol	By acetylation of phenyl ethyl alcohol
Natural occurrence	The *d*-form has been reported found in the essential oils of bitter fennel, Ceylon cinnamon leaves, star anise, *Curcuma longa*, and others. The *l*-form has been reported found in various eucalyptus oils, angelica, *Lantana camara*, and others.	Reported found in natural products
Reported uses[3]	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 28 ppm Candy 130 ppm Baked goods 41 ppm	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 2.2 ppm Candy 4.2 ppm Baked goods 5.6 ppm
Regulatory status	FDA 121.1164; FEMA No. 2856	FDA 121.1164; FEMA No. 2857

REFERENCES

For References 1–5, see end of Part III.
For further information on α-phellandrene see the following:
Berry et al., *J. Chem. Soc.* (London), p. 1418, 1939.
Semmler, *Ber. Dtsch. Chem. Ges.*, 36, 1749, 1903.
Smith et al., *J. Chem. Soc.* (London), 125, 930, 1924.

	Phenethyl alcohol	Phenethylamine
Other names	Benzyl carbinol 2-Phenylethanol Phenylethyl alcohol β-Phenylethyl alcohol	β-Phenylethylamine 1-Amino-2-phenylethane β-Aminoethyl benzene
Empirical formula	$C_8H_{10}O$	$C_8H_{11}N$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, viscous liquid	Liquid; absorbs CO_2 on exposure to air
Assay	99% min	
Molecular weight	122.17	121.18
Melting point	−25.8°C	
Boiling point	220–222°C at 740 mm Hg	194.5–195°C
Congealing point	101°C	
Flash point	1.017–1.020 at 25°/25°C;[2] 1.0242 at 15°C	
Specific gravity	1.5310–1.5340[2] (1.53212) at 20°C	0.9640
Refractive index		1.5290 at 25°C
Solubility	1:2 in 50% alcohol;[2] 1:1 in 60% alcohol; soluble (approx. 1:60) in water; soluble in most common organic solvents	Soluble in water; readily soluble in alcohol and ether
Organoleptic characteristics	Characteristic rose-like odor; initially a slightly bitter taste, then sweet and reminiscent of peach	Fishy odor
Synthesis	From toluene, benzene, or styrene	By reduction of benzyl cyanide with sodium metal in alcohol[6] or with Ni-Raney[7]
Natural occurrence	Reported found (as is or esterified) in several natural products: rose concrete, rose absolute (60% or more), and rose distillation waters; also found in the essential oils of neroli, ylang-ylang, narcissus, hyacinth, lily, tea leaves, *Michelia champaca*, *Pandamus odoratissimus*, Congo and Reunion geranium, tobacco, and others. It has been identified in wines.[8]	Reported found in the oil of bitter almonds
Reported uses[3]	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 8.3 ppm Candy 12 ppm Baked goods 16 ppm Gelatins and puddings 0.15 ppm Chewing gum 21–80 ppm	Non-alcoholic beverages 0.10 ppm Ice cream, ices, etc. 0.10 ppm Candy 0.10 ppm Baked goods 0.10 ppm Gelatins and puddings 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2858	FEMA No. 3220

REFERENCES

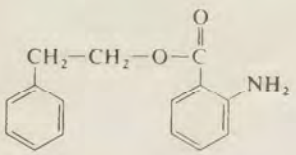
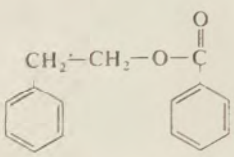
For References 1–5, see end of Part III.

6. **Johnson and Guest,** *Am. Chem. J.*, 42, 346, 1909.
7. **Robinson and Snyder,** in *Organic Syntheses*, Coll. Vol. 3, Horning, E. C., Ed., Wiley & Sons, New York, 1955, 720.
8. **Ayrapas,** *Natuer*, 5, 472, 1962.

For further information on phenethyl alcohol see the following:

Gurunadham, *J. Sci. Ind. Res. (India) Sect. B*, 20(8), 408, 1961.

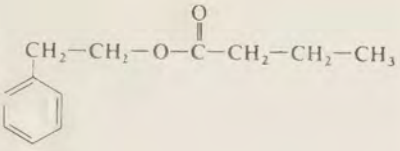
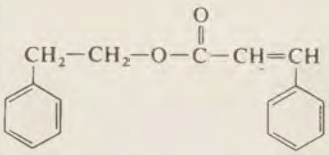
Kishore and Lal, *Indian Oil Soap J.*, 6, 255, 1961.

	Phenethyl anthranilate	Phenethyl benzoate
Other names	Benzyl carbinyl anthranilate β-Phenylethyl-*o*-aminobenzoate	2-Phenylethyl benzoate
Empirical formula	$C_{15}H_{15}NO_2$	$C_{15}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Fused yellow-amber mass (poor quality); white, colorless, crystalline mass	Colorless to yellowish, oily liquid
Assay		98% min
Molecular weight	241.29	226.28
Melting point	42°C	
Boiling point	324°C	189°C (>300°C) at 21 mm Hg
Congealing point	>40°C	
Flash point		>100°C
Specific gravity	1.14 (liquid)	1.092–1.096 at 25°/25°C; 1.023–1.030 at 15°C
Refractive index		1.558–1.562 (1.5591–1.5605) at 20°C
Acid value	1 max	1 max
Solubility	Insoluble in water; 1 gm in 6 ml of 80% alcohol; 1 gm in 1 ml of 90% alcohol	1:1 in 90% alcohol; 1:18 in 80% alcohol; insoluble in water
Organoleptic characteristics	Pure material almost odorless; with other materials it has a characteristic odor reminiscent of neroli and grapefruit with a sweet, grape and orange undertone; not very stable	Sweet, rose and honey-like odor; used in trace quantities for fixation of honey, strawberry, and others
Synthesis	By direct esterification of anthranilic acid with phenylethyl alcohol; pure material from phenylethyl alcohol plus isatoic anhydride; also from phenylethyl alcohol and methylanthranilate	From phenethyl alcohol and benzoyl chloride in the presence of NaOH;[6] from phenylethyl alcohol and methylbenzoate; by esterification of phenylethyl alcohol with benzoic acid
Natural occurrence	Not reported found in nature	Reported found in the essential oil from flowers of rose and orange[7]
Reported uses[3]	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 1.9 ppm Candy 6.2 ppm Baked goods 5.8 ppm	Non-alcoholic beverages 1.0 ppm Ice cream ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 4.0 ppm Chewing gum 3.8 ppm
Regulatory status	FDA 121.1164; FEMA No. 2859	FDA 121.1164; FEMA No. 2860

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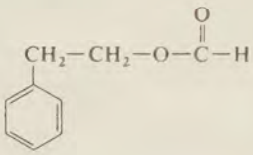
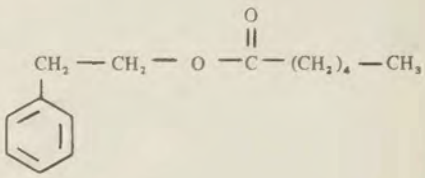
For References 1–5, see end of Part III.

6. Klazes and Allendorf, *Ber. Dtsch. Chem. Ges.*, 31, 1003, 1898.
7. Grignard, *Traite Chim. Org.*, 22, 1047, 1953.

	Phenethyl butyrate	Phenethyl cinnamate
Other names	β-Phenethyl-*n*-butanoate	Benzyl carbinyl cinnamate Phenylethyl cinnamate Phenylethyl-β-phenylacrylate β-Phenethyl-3-phenylpropenoate
Empirical formula	$C_{12}H_{16}O_2$	$C_{17}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	White, crystalline solid
Assay	98% min	98–99% min
Molecular weight	192.26	252.32
Melting point		58°C
Boiling point	238°C	>300°C
Congealing point		>54–56°C
Flash point	>100°C	
Specific gravity	0.991–0.994 (1.00) at 25°/25°C	
Refractive index	1.488–1.492 at 20°C	
Acid value	1 max	
Solubility	1:2 in 80% alcohol; 1:1 in 90% alcohol; almost insoluble in water	1 gm in 10 ml of 95% alcohol with slight turbidity; soluble in hot alcohol
Organoleptic characteristics	Rose-like fragrance; sweet taste suggestive of honey; not as stable as the isobutyrate	Sweet, balsamic odor reminiscent of rose; at low levels sweet, plum-like taste
Synthesis	By esterification of phenylethyl alcohol with *n*-butyric acid	From phenylethyl alcohol and methylcinnamate
Natural occurrence	In passion fruit, grapes, and wine	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 3.2 ppm Ice cream, ices, etc. 8.9 ppm Candy 13 ppm Baked goods 13 ppm	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 0.80 ppm Candy 3.2 ppm Baked goods 3.1 ppm Gelatins and puddings 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2861	FDA 121.1164; FEMA No. 2863

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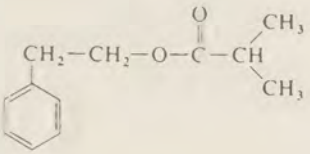
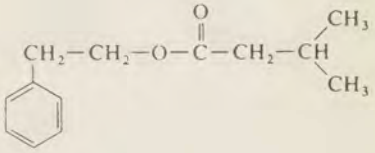
For References 1–5, see end of Part III.

	Phenethyl formate	Phenethyl hexanoate
Other names	Benzyl carbinyl formate Phenethyl methanoate 2-Phenylethyl formate	Phenyl ethyl caproate β-Phenethyl hexoate Benzyl carbinyl hexylate
Empirical formula	$C_9H_{10}O_2$	$C_{14}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless oily liquid
Assay	96% min (90%)	
Molecular weight	150.18	220.31
Boiling point	226 C	263°C
Flash point	91 C (approx 100 C)	
Specific gravity	1.0660–1.0700 at 15°C; 1.056–1.062 at 25 C	0.98
Refractive index	1.5065–1.5090 (1.5060–1.5100) at 20°C	
Acid value	0.1 max (1.0)	
Solubility	Partially soluble in water; soluble in most common organic solvents. For the 96% active product, 1:4 in 70% alcohol	Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Rose-like odor reminiscent of hyacinth and chrysanthemum; bittersweet flavor suggestive of unripe plum; not very stable	Fresh, fruity-green odor reminiscent of pineapple; pleasant taste
Synthesis	By direct esterification of phenethyl alcohol with formic acid	See Reference 6
Natural occurrence	Reported found in several natural products	Reported found in yellow passion fruit[7]
Reported uses[3]	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 11 ppm Candy 13 ppm Baked goods 15 ppm	Non-alcoholic beverages 8.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2864	FEMA No. 3221

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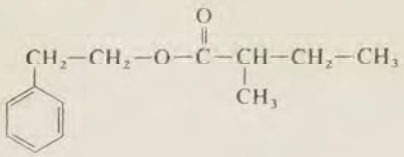
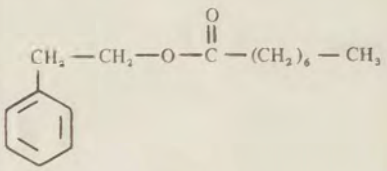
For References 1–5, see end of Part III.

6. Mentani, *Koryo*, (61), 61, 1961; *Chem. Abstr.*, 58, 2400g, 1963.
7. Winter and Klöty, *Helv. Chim. Acta*, 55(6), 1916, 1972.

	Phenethyl isobutyrate	Phenethyl isovalerate
Other names	2-Phenylethyl isobutyrate	Benzyl carbinyl isovalerianate Phenethyl isopentanoate Phenethyl-3-methylbutyrate 2-Phenylethyl isovalerate
Empirical formula	$C_{12}H_{16}O_2$	$C_{13}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to yellowish liquid	Colorless liquid
Assay	98% min	98% min
Molecular weight	192.26	206.28
Boiling point	230°C	263°C
Flash point	>100°C	>100°C
Specific gravity	0.987–0.990 (1.00) at 25°C	0.973–0.976 at 25°C; 0.9845 at 15°C
Refractive index	1.4860–1.4900 at 20°C	1.4840–1.4860 (1.4855) at 20°C
Acid value	1 max	1 max
Solubility	1:3 in 80% alcohol	1:12–14 in 80% alcohol; 1:11 in 70% alcohol; insoluble in water
Organoleptic characteristics	Fruity odor; bittersweet taste reminiscent of unripe plum, pineapple, and banana	Fruity (rose-peach-apricot) odor; bittersweet flavor reminiscent of peach; not very stable
Synthesis	By esterification of phenethyl alcohol with *n*-hexanoic acid	By esterification of phenethyl alcohol with isovaleric acid
Natural occurrence	Reported found in several natural products	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 3.4 ppm Ice cream, ices, etc. 4.0 ppm Candy 13 ppm Baked goods 11 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 2.5 ppm Candy 5.9 ppm Baked goods 6.1 ppm Chewing gum 0.80–45 ppm
Regulatory status	FDA 121.1164; FEMA No. 2862	FDA 121.1164; FEMA No. 2871

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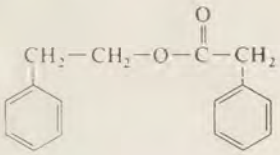
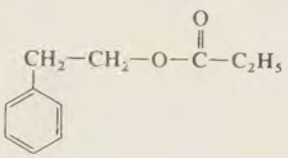
For References 1–5, see end of Part III.

	Phenethyl-2-methylbutyrate	Phenethyl octanoate
Other names	Benzyl carbinyl ethyl methyl acetate Phenethyl-α-methylbutanoate	Phenyl ethyl caprylate Phenethyl octoate Phenyl ethyl octanoate Benzyl carbinyl octylate
Empirical formula	$C_{13}H_{18}O_2$	$C_{16}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless oily liquid
Molecular weight	206.28	248.37
Melting point		295.5°C
Boiling point		143.5°C at 1.5 mm Hg
Specific gravity		0.9473 at 20°C
Refractive index		1.4801 at 20°C
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Sweet, floral, fruity odor with warm, herbaceous notes; sweet, slightly fruity taste	Mild fruity, wine-like odor
Synthesis	By esterification of phenethyl alcohol with α-methylbutyric acid	See Reference 6
Natural occurrence	In mint	
Reported uses[3]	The compound is used sometimes in imitation peppermint	Non-alcoholic beverages 5.0 ppm
Regulatory status	FDA 121.1164	FEMA No. 3222

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For References 1–5, see end of Part III.

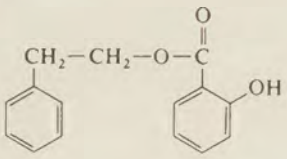
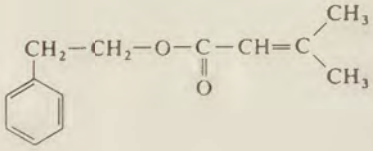
6. Mentani, *Koryo,* (61), 61, 1961; *Chem. Abstr.,* 58, 2400g, 1963.

	Phenethyl phenylacetate	Phenethyl propionate
Other names	Benzyl carbinyl phenylacetate 2-Phenylethyl phenylacetate Phenethyl-α-toluate	Benzyl carbinyl propionate 2-Phenylethyl propionate
Empirical formula	$C_{16}H_{16}O_2$	$C_{11}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid or white crystals at low temperature	Colorless, slightly oily liquid; sometimes yellowish
Assay	98% min	98% min
Molecular weight	240.31	178.23
Melting point	28°C	
Boiling point	325°C (177–178°C at 4–5 mm Hg)	245°C
Congealing point	26°C	
Flash point	>100°C	>100°C
Specific gravity	1.079–1.082 (1.09) at 25°C	1.010–1.014 at 25°/25°C
Refractive index		1.493–1.496 at 20°C
Acid value	1 max	1 max
Solubility	1:4 in 90% alcohol; insoluble in water	1:4 in 70% alcohol; soluble in propylene glycol; insoluble in water
Organoleptic characteristics	Heavy, sweet, floral, and balsamic odor, somewhat rosy; sweet, honey-like flavor	Very sweet odor reminiscent of red rose with a fruity undertone; honey-like flavor; warm, sweet raspberry and strawberry-like flavor
Synthesis	By esterification of phenylacetic acid with phenethyl alcohol in the presence of H_2SO_4;[6] also by direct esterification in the presence of gaseous HCl	By esterification of phenethyl alcohol with propionic acid
Natural occurrence	Not reported found in nature	In peanut (*Arachis hypogaea*)
Reported uses[3]	Non-alcoholic beverages 2.3 ppm Ice cream, ices, etc. 4.2 ppm Candy 4.8 ppm Baked goods 5.3 ppm Maraschino cherries 10 ppm	Non-alcoholic beverages 3.6 ppm Ice cream, ices, etc. 11 ppm Candy 12 ppm Baked goods 16 ppm
Regulatory status	FDA 121.1164; FEMA No. 2866	FDA 121.1164; FEMA No. 2867

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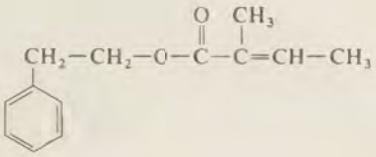
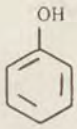
For References 1–5, see end of Part III.

6. **Hibbert and Burt,** *J. Am. Chem. Soc.*, 47, 2242, 1925.

	Phenethyl salicylate	Phenethyl senecioate
Other names	Benzyl carbinyl salicylate Phenethyl-2-hydroxybenzoate Phenethyl-*o*-hydroxybenzoate 2-Phenylethyl salicylate	Phenethyl-3,3-dimethylacrylate Phenethyl-3-methyl-2-butenoate Phenethyl-3-methylcrotonate
Empirical formula	$C_{15}H_{14}O_3$	$C_{13}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White, crystalline solid	Colorless, oily liquid
Assay	98% min	
Molecular weight	242.28	204.27
Melting point	44°C	
Boiling point	370°C	
Congealing point	41°C	
Specific gravity	1.15 (liquid)	
Acid value	1 max	
Solubility	1:16 in 95% alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Faint but persistent rose-like odor, somewhat hyacinth and carnation-like; sweet taste suggestive of peach, apricot, and honey	Faint, deep, sweet odor, somewhat herbaceous and winy; sweet, winy, and deep, fruity flavor
Synthesis	From phenethyl alcohol and methylsalicylate by interchange; also by esterification of phenethyl alcohol with salicylic acid	By esterification of phenethyl alcohol with 3-methylcrotonic acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.75 ppm Ice cream, ices, etc. 0.67 ppm Candy 1.5 ppm Baked goods 2.0 ppm	Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2868	FDA 121.1164; FEMA No. 2869

REFERENCES

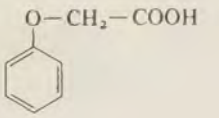
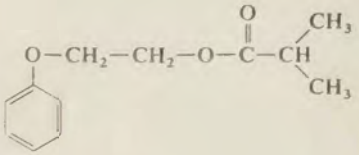
For References 1–5, see end of Part III.

	Phenethyl tiglate	Phenol
Other names	Benzyl carbinyl tiglate Phenethyl *trans*-2,3-dimethylacrylate Phenethyl *trans*-2-methylbutenoate Phenethyl *trans*-2-methylcrotonate Phenylethyl tiglate	Carbolic acid Benzenol Hydroxybenzene Phenic or phenylic acid Phenyl hydroxide Oxybenzene
Empirical formula	$C_{13}H_{16}O_2$	C_6H_5OH
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless or white needles; turns pink on exposure to air
Assay		98% min.
Molecular weight	204.27	94.11
Melting point		43°C
Boiling point	259°C	181.75°C 70.86°C at 10 mm Hg
Congealing point		41°C
Flash point		79°C
Specific gravity	1.02	1.0722 at 20/20°C 1.0576 at 20/4°C
Refractive index		1.5509 at 21°C 1.5418 at 41°C
Solubility	Insoluble in water; soluble in alcohol	Soluble in water, alcohol, chloroform, and carbon disulfide; very soluble in ether; soluble in carbon tetrachloride, acetone, and benzene in all proportions
Organoleptic characteristics	Pleasant, warm, rose-like, sweet odor; sweet, winy taste	
Synthesis	From phenethyl alcohol and tiglyl chloride in the presence of pyridine	See Reference 6
Natural occurrence	Not reported found in nature	Formed in dry distillation of wood, peat, and coal; coal tar is one of the commercial sources of phenol and its homologs; reported found as a constituent in coffee aroma;[7] also reported found in cognac[8] and in yellow passion fruit[9]
Reported uses[3]	Non-alcoholic beverages 0.80–0.90 ppm Ice cream, ices, etc. 4.3 ppm Candy 10 ppm Baked goods 10 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50 ppm Baked goods 0.50 ppm Gelatins and puddings 0.50 ppm
Regulatory status	FDA 121.1164; FEMA No. 2870	FEMA No. 3223

REFERENCES

For References 1–5, see end of Part III.

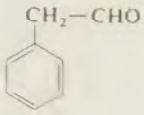
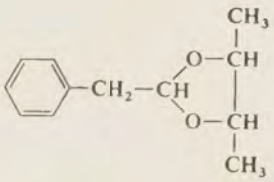
6. **Dierichs and Rubička,** *Phenole und Basen, Vorkommen und Gewinnung,* Akademie-Verlag, Berlin, 1958.
7. **Stoll et al.,** *Helv. Chim. Acta,* 50, 628, 1967.
8. **Schaefer and Timmer,** *J. Food Sci.,* 35(1), 10, 1970.
9. **Winter and Klöty,** *Helv. Chim. Acta,* 55(6), 1916, 1972.

	Phenoxyacetic acid	2-Phenoxyethyl isobutyrate
Other names	Glycolic acid phenyl ether Phenoxyethanoic acid *o*-Phenylglycolic acid Phenylium	Ethyleneglycol monophenylether, isobutyrate 2-Phenoxyethyl isobutanoate Phenylcellosolve isobutyrate
Empirical formula	$C_8H_8O_3$	$C_{12}H_{16}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Crystalline solid	Colorless liquid
Assay		97% min
Molecular weight	152.14	208.26
Melting point	98°C	
Boiling point	285°C (decomposes)	265°C
Flash point		>100°C
Specific gravity		1.044–1.048 at 25°/25°C
Refractive index		1.4920–1.4950 at 20°C
Acid value		1 max
Solubility	Slightly soluble in water; readily soluble in alcohol, ether, and other common organic solvents	1:2 in 70% alcohol
Organoleptic characteristics	Sour, sweet odor; honey-like taste	Faint, rose-like and honey odor; sweet, fruity (peach-like) taste
Synthesis	By reacting phenol and monochloroacetic acid	From the corresponding phenoxyethyl alcohol and isobutyric acid in the presence of boric acid in benzene solution[6]
Natural occurrence	Reported as naturally occurring in cocoa beans	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.37 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.2 ppm Baked goods 2.2 ppm	Non-alcoholic beverages 0.90–5.0 ppm Ice cream, ices, etc. 5.0–30 ppm Candy 15–30 ppm Baked goods 15–30 ppm
Regulatory status	FDA 121.1164; FEMA No. 2872	FDA 121.1164; FEMA No. 2873

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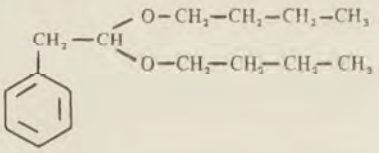
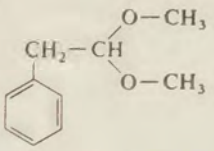
For References 1–5, see end of Part III.

6. Takaharu and Mentani, *Chem. Abstr.*, 58, 2400g, 1963.

	Phenylacetaldehyde	Phenylacetaldehyde-2,3-butylene glycol acetal
Other names	Hyacinthin 1-Oxo-2-phenylethane x-Toluic aldehyde α-Tolualdehyde α-Tolyl aldehyde	4, 5-Dimethyl-2-benzyl-1,3-dioxolan
Empirical formula	C_8H_8O	$C_{12}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow, oily liquid; becomes more viscous on aging	Colorless, viscous liquid
Assay	90% min[2] (95%)	
Molecular weight	120.14	192.26
Melting point	33–34°C	
Boiling point	193–194°C (206°C)	
Flash point	68°C	
Specific gravity	1.025–1.035[2] (1.023–1.040) at 25°/25°C	
Refractive index	1.5240–1.5320 at 20°C[2]	
Acid value	Not more than 5.0[2]	
Solubility	1:2 in 80% alcohol;[2] insoluble in water; soluble in most common organic solvents	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Harsh, green odor reminiscent of hyacinth on dilution; unpleasant, pungent, bitter flavor, turning sweet and fruit-like at low levels	Sweet, floral, somewhat earthy fragrance; fruity flavor
Synthesis	By Darzen glycidic ester synthesis from benzaldehyde;[2] readily oxidizable to phenylacetic acid	By condensation of phenylacetaldehyde with 2,3-butylene glycol
Natural occurrence	Identified among the constituents of several essential oils: neroli, *Citrus sinensis* leaves, other citrus species (flowers and leaves), narcissus, magnolia, lily, rose, tea, and others	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.68 ppm Ice cream, ices, etc. 0.75 ppm Candy 1.6 ppm Baked goods 2.0 ppm Chewing gum 1.7–87 ppm	Candy 4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2874	FDA 121.1164; FEMA No. 2875

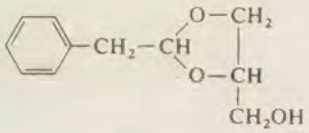
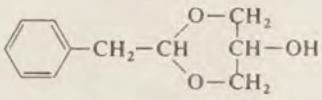
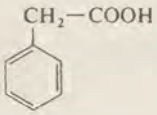
REFERENCES

For References 1–5, see end of Part III.

	Phenylacetaldehyde diisobutyl acetal	Phenylacetaldehyde dimethyl acetal
Other names	1,1-Diisobutoxy-2-phenylethane	1,1-Dimethoxy-2-phenylethane α-Toluic aldehyde dimethylacetal
Empirical formula	$C_{16}H_{26}O_2$	$C_{10}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay		95% min[2]
Molecular weight	250.38	166.22
Boiling point	240°C	221°C
Flash point		88°C
Specific gravity	0.93	1.000–1.006 at 25°/25°C[2]
Refractive index		1.4930–1.4960 at 20°C[2]
Acid value		Not more than 1[2]
Free aldehyde content		3.0% max[2]
Solubility	Almost insoluble in water; soluble in alcohol and oils	1:2–10 in 70% ethanol; insoluble in water
Organoleptic characteristics	Sweet, floral, delicate-green odor	Strong, green odor with hyacinth-like note; at low levels sweet, green, spicy flavor, turning bitter at high levels
Synthesis	From benzyl magnesium chloride and butyl *o*-formate; also from phenyl acetaldehyde and butyl alcohol	By the cold reaction of the corresponding aldehyde with methanol or with orthoformic ester in the presence of acid[2]
Natural occurrence		In Bulgarian tobacco
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Alcoholic beverages 25.0 ppm Ice cream, ices, etc. 30.0 ppm Candy 75.0 ppm Baked goods 50.0 ppm Gelatins and puddings 50.0 ppm	Non-alcoholic beverages 0.40 ppm Ice cream, ices, etc. 0.78 ppm Candy 1.4 ppm Baked goods 8.8 ppm Chewing gum 1.0 ppm
Regulatory status	FEMA No. 3384	FDA 121.1164; FEMA No. 2876

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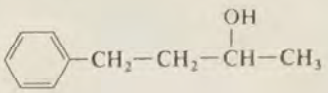
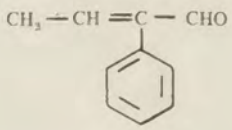
For References 1–5, see end of Part III.

	Phenylacetaldehyde glyceryl acetal	Phenylacetic acid
Other names	Mixture of 60% 5-hydroxymethyl-2-benzyl-1,3-dioxolan and 40% 5-hydroxy-2-benzyl-1,3-dioxan	α-Toluic acid
Empirical formula	$C_{11}H_{14}O_3$	$C_8H_8O_2$
Structure	 60%  40%	
Physical/chemical characteristics[5]		
Appearance	Colorless, viscous liquid	White, crystalline solid (leaf)
Assay		99–100%[2]
Molecular weight	194.23	136.15
Melting point		76–78°C[2]
Boiling point		265.5°C (266°C)
Flash point	95°C	
Specific gravity	1.1650–1.1680 at 15°C	1.080 at 15.5°C
Refractive index	1.5315–1.5345 at 20°C	
Aldehyde content	0.5% max	
Solubility	1:4–7 in 30% alcohol; insoluble in water	Slightly soluble (2%) in cold water; soluble in hot water, alcohol, ether, and propylene glycol
Organoleptic characteristics	Faint, sweet, rosy odor; sweet, green flavor	Geranium-leaf and rose-like odor in dilute solution; persistent and disagreeable in concentrated solution; sweet, honey-like flavor at high levels; at low levels, a sweetener
Synthesis	From phenylacetaldehyde and glycerol	By the treatment of benzyl cyanide with dilute sulfuric acid[6] and other procedures
Natural occurrence	Not reported found in nature	Reported found among the constituents of a few essential oils: tobacco, *Rosa centifolia*,[7] Bulgarian rose,[8] orange flowers absolute,[9] neroli, and *Mentha arvensis* of Japanese origin; also reported present among the volatile constituents of cocoa[10]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 20 ppm Candy 0.06–20 ppm	Non-alcoholic beverages 1.8 ppm Alcoholic beverages 0.10 ppm Ice cream, ices, etc. 5.3 ppm Candy 5.9 ppm Baked goods 12 ppm Gelatins and puddings 27 ppm Chewing gum 5.4–11 ppm Syrups 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2877	FDA 121.1164; FEMA No. 2878

REFERENCES

For References 1–5, see end of Part III.

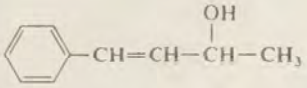
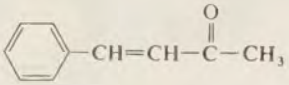
6. Blatt, A. H. (Ed.), *Organic Syntheses*, Coll. Vol. 1, John Wiley & Sons, 1941, 436.
7. Igolen, *Chem. Zentralbl.*, 2, 2718, 1939.
8. Guenther and Garnier, *Chem. Zentralbl.*, 1, 2128, 1931.
9. Elze, *Chem. Zentralbl.*, 2, 660, 1926.
10. Quesnel, *Choc. Confiserie Fr.*, 213, 30, 1965.

	4-Phenyl-2-butanol	2-Phenyl-2-butenal
Other names	Methyl phenethyl carbinol Phenylethyl methyl carbinol	2-Phenyl crotonaldehyde
Empirical formula	$C_{10}H_{14}O$	$C_{10}H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	
Molecular weight	150.22	146.18
Boiling point	123–124°C at 15 mm Hg	177°C at 15 mm Hg
Specific gravity	0.976 at 19°C	1.045 at 18/0°C
Refractive index	1.513 at 17°C	1.5605 at 18°C
Organoleptic characteristics	Characteristic, aromatic, floral odor	
Synthesis	The optically inactive product can be prepared by hydrogenation of benzylidene acetone in alcohol solution; under pressure in the presence of platinum oxide, palladium oxide, or ferrous sulfate;[6] by reduction with magnesium in methanol[7]	From acetaldehyde and phenyl acetaldehyde[8]
Natural occurrence	Not reported found in nature	Reported as the odorous component in black tea[9] and in *Phallus impudicus*[10]
Reported uses[3]	Non-alcoholic beverages 0.12–0.90 ppm Ice cream, ices, etc. 0.60–6.0 ppm Candy 1.5–15 ppm Baked goods 1.5–15 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm Gelatins and puddings 2.0 ppm Chewing gum 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2879	FEMA No. 3224

REFERENCES

For References 1–5, see end of Part III.

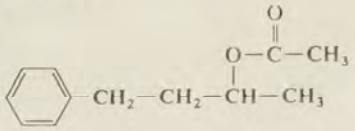
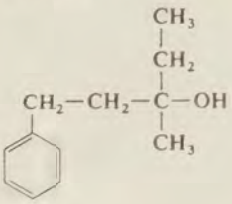
6. **Kern, Shriner and Adams,** *J. Am. Chem. Soc.*, 47, 1157, 1925.
7. **Zechmeister and Rom,** *Ann. Chem.*, 468, 126, 1929.
8. **Kuhn and Michel.,** *Ber. Dtsch. Chem. Ges.*, 71, 1119, 1938.
9. **Bricout, Viani, Muggler-Chavan, Marion, Reymond and Egli,** *Helv. Chim. Acta*, 50(6), 1517, 1967.
10. **List and Freund,** *Naturwissenschaften*, 53(22), 585, 1966.

	4-Phenyl-3-buten-2-ol	4-Phenyl-3-buten-2-one
Other names	Methyl styryl carbinol	Benzylidene acetone Cinnamyl methyl ketone Methyl styryl ketone
Empirical formula	$C_{10}H_{12}O$	$C_{10}H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Dense, oily liquid	Colorless to slightly yellow, crystalline solid
Assay		97% min
Molecular weight	148.20	146.18
Melting point		41–42°C
Boiling point	131°C at 12 mm Hg	260–262°C; 147–149°C at 20 mm Hg
Congealing point		39°C
Specific gravity	1.0134 at 22°C	1.0076 at 47.3°C
Refractive index		1.5824 at 47.3°C
Solubility	Insoluble in water; soluble in most organic solvents	Readily soluble in alcohol, ether, benzene, and chloroform; 1:3 in 60% alcohol
Organoleptic characteristics	Characteristic floral odor	Odor reminiscent of coumarin and rhubarb; sharp, pungent flavor; not very stable
Synthesis	From cinnamic aldehyde and magnesium methyl bromide in ether solution and subsequent hydrolysis of the ester[8]	By condensing benzaldehyde and acetone in the presence of an alkaline condensing agent.[6] For the synthesis of *cis*- and *trans*-benzylidene acetone, see reference 7.
Natural occurrence	Not reported found in nature	In hydrolyzed soy protein
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 20 ppm Candy 0.03–20 ppm Baked goods 20 ppm	Non-alcoholic beverages 0.82 ppm Ice cream, ices, etc. 0.84 ppm Candy 3.7 ppm Baked goods 4.5 ppm Gelatins and puddings 2.1 ppm Shortening 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2880	FDA 121.1164; FEMA No. 2881

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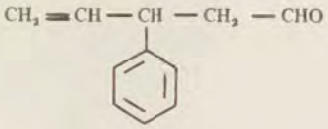
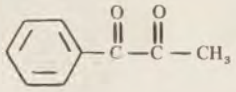
For References 1–5, see end of Part III.

6. **Lawson et al.,** *J. Chem. Soc.*, 125, 636, 1924.
7. **Schinz,** *Riechst. Aromen*, 5, 67, 1955.
8. **Muskat and Ludeman,** *Chem. Ber.*, 62, 2286, 1929.

	4-Phenyl-2-butyl acetate	1-Phenyl-3-methyl-3-pentanol
Other names	Phenylethyl methyl carbinyl acetate	Methyl ethyl phenylethyl carbinol 3-Methyl-1-phenyl-3-pentanol Phenylethyl methyl ethyl carbinol
Empirical formula	$C_{12}H_{16}O_2$	$C_{12}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, slightly viscous liquid
Molecular weight	192.26	178.27
Boiling point	123–124°C at 13 mm Hg; *d*, 130°C at 15 mm Hg	254°C
Specific gravity	0.991 at 16°C; *d*, 0.9874 at 17°C	0.97
Refractive index	1.4895 at 16°C; *d*, 1.5012 at 20°C	
Optical rotation	*d*, +0.83°	
Solubility	Insoluble in water; soluble in alcohol	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Mild, green, fruity odor; sweet, fruity taste	Warm, rose-like odor; fruity, green taste
Synthesis	By acetylation of the corresponding alcohol. The racemic and the *dextro*-rotatory forms are known.	From phenethyl magnesium bromide and methyl ethyl ketone
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.10–3.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Baked goods 0.50–3.0 ppm	Non-alcoholic beverages 0.16 ppm Candy 0.16 ppm Gelatins and puddings 0.60 ppm
Regulatory status	FDA 121.1164; FEMA No. 2882	FDA 121.1164; FEMA No. 2883

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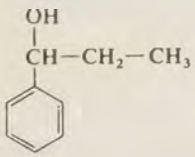
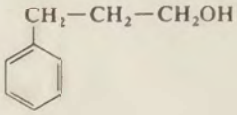
For References 1–5, see end of Part III.

	3-Phenyl-4-pentenal		1-Phenyl-1,2-propanedione	
Other names	β-Vinylhydrocinnamaldehyde		Acetyl benzoyl Methyl phenyl diketone Methyl phenyl glyoxal	
Empirical formula	$C_{11}H_{12}O$		$C_9H_8O_2$	
Structure				
Physical/chemical characteristics[5]				
Appearance			Yellow oily liquid	
Molecular weight	160.21		148.17	
Boiling point			222°C 101°C at 12 mm Hg	
Specific gravity			1.0065 at 20°C	
Refractive index			1.537 at 10°C	
Solubility			Soluble in water, alcohol, and ether	
Organoleptic characteristics			Pungent odor	
Synthesis			By oxidation of propiophenone or benzyl methyl ketone with selenium dioxide;[6,7] by the acid hydrolysis of oximinopropiophenone[8] or other synthetic routes[9]	
Natural occurrence	Not reported found in nature		Reported found as a constituent in coffee aroma[10]	
Reported uses[3]	Non-alcoholic beverages	1.0 ppm	Non-alcoholic beverages	10.0 ppm
	Candy	1.0 ppm	Ice cream, ices, etc.	10.0 ppm
	Baked goods	1.0 ppm	Candy	10.0 ppm
	Meat, meat sauces, soups	1.0 ppm	Gelatins and puddings	10.0 ppm
	Milk, dairy products	1.0 ppm		
	Cereals	1.0 ppm		
Regulatory status	FEMA No. 3318		FEMA No. 3226	

REFERENCES

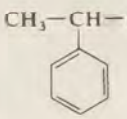
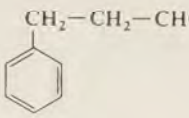
For References 1–5, see end of Part III.

6. **Riley et al.,** *J. Chem. Soc.*, p. 1875, 1932.
7. **Wegmann and Dalm,** *Helv. Chim. Acta*, 29, 1247, 1946.
8. **Hartmann and Roll,** in *Organic Syntheses*, Coll. Vol. 2, Blatt, A. H., Ed., Wiley & Sons, New York, 1943.
9. **Rodd,** *Chemistry of Carbon Compounds*, Vol. 3, Part B, American Elsevier, New York, 1956, 898.
10. **Stoll et al.,** *Helv. Chim. Acta*, 50, 628, 1967.

	1-Phenyl-1-propanol	3-Phenyl-1-propanol
Other names	Dihydro isocinnamic alcohol Dihydro-α-phenyl allyl alcohol Ethyl phenyl carbinol Phenylethyl carbinol *sec*-Phenyl propyl alcohol	Benzyl ethyl alcohol Hydrocinnamyl alcohol Phenyl propyl alcohol
Empirical formula	$C_9H_{12}O$	$C_9H_{12}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless, slightly viscous liquid
Assay		98% min[2]
Molecular weight	136.19	136.19
Boiling point	220°C	233–235°C at 740 mm Hg
Specific gravity	0.99	0.998–1.002 at 25°/25°C;[2] 1.006 at 24°C
Refractive index		1.5240–1.5280 at 20°C;[2] 1.5351 at 23°C
Aldehyde content		0.5% max (as phenylpropyl aldehyde)
Solubility	Insoluble in water; soluble in alcohol	1:1 in 70% alcohol;[2] 1:4 in 45% alcohol; 1:3 in 50% alcohol; soluble in water (1:300) and most common organic solvents
Organoleptic characteristics	Balsamic, floral fragrance; sweet, honey-like taste	Characteristic sweet, hyacinth-mignonette odor; sweet and pungent taste suggestive of apricot
Synthesis	By hydrogenation of phenethyl ketone	By hydrogenation of either cinnamic aldehyde or cinnamic alcohol[2]
Natural occurrence	Not reported found in nature	Frequently occurring in nature—storax, Sumatra benzoin, tea, Peru balsam, and other products (passion fruit, strawberry)
Reported uses[3]	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.50 ppm Candy 1.5 ppm Baked goods 1.5 ppm	Non-alcoholic beverages 0.73 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 1.4 ppm Candy 2.8 ppm Baked goods 3.3 ppm Chewing gum 4.3 ppm
Regulatory status	FDA 121.1164; FEMA No. 2884	FDA 121.1164; FEMA No. 2885

REFERENCES

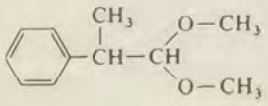
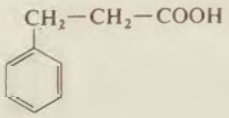
For References 1–5, see end of Part III.

	2-Phenylpropionaldehyde	3-Phenylpropionaldehyde
Other names	Hydratropaldehyde α-Methyl phenylacetaldehyde α-Methyl tolualdehyde 2-Phenylpropanal α-Phenyl propionaldehyde	Benzyl acetaldehyde Dihydrocinnamic aldehyde Hydrocinnamaldehyde Hydrocinnamic aldehyde β-Phenyl propionaldehyde Phenylpropyl aldehyde
Empirical formula	$C_9H_{10}O$	$C_9H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to pale-yellow liquid	Colorless to pale-yellow liquid
Assay	95% min[2] (98% min)	96% min
Molecular weight	134.17	134.17
Boiling point	204°C	104–105°C (222°C) at 13 mm Hg
Flash point	80°C	97°C (95°C)
Specific gravity	0.998–1.006 at 25°/25°C;[2] 1.0050–1.0080 at 15°C	1.0160–1.0200 at 15°C; 1.010–1.020 at 25°C
Refractive index	1.5140–1.5190[2] (1.5155–1.5175) at 20°C	1.5205–1.5240 (1.5200–1.5220) at 20°C
Aldehyde content		3.7 max
Acid value	Not more than 5[2] (0.9)	
Solubility	1:3–10 in 80% alcohol;[2] 1:2–4 in 70% alcohol	Insoluble in water; soluble in most common organic solvents; 1:2 in 70% alcohol; 1:7 in 60% alcohol; 1:19 in 50% alcohol
Organoleptic characteristics	Intense, green, floral odor reminiscent of hyacinth	Strong, floral odor reminiscent of hyacinth; balsamic, green, warm (almost burning) flavor
Synthesis	By alkaline condensation of acetophenone and ethyl chloroacetate; also by distillation of methylphenyl ethylene glycol in 91% yields (under atmospheric pressure). See reference 6.	From phenyl propionitrile; also from cinnamic aldehyde diethylacetal
Natural occurrence	Not reported found in nature	Reported found in the essential oil of Ceylon cinnamon and in strawberry
Reported uses[3]	Non-alcoholic beverages 0.61 ppm Ice cream, ices, etc. 0.30 ppm Candy 0.85 ppm Baked goods 0.85 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.7 ppm Candy 5.0 ppm Baked goods 5.5 ppm Gelatins and puddings 4.3 ppm
Regulatory status	FDA 121.1164; FEMA No. 2886	FDA 121.1164; FEMA No. 2887

REFERENCES

For References 1–5, see end of Part III.

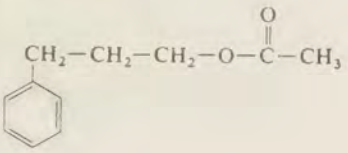
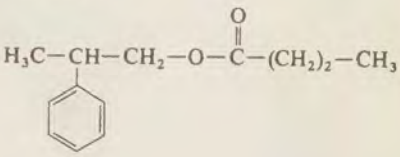
6. **Wagner**, *Die Riechstoffe und ihre Derivate — Die Aldehyde*, Hartleben's ed., 1929, 617.

	2-Phenylpropionaldehyde dimethyl acetal	3-Phenylpropionic acid
Other names	1,1-Dimethoxy-2-phenylpropane Hydratropic aldehyde dimethyl acetal	Benzylacetic acid Hydrocinnamic acid γ-Phenylpropionic acid
Empirical formula	$C_{11}H_{16}O_2$	$C_9H_{10}O_2$
Structure		
Physical/chemical characteristics[4]		
Appearance	Oily liquid	White, crystalline solid
Molecular weight	180.25	150.18
Melting point		47–48°C (49°C)
Boiling point	240–241 C; 111–112°C at 14 mm Hg	280 C; 169–170°C at 28 mm Hg
Specific gravity	0.990 at 15.5°C; 0.9883 at 19°C	1.07 (liquid)
Refractive index	1.4990 at 20°C	
Solubility	Insoluble in water; soluble in alcohol	Slightly soluble in water (0.6%); soluble in alcohol, ether, propylene glycol, and glycerin
Organoleptic characteristics	Strong, warm, spicy odor reminiscent of walnut; warm, mushroom, nut-like taste	Faint, sweet odor, somewhat balsamic and coumarin-like; mildly sweet-sour taste, vanilla-like
Synthesis	By catalytic hydrogenation of cinnamyl aldehyde dimethyl acetal in the presence of colloidal palladium;[6] or from 2-phenylpropionaldehyde and a methanolic solution of HCl[7]	By reduction of cinnamic acid using sodium amalgam
Natural occurrence	Not reported found in nature	Reported found in raspberry and labdanum
Reported uses[3]	Non-alcoholic beverages 0.26 ppm Ice cream, ices, etc. 0.51 ppm Candy 1.5 ppm Baked goods 3.1 ppm Chewing gum 5.0 ppm Condiments 5.0 ppm	Non-alcoholic beverages 0.02–1.0 ppm Ice cream, ices, etc. 0.48–1.0 ppm Candy 0.80–4.0 ppm Baked goods 17 ppm Gelatins and puddings 1.2 ppm Dairy products 2.0 ppm Toppings 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2888	FDA 121.1164; FEMA No. 2889

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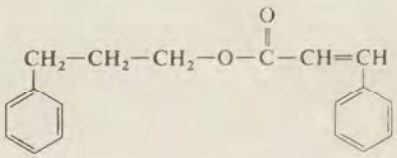
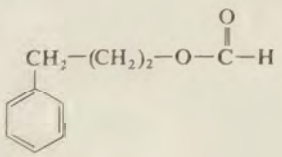
For References 1–5, see end of Part III.

6. Strauss and Berkow, *Ann. Chem.*, 401, 158, 1913.
7. Fischer and Hoffa, *Ber. Dtsch. Chem. Ges.*, 31, 1992, 1898.

	3-Phenylpropyl acetate	2-Phenylpropyl butyrate
Other names	Hydrocinnamyl acetate	Hydratropyl butyrate β-Methyl phenethyl butyrate α-Phenylpropyl alcohol, butyric ester 2-Phenylpropyl-*n*-butyrate
Empirical formula	$C_{11}H_{14}O_2$	$C_{13}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	98% min	
Molecular weight	178.23	206.28
Boiling point	244–245°C	
Specific gravity	1.012–1.015 at 25°C; 1.0285 at 15°C	
Refractive index	1.4940–1.4970 (1.4975) at 20°C	
Solubility	1:2–3 in 70% alcohol; soluble in most common organic solvents	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic floral, spicy odor reminiscent of phenylpropyl alcohol and of geranyl acetate; bittersweet, burning flavor suggestive of currant	Fruity, woody, very sweet odor; sweet flavor reminiscent of plum
Synthesis	By acetylation of the corresponding alcohol	By esterification of the alcohol with *n*-butyric acid
Natural occurrence	Reported found among the constituents of the essential oils of narcissus and *Heracleum candicans* and probably in cinnamon	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.2 ppm Ice cream, ices, etc. 4.8 ppm Candy 4.6 ppm Baked goods 6.3 ppm Chewing gum 10 ppm Condiments 0.10 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2890	FDA 121.1164; FEMA No. 2891

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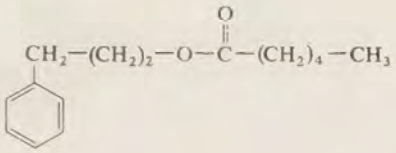
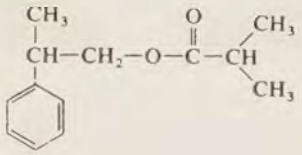
For References 1–5, see end of Part III.

	3-Phenylpropyl cinnamate	3-Phenylpropyl formate
Other names	Hydrocinnamyl cinnamate 3-Phenylpropyl-β-phenylacrylate 3-Phenylpropyl-3-phenyl-2-propenoate	Hydrocinnamyl formate 3-Phenyl-1-propyl methanoate
Empirical formula	$C_{18}H_{18}O_2$	$C_{10}H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow liquid	Colorless liquid
Assay	98% min	90% min
Molecular weight	266.33	164.21
Boiling point	> 300°C (decomposes)	238°C (approx 280°C)
Flash point	> 100°C	> 100°C
Specific gravity	1.074–1.078 at 25°C	1.035–1.038 at 25°C
Refractive index	1.585–1.588 at 20°C	1.5030–1.5060 at 20°C
Acid value	1 max	2 max
Solubility	Slightly soluble in 95% alcohol; soluble in benzyl benzoate and in diethylphthalate	Insoluble in water; soluble in most common organic solvents; 1:2 in 80% alcohol
Organoleptic characteristics	Sweet, heavy, floral-fruity odor with a balsamic note; sweet flavor suggestive of cocoa	Sweet, floral odor reminiscent of honey and hyacinth; powerful, sweet, fruity, herbaceous taste
Synthesis	From phenylpropyl alcohol and methylcinnamate	Cold formylation of phenylpropyl alcohol
Natural occurrence	Reported found in Oriental storax,[6-8] American storax,[9-10] Peru balsam from Honduras,[11-13] and Sumatra benzoin[14]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.4 ppm Ice cream, ices, etc. 4.1 ppm Candy 4.3 ppm Baked goods 5.3 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 0.90–1.5 ppm Candy 3.0–5.0 ppm Baked goods 2.7 ppm
Regulatory status	FDA 121.1164; FEMA No. 2894	FDA 121.1164; FEMA No. 2895

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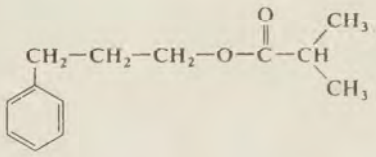
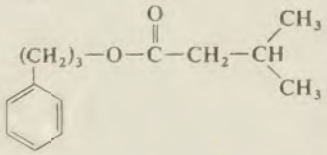
For References 1–5, see End of Part III.

6. Miller, *Chem. Ber.*, 9, 275, 1876.
7. Miller, *Chem. Ann.*, 188, 201, 1877; 189, 353, 1877.
8. Tschirch and van Itallie, *Arch. Pharm.*, 239, 513, 1901.
9. Miller, *Arch. Pharm.*, 220, 648, 1882.
10. Tschirch and van Itallie, *Arch. Pharm.*, 239, 536, 1901.
11. Thoms and Blitz, *Chem. Zentralbl.*, 2, 1047, 1904.
12. Hellstrom, *Arch. Pharm.*, 218, 243, 1881.
13. Tschirch and Werdmüller, *Arch. Pharm.*, 248, 421, 1910.
14. Tschirch and Ludy, *Arch. Pharm.*, 231, 54, 1893.

	3-Phenylpropyl hexanoate	2-Phenylpropyl isobutyrate
Other names	Hydrocinnamyl hexanoate 3-Phenylpropyl caproate Phenylpropyl capronate Phenylpropyl hexylate	Hydratropyl isobutyrate β-Methyl phenethyl isobutyrate α-Phenylpropyl alcohol, isobutyric ester
Empirical formula	$C_{15}H_{22}O_2$	$C_{13}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	234.35	206.28
Boiling point	292°C	
Specific gravity	1.01	
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Sweet, fruity, green odor; powerful, warm, fruity taste of peach and pineapple	Fruity, woody, highly sweet odor; fruity, sweet taste
Synthesis	By esterification of phenylpropyl alcohol with *n*-hexanoic acid	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.6 ppm Ice cream, ices, etc. 1.3 ppm Candy 3.3 ppm Baked goods 3.7 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 20 ppm Candy 20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2896	FDA 121.1164; FEMA No. 2892

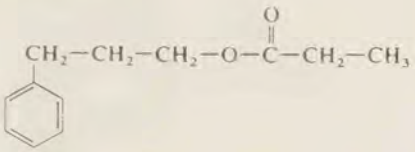
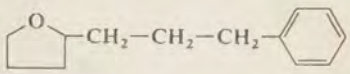
REFERENCES

For References 1–5, see end of Part III.

	3-Phenylpropyl isobutyrate	3-Phenylpropyl isovalerate
Other names	Hydrocinnamyl isobutyrate	Hydrocinnamyl isovalerate 3-Phenylpropyl-β-methylbutyrate
Empirical formula	$C_{13}H_{18}O_2$	$C_{14}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	206.28	220.31
Boiling point	258°C	280°C
Specific gravity	0.99	1.00
Solubility	Insoluble in water; soluble in propylene glycol and alcohol	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Sweet, balsamic odor, finer and fresher than the corresponding *n*-butyrate; bittersweet flavor reminiscent of peach	Complex, fruity (strawberry-raspberry) odor with a plum-like undertone; sweet, jam-like, fruity taste with nut-like undernotes
Synthesis	By esterification of hydrocinnamic alcohol with *n*-butyric acid	By esterification of phenylpropyl alcohol with isovaleric acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 3.0 ppm Candy 5.0 ppm Baked goods 5.8 ppm	Non-alcoholic beverages 0.90 ppm Ice cream, ices, etc. 0.90 ppm Candy 1.8 ppm Baked goods 1.7 ppm
Regulatory status	FDA 121.1164; FEMA No. 2893	FDA 121.1164; FEMA No. 2899

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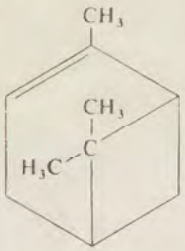
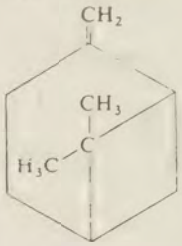
For References 1–5, see end of Part III.

	3-Phenylpropyl propionate	2-(3-Phenylpropyl)-tetrahydrofuran
Other names	Hydrocinnamyl propionate 3-Phenylpropyl propanoate β-Phenylpropyl propionate	2-Hydrocinnamyl tetrahydrofuran α-(3-Phenylpropyl)-tetrahydrofuran
Empirical formula	$C_{12}H_{16}O_2$	$C_{13}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to pale, straw yellow liquid
Molecular weight	192.26	190.28
Boiling point	265°C (247°C)	105–107°C at 1 mm Hg
Specific gravity	1.010 at 15.5°C	
Refractive index	1.5125 at 20°C	1.5142 at 20°C
Solubility	Almost insoluble in water; soluble in alcohol	Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Heavy floral, balsamic odor with hyacinth and mimosa undertone; sweet, fruity, slightly green taste at low concentrations	Sweet, fruity odor; honey-like, sweet flavor
Synthesis	By esterification of phenylpropyl alcohol with propionic acid	From β-[2-(5-phenyl furyl)]-propionic acid butyl ester by catalytic hydrogenation with copper chromite under pressure and subsequent ring closure by heating the intermediate 7-phenyl-heptan-1,4-diol in the presence of Al_2O_3[6]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.49 ppm Ice cream, ices, etc. 0.52 ppm Candy 2.0 ppm Baked goods 2.4 ppm Chewing gum 0.80–50 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 2.0 ppm Candy 0.03–2.0 ppm Gelatins and puddings 2.0 ppm Chewing gum 2.3 ppm
Regulatory status	FDA 121.1164; FEMA No. 2897	FDA 121.1164; FEMA No. 2898

REFERENCES

For References 1–5, see end of Part III.

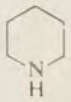
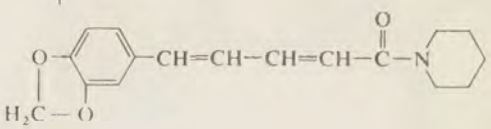
6. **Thewalt and Rudolph,** *Ber. Dtsch. Chem. Ges.*, 96, 136, 1963.

	α-Pinene	β-Pinene
Other names	2-Pinene 2,6,6-Trimethylbicyclo-(3,1,1)-2-heptene	6,6-Dimethyl-2-methylene norpinane Nopinene 2(10)-Pinene
Empirical formula	$C_{10}H_{16}$	$C_{10}H_{16}$
Structure		
Physical/chemical characteristics[5]		
Appearance	Mobile, colorless liquid	Colorless liquid
Assay		85–90%; 96% (1% α-pinene content)
Molecular weight	136.23	136.23
Melting point	−62.5°C	
Boiling point	156°C at 760 mm Hg	*d*-, 164–166°C; *l*-, 162–163°C
Specific gravity	0.8625 at 15°C	*d*-, 0.8660 at 20°C; *l*-, 0.8666 at 25°C
Refractive index	1.4680 at 15°C	*d*-, 1.4746 at 20°C; *l*-, 1.4762 at 25°C
Optical rotation	*d*-, +51°8′; *l*-, −51°17′, −58°	*d*-, +28.6°; *l*-, −23.4°
Solubility	Insoluble in water; soluble in alcohol, chloroform, and ether; almost insoluble in propylene glycol and glycerin	Insoluble in water; soluble in alcohol; almost insoluble in propylene glycol
Organoleptic characteristics	Characteristic odor of pine; turpentine-like; oxidized material rosin-like odor.	Characteristic turpentine odor; dry, woody or resinous aroma
Synthesis	From turpentine, by distillation. For total synthesis see Reference 6.	Isolated from American turpentine; also by conversion from α-pinene; as an intermediate extremely important for the manufacture of citral, citronellol, hydroxycitronellal, geraniol, citronellal, linalool, ionones, methylionones, and menthol
Natural occurrence	The structure would account for the presence of four optically active and two optically inactive isomers. Only *d*-, *l*-, and *dl*-α-pinene are known, however. Its presence in nature has been reported in more than 400 essential oils. In the largest amounts it has been reported found in: *Achillea millefolium* (*d*-), *Artemisia tridentata* (*d*-), Italian rosemary (*l*-), wild thyme (*l*-), French lavender (*l*-), coriander (*d*-, *dl*-), cumin (*d*-, *dl*-), labdanum (*l*-), neroli (*l*-), lemon, *Litsea cubeba* (*d*-), and ylang-ylang (*d*-).	Usually occurring together with α-pinene but in smaller amounts. The *d*- and *l*-forms are reported found in the essential oils of various *Artemisiae* and several *Cupressaceae*, in coriander and cumin. The *l*-form is a constituent of several citrus oils
Reported uses[3]	Non-alcoholic beverages 16–54 ppm Ice cream, ices, etc. 64 ppm Candy 48 ppm Baked goods 160 ppm Condiments 2.6–150 ppm	Non-alcoholic beverages 0.05–16 ppm Ice cream, ices, etc. 64 ppm Candy 48–600 ppm Baked goods 48–600 ppm
Regulatory status	FDA 121.1164; FEMA No. 2902	FDA 121.1164; FEMA No. 2903

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For References 1–5, see end of Part III.

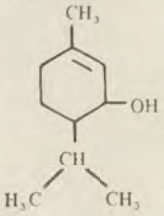
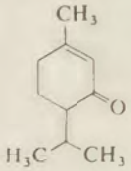
6. Komppa, *Ann. Acad. Sci. Fenn. Ser. A*, 59, 3, 1943.

	Piperidine	Piperine
Other names	Hexahydropyridine Hexazane Pentamethylenimine	1-Piperoylpiperidine
Empirical formula	$C_5H_{11}N$	$C_{17}H_{19}NO_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless prisms (from alcohol and other solvents)
Assay	95–98%	
Molecular weight	85.15	285.32
Melting point	−7° to −9°C	128–129.5°C
Boiling point	106°C	
Congealing point	−13 to −17°C	
Flash point	16°C	
Specific gravity	0.8628 at 18.7°C (0.8615 at 20°C)	1.193 (liquid)
Refractive index	1.4535 at 18.7°C (1.4530 at 20°C)	
Optical rotation		
Solubility	Soluble in water, alcohol, ether, and chloroform	Almost insoluble in water; soluble in alcohol (10%), chloroform, and ether
Organoleptic characteristics	Heavy, sweet, floral, animal odor; burning peppery taste	Odorless; tasteless at first, but developing a burning aftertaste of pepper
Synthesis	Usually prepared by electrolytic reduction of pyridine	From piperoyl chloride and piperidine[12]
Natural occurrence	Reported found in black pepper,[6,7] *Piper officinarum*,[8] *Psilocaulon absimile* N.E. Br.,[9] tobacco,[10] and *Petrosimonia monandra*[11]	Reported found in black pepper; also in *Piper longum*, *Piper officinarum*, *Piper lowong* Bl.,[13] *Piper famechoni*,[14] *Piper chaba*,[15] and the leaves of *Rhododendron fauriae* var. *rupescens*[16]
Reported uses[3]	Non-alcoholic beverages 3.0 ppm Candy 5.0 ppm Baked goods 0.05–5.0 ppm Condiments 0.05 ppm Meats 0.05 ppm Soups 0.05 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2908	FDA 121.1164; FEMA No. 2909

REFERENCES

For References 1–5, see end of Part III.

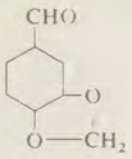
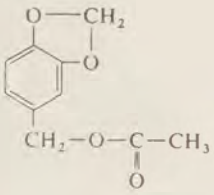
6. Johnstone, *Ber. Dtsch. Chem. Ges.*, 22, 61, 1889.
7. Englaender, *Ber. Dtsch. Chem. Ges.*, 58, 2218, 1935.
8. Wangerin, *Chem. Zentralbl.*, 2, 214, 1903.
9. Rimington, *Chem. Zentralbl.*, 1, 80, 1936.
10. Spath et al., *Ber. Dtsch. Chem. Ges.*, 69, 2448, 1936.
11. Juraschewski et al., *Chem. Zentralbl.*, 1, 1841, 1940.
12. Rugheimer, *Ber. Dtsch. Chem. Ges.*, 15, 1390, 1882.
13. Peinemann, *Arch. Pharm.*, 234, 204, 245, 1896.
14. Barilli, *Chem. Zentralbl.*, 2, 384, 1901.
15. Bose, *Chem. Zentralbl.*, 1, 4315, 1936.
16. Kawaguchi et al., *Chem. Abstr.*, 44, 9634, 1950.

	Piperitol	*d*-Piperitone
Other names	1-Methyl-4-isopropyl-1-cyclohexen-3-ol *p*-Menth-1-en-3-ol Neopiperitol (*trans*-form)	*p*-Menth-1-en-3-one 4-Isopropyl-1-methyl-1-cyclohexen-3-one
Empirical formula	$C_{10}H_{18}O$	$C_{10}H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Crystals; *cis*- and *trans*-form optically active	Colorless liquid
Molecular weight	154.24	152.23
Melting point	*cis*-, *l*-, 36°C *cis*-, *dl*-, 28°C	*l*-, −29°C
Boiling point	*trans*-, *dl*-, 57°C at 0.15 mm Hg *trans*-, *dl*-, 66–69°C at 0.2 mm Hg	*d*-, 116–118.5°C at 20 mm Hg; *dl*-, 235–237°C; *l*-, 232.5–234.7°C
Specific gravity	*trans*-, *d*-, 0.9203 at 25°C *trans*-, *dl*-, 0.9217 at 25°C	*d*-, 0.9344 at 20°C; *dl*-, 0.9375 at 19°C; *l*-, 0.9330 at 20°C
Refractive index	*trans*-, *d*-, 1.4762 at 25°C	*d*-, 1.4848 at 20°C; *dl*-, 1.4845 at 20°C; *l*-, 1.4815 at 20°C
Optical rotation	*cis*-, *l*-, −246° at 17°C (c = 2 in benzene) *trans*-, *d*-, +28° at 17°C (c = 2 in benzene)	*d*-, +49°8′ at 20°C; *l*-, −67.6° or −51.53°
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics	Fresh pungent odor and taste	Camphor-like odor; sharp, minty flavor
Synthesis	By reduction of racemic piperitone with lithium aluminum hydride or aluminum isopropoxide;[6] the *d*-form is isolated from natural sources[7]	Isolated from Japanese mint oil; *l*-form from *Eucalyptus dives* oil; by hydrogenation of diosphenol; by reduction of 5-methyl-2-isopropylanisole with sodium in liquid NH_3
Natural occurrence	Reported found in several naturally occurring oils[7,8] originally isolated from the oil of *Eucalyptus radiata*[7]	The structure has been defined by the work of several authors.[9–13] The *d*-, *l*-, and *dl*-forms are known. The *d*-form is found in the essential oils of *Mentha silvestris*, *Cymbopogon sennaarensis*, and Japanese peppermint oil. The *dl*-form is found in the essential oils of: *Andropogon iwarancusa*, *Mentha pulegium* var. *hirsuta*,[12–14] and, in mixture with the *l*-form, *Eucalyptus dives*. The *l*-form, the most abundant, is found in about 30 varieties of eucalyptus and in other plants.
Reported uses[3]	Non-alcoholic beverages 20.0 ppm Ice cream, ices, etc. 20.0 ppm Candy 20.0 ppm	Non-alcoholic beverages 1.0–11 ppm Ice cream, ices, etc. 18 ppm Candy 18 ppm Baked goods 18 ppm
Regulatory status	FEMA No. 3179	FDA 121.1164; FEMA No. 2910

REFERENCES

For References 1–5, see end of Part III.

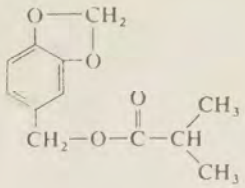
6. Macbeth, Milligan and Shannon, *J. Chem. Soc.*, p. 901, 1953.
7. Baker and Smith, *Research on the Eucalyptus*, 2nd ed., Government of the State of New South Wales, Sydney, 1920, 373.
8. Simonsen, *Indian For. Rec.*, 10, 161, 1924.
9. Penfold, *J. Proc. R. Soc. N. S. W.*, 54, 40, 1920.
10. Wallach and Meister, *Annalen*, 362, 272, 1908.
11. Simonsen, *J. Chem. Soc.* (London), 119, 1646, 1921.
12. Morani, *Ann. Chim. Appl.*, 14, 293, 1924.
13. Morani, *Riv. Ital. EPPOS*, 7, 65, 1925.
14. Romeo and Giuffre, *Ann. Chim. Appl.*, 15, 368, 1925.

	Piperonal	Piperonyl acetate
Other names	Heliotropine 3,4-Methylenedioxybenzaldehyde Piperonylaldehyde Protocatechualdehyde methylene ether	Heliotropyl acetate 3,4-Methylenedioxybenzyl acetate
Empirical formula	$C_8H_6O_3$	$C_{10}H_{10}O_4$
Structure		
Physical/chemical characteristics[5]		
Appearance	White, lustrous crystals; tends to yellow on exposure to air or light	Oily liquid (see references 12 and 13.)
Assay	99.0% min[2]	
Molecular weight	150.14	194.19
Melting point	37°C	
Boiling point	263°C (140°C at 15 mm Hg)	153–154°C at 14 mm Hg
Congealing point	35°C min[2]	
Specific gravity		1.240 at 18°C
Refractive index		1.528 at 18°C
Solubility	1 gm in 4 ml of 70% alcohol;[2] 0.2% in cold water; somewhat soluble in propylene glycol	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Sweet, flowery odor reminiscent of heliotrope; bittersweet taste	Very sweet, floral odor with cherry-like undernotes; sweet, fruity flavor at low levels, bitter at high levels
Synthesis	By the oxidation of isosafrole with potassium dichromate and sulfuric acid and subsequent steam distillation of piperonal[6]	By acetylation of the corresponding alcohol;[10] or by boiling dimethylpiperonyl amine with acetic anhydride[11]
Natural occurrence	Reported found in the essential oils of *Robinia pseudo-acacia*[7] and *Eryngium poterium*;[8] in the oils of *Spirea ulmaria*[9] and of leaves of *Doryphora sassafras*. Also reported found in Tahitian vanilla, camphor wood oil, and violet flowers concrete and absolute	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 6.0 ppm Ice cream, ices, etc. 7.0 ppm Candy 7.4 ppm Baked goods 18 ppm Gelatins and puddings 5.8 ppm Chewing gum 36 ppm	Non-alcoholic beverages 27–50 ppm Ice cream, ices, etc. 80–110 ppm Candy 70–80 ppm Baked goods 55–80 ppm
Regulatory status	FDA GRAS; FEMA No. 2911	FDA 121.1164; FEMA No. 2912

REFERENCES

For References 1–5, see end of Part III.

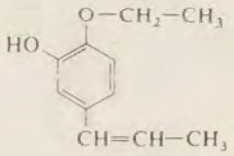
6. **Ciamician and Silber,** *Gazz. Chim. Ital.*, 20, 571, 1890.
7. **Elze,** *Chem. Ztg.*, 34, 814, 1910.
8. **Salgue,** *C. R. Séances Acad. Sci. Paris*, 241, 987, 1955.
9. **Ikeda,** *J. Chem. Soc. Jap.*, 61, 583, 1940.
10. **Tiffenau,** *Bull. Soc. Chim. Fr.*, 4(9), 932, 1911.
11. **Tiffenau and Fuhrer,** *Bull. Soc. Chim. Fr.*, 4(15), 172, 1914.
12. **Vavon,** *Compt. Rend.*, 154, 361, 1912.
13. **Vavon,** *Ann. Chim. Paris*, 9(1), 166, 1914.

	Piperonyl isobutyrate	L-Proline
Other names	Heliotropyl isobutyrate 3,4-Methylenedioxybenzyl isobutyrate	2-Pyrrolidine carboxylic acid
Empirical formula	$C_{12}H_{14}O_4$	$C_5H_9NO_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	White needles or prisms
Molecular weight	222.24	115.13
Melting point		220–222°C (decomposes)
Optical rotation		-80.9° at 20°C (c = 1 in water) -52.6° at 20°C (c = 0.58 in 0.5*N* HCl) -93° at 20°C (c = 0.24 in 0.6*N* KOH)
Solubility	Almost insoluble in water; soluble in alcohol	Very soluble in water; slightly soluble in alcohol, acetone, and benzene; insoluble in ether
Organoleptic characteristics	Very sweet but mild, fruity, and berry-like fragrance with some jam-like qualities; intense, sweet, plum-like flavor	
Synthesis	By esterification of the corresponding alcohol with isobutyric acid	From α-piperidone,[6] from cyclopentanone,[7] or from *l*-glutamic acid[8]
Natural occurrence	Not reported found in nature	Reported found as a component in many proteins; also widely occurring as the free acid in natural products
Reported uses[3]	Non-alcoholic beverages 0.05–1.0 ppm Ice cream, ices, etc. 0.05 ppm Candy 0.05–3.5 ppm Baked goods 0.10–3.5 ppm	Non-alcoholic beverages 50.0 ppm Baked goods 50.0 ppm Condiments, pickles 50.0 ppm Meat, meat sauces, soups 50.0 ppm Milk, dairy products 50.0 ppm Cereals 50.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2913	FEMA No. 3319

REFERENCES

For References 1–5, see end of Part III.

6. Heymons, *Berichte.*, 66, 846, 1933.
7. Schmidt, *Chemistry of Amino Acids and Proteins*, 2nd ed., C C Thomas, Springfield, 1944, 89.
8. Buyle, *Chem. Ind.* (London), p. 380, 1966.

	Propenylguaethol	Propenyl propyl disulfide
Other names	6-Ethoxy-*m*-anol 1-Ethoxy-2-hydroxy-4-propenylbenzene 2-Ethoxy-5-propenylphenol Hydroxymethyl anethole 2-Propenyl-6-ethoxyphenol	
Empirical formula	$C_{11}H_{14}O$	$C_6H_{12}S_2$
Structure		$CH_3-CH_2-CH_2-S-S-CH=CH-CH_3$
Physical/chemical characteristics		
Appearance	Colorless, crystalline solid	
Molecular weight	162.23	148.29
Melting point	85–86°C (sublimes under vacuum)	
Boiling point		78 - 80°C at 13 mm Hg
Refractive index		n_D^{20} 1.5219
Solubility	10% in alcohol; 4% in propylene glycol; 4% in polysorbate 80; 20% in benzyl alcohol; slightly soluble in water	
Organoleptic characteristics	Vanilla-like odor and flavor	Odor and taste like that of cooked onions
Synthesis	By alkaline hydrolysis of 1-ethoxy-2-methoxy-4-propenyl benzene in ethanol or methanol solution at 150–190°C under pressure,[9] or in ethylene glycol solution at the same temperature under atmospheric pressure; by saponification and contemporary transposition of the double bond starting from 1-ethoxy-2-methoxy-4-allyl benzene	Treatment of 1-ethylthio-2-propenylthioethene with $NaNH_2$ in liquid ammonia results in formation of Na-1-propenethiolate, which reacts with S-propyl propanethiosulfonate to give propenyl propyl disulfide in good yield[6]
Natural occurrence	Not reported found in nature	Flavor component of onion oil (*trans*-form);[7] volatile component from chives (*Allium schoenoprosum*)[8]
Reported uses[3]	Non-alcoholic beverages 5.9 ppm Ice cream, ices, etc. 6.3 ppm Candy 20 ppm Baked goods 20 ppm Gelatins and puddings 2.5 ppm	Baked goods 2.0 ppm Condiments, pickles 2.0 ppm Meat, meat sauces, soups 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2922	FEMA No. 3227

REFERENCES

For References 1–5, see end of Part III.

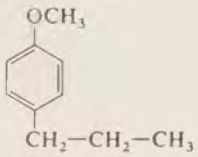
6. **Wijers, Boelens and Van der Ojeu,** *Recl. Trav. Chim. Pays-Bas,* 88(5), 519, 1969.
7. **Brodnitz, Pollack and Vallon,** *J. Agric. Food Chem.,* 17(4), 760, 1969.
8. **Wahlroos and Virtanen,** *Acta Chem. Scand.,* 19(6), 1327, 1965.
9. **Junge,** *Riechstoffind. Kosmet.,* 8, 81, 1933.

	Propionaldehyde	Propyl acetate
Other names	Methylacetaldehyde Propanal Propyl aldehyde	*n*-Propyl acetate
Empirical formula	C_3H_6O	$C_5H_{10}O_2$
Structure	CH_3-CH_2-CHO	$CH_3-CH_2-CH_2-O-\overset{\overset{O}{\|\|}}{C}-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Highly mobile, colorless liquid
Molecular weight	58.08	102.13
Melting point	−81°C	
Boiling point	47.5–49°C	101.6°C
Specific gravity	0.8074 at 21°C	0.8905–0.8992 at 15°C
Refractive index	1.3695 at 16.6°C	1.3840–1.3884 at 20°C
Solubility	Soluble in water (1:5 at 20°C); soluble in alcohol, ether, and chloroform	Fairly soluble in water (1:60); 1:17 in 30% alcohol; soluble in most common organic solvents
Organoleptic characteristics	Characteristic odor similar to acetaldehyde	Fruity (pear-raspberry) odor; pleasant, bittersweet flavor reminiscent of pear on dilution
Synthesis	By oxidation of propyl alcohol, or by dry distillation of barium propionate with calcium formate[6]	By direct acetylation of propyl alcohol
Natural occurrence	Reported found in apple aroma[7] and in the essential oils of: camphor,[8] *Rosa centifolia*,[9] clary sage,[10] *Pinus excelsa*, *Pinus silvestris*,[11] and others	In raspberry, banana, and tomato
Reported uses[3]	Non-alcoholic beverages 3.9 ppm Ice cream, ices, etc. 12 ppm Candy 11 ppm Baked goods 13 ppm	Non-alcoholic beverages 4.0 ppm Ice cream, ices, etc. 16 ppm Candy 12 ppm Baked goods 14 ppm
Regulatory status	FDA 121.1164; FEMA No. 2923	FDA 121.1164; FEMA No. 2935

REFERENCES

For References 1–5, see end of Part III.

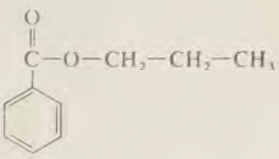
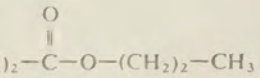
6. Limpricht, *Justus Liebigs Ann. Chem.*, 97, 361, 1856.
7. Huelin, *J. Sci. Res. Aust.*, 5, 328, 1952.
8. Ono and Imoto, *J. Chem. Soc. Jap.*, 59, 1014, 1938.
9. Calvarano, *Essenze Deriv. Agrum.*, 28, 157, 1958.
10. Panayotov, *Perfum. Essent. Oil Rec.*, 49, 233, 1958.
11. Aschau, *Chem. Zentralbl.*, 1, 147, 1914.

	Propyl alcohol	*p*-Propyl anisole
Other names	Albacol Optal 1-Propanol Propylic alcohol *n*-Propyl alcohol	Dihydroanethole 1-Methoxy-4-*n*-propylbenzene Methyl *p*-propylphenyl ether Propylmethoxybenzene
Empirical formula	C_3H_8O	$C_{10}H_{14}O$
Structure	$CH_3-CH_2-CH_2OH$	
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to pale-yellow, oily liquid
Molecular weight	60.09	150.22
Melting point	−127°C	
Boiling point	97.2°C	212–213°C (104–107°C at 20 mm Hg)
Flash point	22°C	
Specific gravity	0.8044 at 20°C	0.940–0.943 at 25°/25°C;[2] 0.94718 at 20°C
Refractive index	1.38543 at 20°C	1.5025–1.5055[2] (1.5045) at 20°C
Solubility	Miscible with water, alcohol, ether, and propylene glycol	1:5 in 80% alcohol[2]
Organoleptic characteristics	Alcoholic odor; characteristic ripe, fruity flavor	Characteristic anise-type odor with a sassafras undertone
Synthesis	Can be isolated from the head fractions during the distillation of wine, or from the tail fractions during rectification of spirits	By partial hydrogenation of anethole in the presence of nickel at 60–95°C under pressure,[7–9] or under atmospheric pressure[10,11]
Natural occurrence	Reported found in the natural aromas of apple, cognac, and rum;[6] also forms during alcoholic fermentation	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.50–5.0 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50 ppm Baked goods 0.65 ppm	Non-alcoholic beverages 4.3 ppm Ice cream, ices, etc. 9.9 ppm Candy 64 ppm Baked goods 67 ppm
Regulatory status	FDA 121.1164; FEMA No. 2928	FDA 121.1164; FEMA No. 2930

REFERENCES

For References 1–5, see end of Part III.

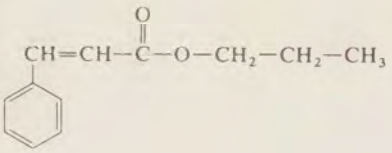
6. **Fenaroli et al.,** *Riv. Ital. EPPOS*, 9, 484, 1965; 2, 75, 1966.
7. **Ipatjew,** *Chem. Ber.*, 46, 3590, 1913.
8. **Brochet and Bauer,** *Compt. Rend.*, 154, 192, 1914.
9. **Brochet and Bauer,** *Bull. Soc. Chim. Fr.*, 4(17), 53, 1915.
10. **Brochet and Cavaret,** *Comp. Rend.*, 159, 328, 1914.
11. **Brochet and Cavaret,** *Bull. Soc. Chim. Fr.*, 4(17), 58, 1915.

	Propyl benzoate	Propyl butyrate
Other names	*n*-Propyl benzoate	*n*-Propyl-*n*-butanoate *n*-Propyl butyrate
Empirical formula	$C_{10}H_{12}O_2$	$C_7H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Molecular weight	164.21	130.18
Melting point	51 to −52 C	
Boiling point	230°C (230-231°C)	142-143°C
Specific gravity	1.039 at 15.5°C; 1.0274 at 15°C	0.8722 at 20°C
Refractive index	1.5100 at 20°C; 1.50139 at 15°C	1.3995 at 20°C
Solubility	Insoluble in water; soluble in alcohol	Almost insoluble in water; miscible with alcohol and ether
Organoleptic characteristics	Balsamic odor reminiscent of nut; sweet, fruity, nut-like taste	Pineapple and apricot-like odor; sweet, fruity flavor of banana and pineapple
Synthesis	By exchange between methyl benzoate and propyl alcohol in the presence of potassium propylate;[6] or by heating benzamide sulfate with propyl alcohol at 90–95 C[7]	From propyl alcohol and butyric acid in the presence of *p*-toluenesulfonic acid in benzene solution at the boil[8]
Natural occurrence	Reported found in several natural products	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 44 ppm Candy 33 ppm Baked goods 33 ppm	Non-alcoholic beverages 6.8 ppm Ice cream, ices, etc. 4.6 ppm Candy 24 ppm Baked goods 16 ppm
Regulatory status	FDA 121.1164; FEMA No. 2931	FDA 121.1164; FEMA No. 2934

REFERENCES

For References 1–5, see end of Part III.

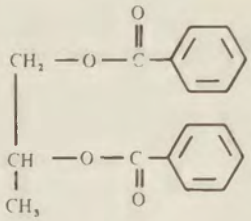
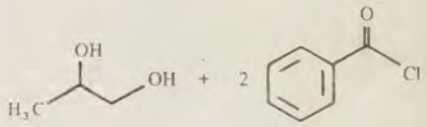
6. Reimer and Downes, *J. Am. Chem. Soc.*, 43, 949, 1921.
7. Roessler (Hasslacher Chemical Co.). German Patent 463,721, 1928.
8. Salmi and Leimu, *Suom. Kemistil. B*, 20, 46, 1947.

	Propyl cinnamate
Other names	*n*-Propyl cinnamate Propyl-β-phenyl acrylate Propyl-3-phenylpropenoate
Empirical formula	$C_{12}H_{14}O_2$
Structure	
Physical/chemical characteristics[2]	
Appearance	Colorless, viscous liquid; solidifies into crystalline mass when cold
Molecular weight	190.24
Melting point	13°C
Boiling point	283–284°C; 102–104°C at 1 mm Hg
Specific gravity	1.0435 at 0°/0°C
Refractive index	1.5510 at 20°C; 1.5530 at 14°C
Solubility	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic peach-apricot flavor; wine-like odor
Synthesis	By esterification of cinnamic acid with propyl alcohol in the presence of HCl as a catalyst;[6] or by direct esterification in the presence of benzene
Natural occurrence	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.6 ppm Ice cream, ices, etc. 2.9 ppm Candy 4.9 ppm Baked goods 4.3 ppm Gelatins and puddings 0.07 ppm
Regulatory status	FDA 121.1164; FEMA No. 2938

REFERENCES

For References 1–5, see end of Part III.

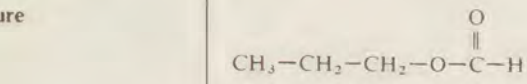
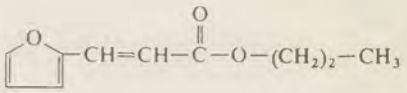
6. Weger, *Chem. Ann.*, 221, 76, 1883.
7. Challenger and Rawling, *J. Chem. Soc.*, p. 872, 1937.

	Propyl disulfide	Propylene glycol dibenzoate
Other names	Dipropyl disulfide Propyldithiopropane Di-*n*-propyl disulfide 1-Propyl disulfide	1,2-Propanediol dibenzoate
Empirical formula	$C_6H_{14}S_2$	$C_{17}H_{16}O_4$
Structure	$CH_3-CH_2-CH_2-S-S-CH_2-CH_2-CH_3$	
Physical/chemical characteristics		
Appearance	Colorless liquid	
Molecular weight	150.29	286.31
Boiling point	193.5°C at 750 mm Hg	
Specific gravity	0.9599 at 20°C	
Refractive index	1.4981 at 20°C	
Solubility	Almost insoluble in water; soluble in alcohol	
Organoleptic characteristics	Pungent sulfur-like odor penetrating odor of onion and garlic	
Synthesis	By boiling propyl bromide and Na_2S_2 in propyl alcohol;[6] from iodine and *n*-propyl mercaptan; from propyl iodide and sodium thiosulfate by way of sodium propyl thiosulfate, followed by heating	
Natural occurrence	In cabbage,[7-9] onion and garlic,[10-25] and roasted peanut[26]	
Reported uses[3]	Soups 6.0 ppm Spices 10.0 ppm The compound has been used in reconstructing concentrated onion and garlic flavor; levels are from 0.3 to 3 ppm.	Non-alcoholic beverages 85.0 ppm
Regulatory status	FEMA No. 3228; FDA 121.1164	FEMA No. 3419

REFERENCES

For References 1–5, see end of Part III.

6. Challenger et al., *J. Chem. Soc.*, p. 872, 1937.
7. Bailey et al., *J. Food Sci.*, 26, 163, 1960.
8. Hewit, *J. Agric. Food Chem.*, 11, 14, 1963.
9. Johnson et al., *Chem. Ind.* (London), p. 556, 1971.
10. Niegisch et al., *Food Res.*, 21, 657, 1956.
11. Carson et al., *Am. Chem. Soc. Div. Pet. Chem. Prepr.*, 2(4), Abstr., D 115, 1957.
12. Carson et al., *J. Agric. Food Chem.*, 9, 140, 1961.
13. Jacobsen et al., *Arch. Biochem. Biophys.*, 104, 473, 1964.
14. Saghir et al., *Proc. Am. Soc. Hort. Sci.*, 84, 386, 1964.
15. Wilkens, *Memo No. 385, Cornell University, Agricultural Experimental Station*, Ithaca, N.Y., 1964.
16. Wahlroos et al., *Acta Chem. Scand.*, 19, 1327, 1965.
17. Schwob et al., *Ann. Nutr. Aliment.*, 19, 1327, 1965.
18. Saghir et al., *Plant Physiol.*, 40, 681, 1965.
19. Bernhard, *Adv. Chem. Ser.*, 56, 131, 1966.
20. Bernhard, *J. Food Sci.*, 33, 298, 1968.
21. Brodnitz et al., *J. Agric. Food Chem.*, 17, 760, 1969.
22. Bernhard, *Qual. Plant. Mater. Veg.*, 18, 72, 1969.
23. Brodnitz et al., *Food Technol.*, 24, 78, 1970.
24. Boelens et al., *J. Agric. Food Chem.*, 19, 984, 1971.
25. Dubois et al., *Ind. Aliment. Agric.*, p. 127, 1972.
26. Walradt et al., *J. Agric. Food Chem.*, 19, 972, 1971.

	Propyl formate	Propyl 2-furanacrylate
Other names	*n*-Propyl formate *n*-Propyl methanoate	Propyl β-furylacrylate Propyl-3-(2-furyl)-acrylate Propyl-3-furylpropenoate
Empirical formula	$C_4H_8O_2$	$C_{10}H_{12}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid (sometimes very pale-yellow)
Molecular weight	88.10	180.21
Melting point	−92.9°C	
Boiling point	81–81.3°C	119°C (236°C) at 7 mm Hg
Flash point	27°C	
Specific gravity	0.9039 at 20°C	1.0744 at 20°C
Refractive index	1.3769 at 20°C	1.5229 at 20°C
Solubility	Scarcely soluble in water; miscible with alcohol, ether, and most common organic solvents	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic fruity (rum-plum) odor; corresponding bittersweet flavor	Light strawberry-, apple-, pear-like odor; fruity, caramellic flavor at low levels, turning bitter at higher levels
Synthesis	By action of sulfuric acid on a mixture of propyl alcohol, formic acid, and sodium formate;[6] also by distilling propyl alcohol with anhydrous formic acid in the presence of sodium formate[7]	By esterification of *n*-propanol with furanacrylic acid
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 20 ppm Ice cream, ices, etc. 57 ppm Candy 65 ppm Baked goods 85 ppm	Non-alcoholic beverages 3.0 ppm Candy 0.03 ppm
Regulatory status	FDA 121.1164; FEMA No. 2943	FDA 121.1164; FEMA No. 2945

REFERENCES

For References 1–5, see end of Part III.

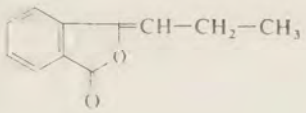
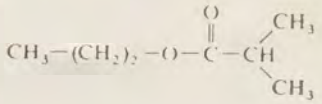
6. **Wagner,** German Patent 546,806, 1929.
7. **Adickes,** *J. Prakt. Chem.*, 2(145), 236, 1936.

	Propyl heptanoate	*n*-Propyl hexanoate
Other names	*n*-Propyl heptoate *n*-Propyl heptylate	*n*-Propyl caproate *n*-Propyl-*n*-hexoate *n*-Propyl hexylate
Empirical formula	$C_{10}H_{20}O_2$	$C_9H_{18}O_2$
Structure	$CH_3-CH_2-CH_2-O-\overset{O}{\overset{\|}{C}}-(CH_2)_5-CH_3$	$CH_3-(CH_2)_2-O-\overset{O}{\overset{\|}{C}}-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	172.27	158.24
Melting point	64.8°C (from pentane)	−69°C
Boiling point	207.9°C (206°C)	187°C; 84–85 C at 20 mm Hg
Specific gravity	0.870 at 15.5°C; 0.85705 at 20°C	0.8632 at 25 C
Refractive index	1.4160 (1.41894) at 20°C	1.4109 at 25 C
Solubility	Soluble in most common organic solvents; insoluble in water	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic, strong ether-like odor; corresponding flavor reminiscent of grape	Ether-like odor with a pineapple-blackberry undertone; sweet, fruity flavor of blackberry and plum
Synthesis	By treating heptanoic acid with propyl alcohol in the presence of mineral acids,[6,7] or in benzene solution in the presence of *p*-toluenesulfonic acid[8]	By esterification of hexanoic acid with propyl alcohol in benzene solution in the presence of *p*-toluenesulfonic acid[8]
Natural occurrence	Not reported found in nature	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 3.8 ppm Alcoholic beverages 3.0 ppm Ice cream, ices, etc. 5.1 ppm Candy 5.9 ppm Baked goods 18 ppm	Non-alcoholic beverages 2.2 ppm Ice cream, ices, etc. 3.0 ppm Candy 8.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2948	FDA 121.1164; FEMA No. 2949

REFERENCES

For References 1–5, see end of Part III.

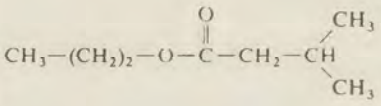
6. **Gartenmeister,** *Justus Liebigs Ann. Chem.*, 233, 282, 1886.
7. **Bilterys and Gisseleire,** *Bull. Soc. Chim. Belg.*, 44, 569, 572, 1935.
8. **Hoback, Parsons and Bartlett,** *J. Am. Chem. Soc.*, 65, 1606, 1943.

	3-Propylidene phthalide	Propyl isobutyrate
Other names		*n*-Propyl isobutyrate *n*-Propyl-2-methylpropanoate
Empirical formula	$C_{11}H_{10}O_2$	$C_7H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to very pale, yellow liquid	Colorless liquid
Molecular weight	174.20	130.18
Boiling point	169 C (273 C) at 12 mm Hg	134 C (135 C) at 752 mm Hg
Specific gravity	1.08	0.8643 at 20°C
Refractive index		1.3955 at 20°C
Solubility	Almost insoluble in water; soluble in alcohol	Insoluble in water; soluble in most common organic solvents, including alcohol
Organoleptic characteristics	Very powerful and warm, spicy odor; warm, spicy, herbaceous flavor	Pineapple-like odor; corresponding sweet flavor
Synthesis	By condensing at 175 C phthalic anhydride and butyric anhydride in the presence of sodium butyrate[6]	From propyl alcohol and isobutyric acid in benzene solution in the presence of concentrated H_2SO_4[7]
Natural occurrence	Not reported found in nature	Reported found in several natural products
Reported uses[3]	Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm	Non-alcoholic beverages 6.8 ppm Ice cream, ices, etc. 4.8 ppm Candy 24 ppm Baked goods 20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2952	FDA 121.1164; FEMA No. 2936

REFERENCES

For References 1–5, see end of Part III.

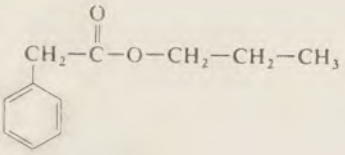
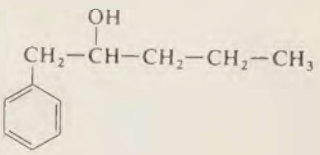
6. **Bromberg,** *Ber. Dtsch. Chem. Ges.*, 29, 1436, 1896.
7. **Vogel,** *J. Chem. Soc.*, p. 637, 1948.

	Propyl isovalerate	Propyl mercaptan
Other names	*n*-Propyl isovalerate *n*-Propyl-β-methylbutyrate	*n*-Propane thiol Propanthiol-1 *n*-Propyl mercaptan *n*-Thiopropyl alcohol
Empirical formula	$C_8H_{16}O_2$	C_3H_8S
Structure		$CH_3-CH_2-CH_2-SH$
Physical/chemical characteristics[5]		
Appearance	Colorless, mobile liquid	Colorless, mobile liquid
Molecular weight	144.21	76.165
Melting point		−111.5°C
Boiling point	156–157°C; 49°C at 13 mm Hg	67°–68°C
Flash point		−20°C
Specific gravity	0.8617 at 20°C	0.8408 at 20°C
Refractive index	1.4031 at 20°C	1.4380 at 20°C
Solubility	Insoluble in water; soluble in most common organic solvents, including alcohol	Forms binary azeotropic mixtures with propyl alcohol (91.35%) and a ternary azeotrope with water and propyl alcohol; slightly soluble in water; soluble in alcohol and propylene glycol
Organoleptic characteristics	Fruity odor; bittersweet flavor similar to apple	Characteristic odor of cabbage; below 2–3 ppm sweet onion and cabbage-like flavor
Synthesis	By prolonged boiling of propyl alcohol with isovaleric acid in benzene in the presence of concentrated H_2SO_4[6]	By reacting propyl alcohol and H_2S under particular conditions;[7] from propyl alcohol or propyl disulfide and naphthalene;[8,9] from *n*-propyl chloride and potassium hydrosulfide; also from *n*-propanol plus bromine plus red phosphorus in the presence of sodium sulfate
Natural occurrence	Reported found in several natural products	Reported found in *Allium cepa*[10]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 16 ppm Candy 17 ppm Baked goods 20 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2960	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.

6. Vogel, *J. Chem. Soc.*, p. 640, 1948.
7. Sabatier et al., C. R. *Séances Acad. Sci. Paris*, 150, 1219, 1910.
8. Mereshkoski, *Chem. Zentralbl.*, 86, 982, 1915.
9. Faragher et al., *Chem. Zentralbl.*, 99, 119, 1928.
10. Challenger and Greenwood, *Biochem. J.*, 44, 87, 1949.

	Propyl phenylacetate	α-Propylphenylethyl alcohol
Other names	*n*-Propyl-α-toluate	Benzylbutyl alcohol Benzyl-*n*-propyl carbinol 1-Phenyl-2-pentanol 1-Phenylpentan-2-ol *n*-Propyl benzyl carbinol
Empirical formula	$C_{11}H_{14}O_2$	$C_{11}H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless and somewhat oily liquid
Molecular weight	178.23	164.25
Boiling point	253°C	247°C
Specific gravity	0.990 at 15.5°C	0.98
Refractive index	1.4955 at 20°C	
Solubility	Almost insoluble in water; soluble in alcohol	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic honey-like, apricot-rose odor; sweet, honey-like taste	Mild, green, sweet odor with an earthy undernote; tart, fruit-like, green, sweet taste
Synthesis	By esterification of *n*-propanol with phenylacetic acid	From phenyl acetaldehyde and propyl magnesium bromide; also by hydrogenation of propyl benzyl ketone
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.30–1.0 ppm Ice cream, ices, etc. 0.30–1.5 ppm Candy 2.7 ppm Baked goods 1.0–5.0 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm Gelatins and puddings 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2955	FDA 121.1164; FEMA No. 2953

REFERENCES

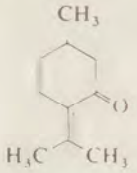
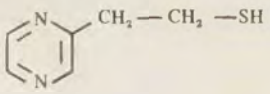
For References 1–5, see end of Part III.

	Propyl propionate	Propyl thioacetate
Other names	*n*-Propyl propionate	
Empirical formula	$C_6H_{12}O_2$	$C_5H_{10}OS$
Structure	$CH_3-CH_2-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_2-CH_3$	$CH_3-\overset{\overset{O}{\|}}{C}-S-CH_2-CH_2-CH_3$ or $CH_3-\overset{\overset{O}{\|}}{C}-O-CH_2-CH_2-CH_3$ (S)
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Molecular weight	116.16	118.96
Boiling point	122–125°C	137–139°C
Flash point	79°C	
Specific gravity	0.883 at 15.5°C	
Refractive index	1.3910 (1.3935) at 20°C	
Solubility	0.5% soluble in water; miscible with alcohol, propylene glycol, and ether	
Organoleptic characteristics	Complex, fruity odor reminiscent of apple, banana, and pineapple; somewhat pleasant, bitter flavor	
Synthesis	By esterification of propyl alcohol with the corresponding acid in the presence of concentrated H_2SO_4,[6,7] or in the presence of BF_3[8]	From acetyl chloride and phenyldipropylarsin sulfide at 80–90°C[10]
Natural occurrence	Reported found among the volatile constituents of grape var. white Sauvignon[9]	
Reported uses[3]	Non-alcoholic beverages 6.0 ppm Ice cream, ices, etc. 12 ppm Candy 25 ppm Baked goods 25 ppm	Non-alcoholic beverages 1.0 ppm Candy 1.0 ppm Condiments, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm Cereals 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2958	FEMA No. 3385

REFERENCES

For References 1–5, see end of Part III.

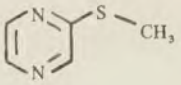
6. **Vogel,** *J. Chem. Soc.*, p. 629, 1948.
7. **Salmi and Leimu,** *Chem. Abstr.*, 42, 4031, 1948.
8. **Hinton and Nieuwland,** *J. Am. Chem. Soc.*, 54, 2018, 1932.
9. **Chandhery et al.,** *Am. J. Enol. Vitic.*, 15, 190, 1964.
10. *Chem. Abstr.* 69, 52239d, 1968.

	Pulegone	Pyrazine ethanethiol
Other names	*p*-Menth-4(8)-en-3-one 1-Methyl-4-isopropylidenecyclohexan-3-one	2-(Pyrazinyl)ethanethiol 2-Pyrazinyl ethylmercaptan
Empirical formula	$C_{10}H_{16}O$	$C_6H_8N_2S$
Structure		
Physical/chemical characteristics		
Appearance	Colorless, oily liquid	
Assay		C: 51.40%; H: 5.75%; N: 19.98%; S: 22.87%
Molecular weight	152.23	140.04
Boiling point	*dl*, 220–222°C; *d*, 224°C at 750 mm Hg	57–69°C at 0.05 mm Hg
Specific gravity	*d*, 0.9405 at 15°C	
Refractive index	*d*, 1.48796 at 20°C; *dl*, 1.4846 at 18°C	
Optical rotation	*d*, +20.48′	
Solubility	Insoluble in water; miscible with alcohol, ether, and chloroform	
Organoleptic characteristics	Pleasant odor, somewhat similar to peppermint and camphor	
Synthesis	Isolated from pennyroyal oil (Moroccan or Spanish); synthesis from 3-methyl cyclohexanone	From 2-vinylpyrazine by reaction with thiolactic acid, followed by conversion of the thiolester to 2-(pyrazinyl) ethanethiol[6]
Natural occurrence	The structure has been defined by the work of several authors.[7-10] The *d*-, *l*-, and *dl*-forms are known. The *dl*-form is prepared synthetically and is not found in nature. The *l*-form[11] is found in the essential oils of *Agastache formosana*, Israeli orange, *Barosma betulina*, and *Barosma crenulata*. The *d*-form is the most abundant and is found in pennyroyal oils.	
Reported uses[3]	Non-alcoholic beverages 5.0–8.0 ppm Ice cream, ices, etc. 5.0–32 ppm Candy 17 ppm Baked goods 24–25 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Baked goods 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2963	FEMA No. 3230

REFERENCES

For References 1–5, see end of Part III.

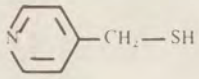
6. **Bardwell and Hewett,** *J. Org. Chem.*, 22, 980, 1957.
7. **Beckmann and Pleissner,** *Annalen*, 262, 1, 1891.
8. **Semmler,** *Ber. Dtsch. Chem. Ges.*, 25, 3519, 1892.
9. **Wallach,** *Annalen*, 289, 337, 1896.
10. **Fredga and Leskinen,** *Ark. Kem. B*, 19, 1, 1944.
11. **Fujita,** *Bot. Mag.* (Tokyo), 64, 165, 1951.

	Pyrazinylmethylsulfide	Pyridine
Other names	Methylthiopyrazine	
Empirical formula	$C_5H_6N_2S$	C_5H_5N
Structure		
Physical/chemical characteristics		
Appearance		Flammable, colorless liquid
Assay	C: 47.59%; H: 4.79%; N: 22.20%; S: 25.41%	
Molecular weight	126.18	79.10
Melting point		−42°C
Boiling point		115.2°C
Flash point		21°C
Specific gravity		0.9808 at 21°C
Refractive index		1.5092 at 21°C
Solubility		Miscible with water, alcohol, ether, propylene glycol, and most oils
Organoleptic characteristics		Characteristic, penetrating odor; sharp taste
Synthesis	Sodium methyl mercaptide is added to 2-chloropyrazine, which is prepared from 2-hydroxypyrazine[6]	From coal-tar distillation
Natural occurrence		Reported found in wood oil, the leaves and roots of *Atropa belladonna*,[7,8] and in other plants (coffee, tobacco)
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Baked goods 1.0 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 0.02–0.12 ppm Candy 0.40 ppm Baked goods 0.40 ppm
Regulatory status	FEMA No. 3231	FDA 121.1164; FEMA No. 2966

REFERENCES

For References 1–5, see end of Part III.

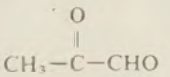
6. Karmas and Spoerri, *J. Am. Chem. Soc.*, 74, 1580, 1952.
7. Goris and Larsonneau, *Chem. Zentralbl.*, 1, 757, 1922.
8. King and Ware, *J. Chem. Soc.* (London), 331, 1941.

	2-Pyridine methanethiol	Pyroligneous acid, extract
Other names	2-Pyridyl methanethiol 2-Pyridyl methyl mercaptan 4-(Methylthio)pyridine	"Liquid smoke" Pyroligneous vinegar Wood vinegar
Empirical formula	C_6H_7SN	A mixture of material from wood distillation; chief component is water containing nearly 10% acid (formic, acetic, and propionic). The extract is free of water, acid, and tar.
Structure		
Physical/chemical characteristics[5]		
Appearance		Yellow to red liquid
Molecular weight	125.19	
Boiling point	57–58°C at 0.6 mm Hg	
Specific gravity	1.1533 at 25°C	1.018–1.030
Refractive index	1.5758 at 25°C	
Solubility		Miscible with water, alcohol, and propylene glycol but not oils. A tar-like phase can separate on standing; it is insoluble in alcohol and water.
Organoleptic characteristics		Smoke odor
Synthesis	By hydrolysis of 2-pyridylmethyl-*tert*-butyl sulfide with sulfuric acid in aqueous solution;[6] from 2-pyridylmethyl chloride[7]	Obtained by destructive distillation of wood, preferably birch. The crude product contains methanol, acetic acid, acetone, furfural, and various tar and related products. The extract is rendered free of water, acid, and tar by (1) alkali washing, followed by (2) re-acidification and (3) solvent extraction.
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Gelatins and puddings 2.0 ppm	Alcoholic beverages 20 ppm Baked goods 50–200 ppm Meats 100–300 ppm
Regulatory status	FEMA No. 3232	FDA 121.1164; FEMA No. 2968

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For References 1–5, see end of Part III.

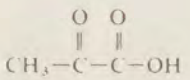
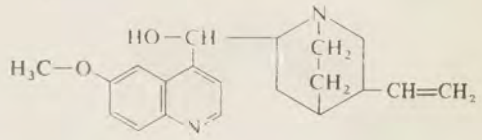
6. **Loev and Olin,** U.S. Patent 3,069,472.
7. **Maneszewska-Wieczorkowska and Michalski,** *Rocz. Chem.*, 31, 543, 1957; *Chem. Abstr.*, 50, 12046h, 1956; *Chem. Abstr.*, 51, 11347a, 1957.

	Pyrrole	Pyruvaldehyde
Other names	Azole Imidole Divynyleneimine	Acetyl formaldehyde 1,2-Ketopropionic aldehyde α-Ketopropionic aldehyde Methyl glyoxal 2-Oxopropanal Pyruvic aldehyde
Empirical formula	C_4H_5N	$C_3H_4O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid; tends to darken on aging	Mobile, yellow liquid; hygroscopic; in air readily polymerizes to a viscous, non-pourable glass
Molecular weight	67.09	72.06
Melting point	−24°C	
Boiling point	130°C at 761 mm Hg (decomposes)	72°C
Specific gravity	0.968–0.969 at 20°C	1.0455 at 24°C
Refractive index	1.5091–1.5095 at 20°C	1.4002 at 17.5°C
Solubility	Insoluble in water and in alkalis; soluble in alcohol, ether, and organic solvents; dissolves slowly in acids, with polymerization, gradual separation of "pyrrole red," and liberation of ammonia	Soluble in alcohol, ether, and benzene; yields colorless solution with alcohol and yellow solutions with the latter two solvents
Organoleptic characteristics	Sweet, warm-ethereal odor reminiscent of chloroform	Characteristic, pungent, stinging odor with a pungent, caramellic, sweet flavor
Synthesis	By fractional distillation of bone oil and subsequent purification via the corresponding potassium salt; by thermal decomposition of ammonium mucate in glycerol or mineral oil[6,7]	By distilling a dilute solution of dihydroxyacetone from calcium carbonate; by oxidation of acetone with selenium dioxide; by heating dihydroxy acetone with phosphorus pentoxide; by warming isonitroso acetone with diluted H_2SO_4
Natural occurrence	Reported found in coal tar and in bone oil (together with several methyl homologs) also reported found in lemon and orange trees and in vervain leaves	Reported found in the dry distillate of *Manilla copal*
Reported uses[3]	Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm Gelatins and puddings 3.0 ppm Meat, meat sauces, soups 3.0 ppm Cereals 3.0 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 0.03–5.0 ppm Baked goods 0.03–5.0 ppm
Regulatory status	FEMA No. 3386	FDA 121.1164; FEMA No. 2969

REFERENCES

For References 1–5, see end of Part III.

6. **Blicke and Powers,** *Ind. Eng. Chem.*, 19, 1334, 1927.
7. **McElrain and Bollinger,** in *Organic Syntheses,* Coll. Vol. 1, Gilman, H. and Blatt, A. H., Eds., Wiley & Sons, New York, 1941, 437.

	Pyruvic acid	Quinine
Other names	Acetylformic acid α-Ketopropionic acid 2-Oxopropanoic acid Pyroracemic acid	
Empirical formula	$C_3H_4O_3$	$C_{20}H_{24}N_2O \cdot 3\,H_2O$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid; tends to darken and decompose unless kept free of minor contaminants and in tightly sealed containers	Triboluminescent, orthorhombic needles; colorless or white, turning brown on exposure to air. Solutions (dilute) show blue fluorescence
Molecular weight	88.06	324.43 (anhydrous); 378.47 (hydrous, 3 moles H_2O)
Melting point	12–14°C (11.8°C)	177°C (anhydrous); 57°C (hydrous)
Boiling point	165 C with decomposition; 65°C at 12 mm Hg	Sublimes in high vacuum at 120–180°C
Specific gravity	1.267 at 15°C	
Refractive index	1.4138 at 20°C	At 15°C: 169° (c = 2 in 97% alcohol) At 17°C: 117° (c = 1.5 in chloroform) At 25°C: 285° (c = 0.4 molar on 0.1 N H_2SO_4)
Solubility	Completely miscible with water, alcohol, and ether	0.05% in water at room temperature, 0.14% in boiling water; soluble in alcohol; slightly soluble in hydrocarbons
Organoleptic characteristics	Sour, acetic odor (similar to acetic acid); pleasant, sour taste with a burning, somewhat sweet note	Odorless; intense, bitter taste
Synthesis	By distillation of tartaric acid in the presence of potassium acid sulfate as a dehydrating agent; from acetyl chloride and potassium cyanide to yield the nitrile, which is subsequently acid hydrolyzed to the acid. Pyruvic acid must be rectified under vacuum.	By extraction from cinchona bark (*Cinchona officinalis*), where it is present at approximately 8%
Natural occurrence	Isolated from cane sugar fermentation broth and from a few plants; also reported found in peppermint[6]	In *Cinchona officinalis*
Reported uses[3]	Non-alcoholic beverages 0.25 ppm Ice cream, ices, etc. 0.25–20 ppm Candy 27 ppm Baked goods 30 ppm Chewing gum 110 ppm	The alkaloid as such is not used in food flavors; *see* bisulfate, sulfate, and hydrochloride salts. In the United States the salts are permitted in carbonated beverages at 83 ppm calculated as quinine alkaloid base
Regulatory status	FDA 121.1164; FEMA No. 2970	*See* bisulfate, sulfate, and hydrochloride salts.

REFERENCES

For References 1–5, see end of Part III.

6. Towers et al., *J. Am. Chem. Soc.*, 76, 2392, 1954.

	Quinine bisulfate	Quinine hydrochloride
Other names		Quinine chloride Quinine monohydrochloride
Empirical formula	$C_{20}H_{24}N_2O_2 \cdot H_2SO_4 + 7\,H_2O$	$C_{20}H_{24}N_2O_2 \cdot HCl + 2\,H_2O$
Structure	*See* Quinine	*See* Quinine
Physical/chemical characteristics[5]		
Appearance	White, crystalline powder; turns brown on exposure to air	Brilliant, silky needles; colorless to white
Molecular weight	548.62	
Solubility	10% in water; 4% in alcohol; 6% in glycerin	6% in water; 50% in alcohol; 12% in glycerin
Organoleptic characteristics	Odorless; bitter taste	Odorless; intensely bitter flavor
Uses	Non-alcoholic beverages 95–100 ppm[3]	Non-alcoholic beverages 110 ppm
Regulatory status	FDA 121.1081; FEMA No. 2975	FDA 121.1081; FEMA No. 2976

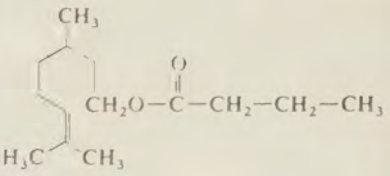
REFERENCES

For References 1–5, see end of Part III.

	Rhodinol	Quinine sulfate
Other names	*l*-Citronellol (3,7-Dimethyl-6-octen-1-ol) 3,7-Dimethyl-7-octen-1-ol	
Empirical formula	$C_{10}H_{20}O$	$(C_{20}H_{24}N_2O_2)_2 \cdot H_2SO_4 + 7\,H_2O$
Structure	The constitution of commercial rhodinol is still controversial. We define rhodinol as the isolate of Reunion geranium oil containing in larger portion *l*-citronellol.	*See* Quinine
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Dull-white, needle-like crystals
Assay	82% min[2]	
Molecular weight	156.26	873.05
Specific gravity	0.860–0.880 at 25°/25°C[2]	
Refractive index	1.4630–1.4730 at 20°C[2]	
Optical rotation	−4° to −9°;[2] −5° to −9°	
Ester content	Not more than 1% (as rhodinyl acetate)[2]	
Solubility	1:1.2 in 70% alcohol;[2] 1:1.5 in 60% alcohol; insoluble in water; soluble in most common organic solvents	0.12% in water; 0.9% in alcohol
Organoleptic characteristics	Very pleasant, rose-like odor	Odorless; intensely bitter flavor
Synthesis	By fractional distillation of Reunion geranium oil	
Natural occurrence	Geranium oil	
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.1 ppm Candy 7.6 ppm Baked goods 8.1 ppm Gelatins and puddings 2.9 ppm Chewing gum 31 ppm Jellies 0.92 ppm	Non-alcoholic beverages 100 ppm
Regulatory status	FDA 121.1164; FEMA No. 2980	FDA 121.1081; FEMA No. 2977

REFERENCES

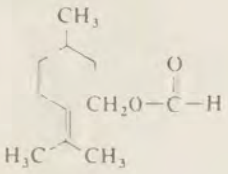
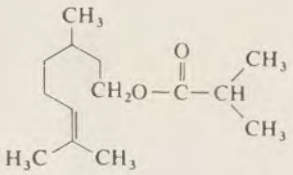
For References 1–5, see end of Part III.

	Rhodinyl acetate	Rhodinyl butyrate
Other names		Citronellyl butyrate
Empirical formula		$C_{14}H_{26}O_2$
Structure	Rhodinyl acetate is chiefly a mixture of acetates of various terpene alcohols derived from geranium oil, in which *l*-citronellyl acetate predominates[2]	
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow liquid	Colorless to yellowish or greenish liquid
Assay	87% min[2]	90%–93% min
Molecular weight		226.36
Boiling point	Approx 237°C	137°C at 13 mm Hg
Flash point		>100 C
Specific gravity	0.895–0.908 at 25°/25°C;[2] 0.8777–0.8810 at 15°C	0.886–0.890 at 25°/25°C; 0.8924 at 15°C
Refractive index	1.4530–1.4580[2] (1.4668–1.4690) at 20°C	1.451–1.455 at 20°C; 1.4474 at 20°C[6]
Acid value	Not more than 1[2]	1 max
Optical rotation	2° to −6°;[2] −6.5 to −8.2	
Solubility	1:2 in 80% alcohol;[2] 1:3.5-5.5 in 60% alcohol; insoluble in water	1:8 in 80% alcohol; 1:1 in 90% alcohol
Organoleptic characteristics	Characteristic fresh, rose-like odor; analogous taste on dilution, bitter when concentrated	Fruity, sweet odor similar to rose; sweet taste reminiscent of blackberry
Synthesis	By acetylation of rhodinol from geranium oil	By esterification of rhodinol, as for geraniol and linalool
Natural occurrence		Reported found in geranium essential oil
	Non-alcoholic beverages 2.8 ppm Ice cream, ices, etc. 1.4 ppm Candy 9.4 ppm Baked goods 18 ppm	Non-alcoholic beverages 0.94 ppm Ice cream, ices, etc. 1.1 ppm Candy 3.0 ppm Baked goods 9.7 ppm Chewing gum 1.1 ppm
Regulatory status	FDA 121.1164; FEMA No. 2981	FDA 121.1164; FEMA No. 2982

REFERENCES

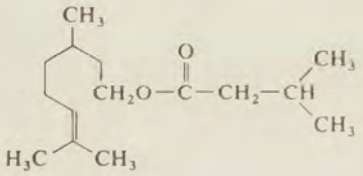
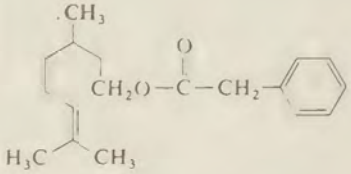
For References 1–5, see end of Part III.

6. Bedoukian, *Perfumery and Flavoring Synthetics*, 2nd ed., American Elsevier, 1967.

	Rhodinyl formate	Rhodinyl isobutyrate
Other names	Citronellyl formate	Citronellyl isobutyrate
Empirical formula	$C_{11}H_{20}O_2$	
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to yellowish liquid	Colorless, oily liquid
Assay	85% min	
Molecular weight	184.26	226.26
Boiling point		Approx 260°C
Flash point	>100°C	
Specific gravity	0.901–0.906 at 25°C	0.89
Refractive index	1.453–1.458 at 20°C	
Acid value	2 max	
Solubility	1:2 in 80% alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Rose-like, leafy odor; bittersweet taste suggestive of cherry	Fruity, sweet, floral odor; fruity, floral, pineapple-like flavor, intensely sweet
Synthesis	By treating rhodinol with formic acid; the rhodinol is extracted from geranium essential oil. Its composition is dependent on the geraniol-citronellol ratio existing in the rhodinol used for esterification.	From rhodinol and isobutyric anhydride
Natural occurrence	Geranyl and citronellyl formate have been found in geranium essential oil. Rhodinyl formate as such has not been reported found in nature.	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 1.8 ppm Candy 4.3 ppm Baked goods 4.9 ppm Gelatins and puddings 0.08 ppm	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 1.8 ppm Candy 3.3 ppm Baked goods 4.5 ppm Gelatins and puddings 0.01 ppm
Regulatory status	FDA 121.1164; FEMA No. 2984	FDA 121.1164; FEMA No. 2983

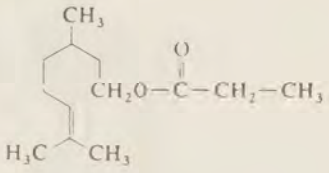
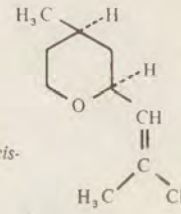
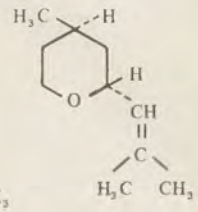
REFERENCES

For References 1–5, see end of Part III.

	Rhodinyl isovalerate	Rhodinyl phenylacetate
Other names	Citronellyl isovalerate Rhodinyl-β-methylbutyrate	Citronellyl phenylacetate Rhodinyl α-toluate
Empirical formula		$C_{18}H_{26}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless to very pale yellow-greenish liquid
Assay		92%–95% min
Molecular weight	240.26	274.26
Boiling point	147°C (approx 270°C) at 14 mm Hg	Approx 340°C
Flash point		>100°C
Specific gravity	0.8829 at 15°C	0.965–0.972 at 25°/25°C
Refractive index	1.4465 at 20°C	1.5000–1.5040 at 20°C
Acid value		1 max
Solubility	Almost insoluble in water; soluble in alcohol	1:3 in 90% alcohol; insoluble in alcohol
Organoleptic characteristics	Lasting, deep, sensual, red rose-like fragrance; bittersweet flavor reminiscent of cherry	Odor reminiscent of rose absolute with a honey-like undertone; very sweet, rose-honey taste
Synthesis		By esterification of rhodinol with phenylacetic acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.3 ppm Candy 7.2 ppm Baked goods 7.2 ppm	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 1.2 ppm Candy 3.8 ppm Baked goods 4.4 ppm
Regulatory status	FDA 121.1164; FEMA No. 2987	FDA 121.1164; FEMA No. 2985

REFERENCES

For References 1–5, see end of Part III.

	Rhodinyl propionate	Rose oxide
Other names	Citronellyl propionate	Tetrahydro-4-methyl-2-(2-methylpro-pen-1-yl)-pyran
Empirical formula		$C_{10}H_{18}O$
Structure		*cis-*   *trans*
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless mobile liquid
Molecular weight	212.26	154.24
Boiling point	122°C (255°C) at 14 mm Hg	70°C at 12 mm Hg (pure material)
Flash point	100°C	
Specific gravity	0.910 at 15.5°C; 0.8959 at 15°C[13]	0.8751 (pure material)
Refractive index	1.4570 at 20°C; 1.4452 at 20°C[13]	1.4566 (pure material)
Solubility	Almost insoluble in water; soluble in alcohol	Very slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics	Sweet odor reminiscent of rose and geranium with a verbena-like undertone; rich, sweet flavor	Powerful, distinctive geranium top-note
Synthesis	From rhodinol and propionic acid (or anhydride)	Several patented syntheses for the preparation of rose oxide are available[6-9]
Natural occurrence	Not reported found in nature	Reported as occurring naturally in the oils of rose (Bulgarian) and geranium (Reunion);[11] both the *cis-* and the *trans*-form have been reportedly isolated from geranium oil;[12] rose oxide exhibits different optical rotations, depending on the source and method of preparation; the highest value (−41.5°C) has been measured on material obtained from Bulgarian attar of roses
Reported uses[3]	Non-alcoholic beverages 1.8 ppm Ice cream, ices, etc. 2.4 ppm Candy 4.9 ppm Baked goods 5.8 ppm	Non-alcoholic beverages 0.40 ppm Candy 2.0 ppm Baked goods 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2986	FEMA No. 3236

REFERENCES

For References 1–5, see end of Part III.

6. **Eschenmoser and Seidel,** U.S. Patent 3,161,657, 1964.
7. **Eschinasi and Cotter,** U.S. Patent 3,163,658, 1964.
8. **Markus,** U.S. Patent 3,166,576, 1965.
9. **Schenk, Ohloff and Klein,** German Patent 1,137,730, 1962.
10. **Seidel and Stoll,** *Helv. Chim. Acta,* 42, 1830, 1959.
11. **Seidel et al.,** *Helv. Chim. Acta,* 44, 598, 1961.
12. **Naves et al.,** *Bull. Soc. Chim. Fr.,* p. 645, 1961.
13. **Bedoukian,** *Perfumery and Flavoring Synthetics,* 2nd ed., American Elsevier, 1967.

Rum ether

Other names

Ethyl oxyhydrate

Empirical formula

Defined as the mixture resulting from the oxidation and the hydration of ethyl alcohol

Structure

Physical/chemical characteristics[5]

Appearance

Rum ether consists of at least 99% water, ethyl alcohol, ethyl acetate, methanol, ethyl formate, acetone, acetaldehyde, and formaldehyde. It all distills at a temperature not exceeding 100°C at atmospheric pressure and leaves no residue on evaporation. The methanol and formaldehyde content, combined, should not exceed 5%.

Boiling point

Rectified material, 65–87°C

Organoleptic characteristics

Rum-like odor and flavor

Synthesis

Place 95% ethanol and manganese dioxide in the reaction flask equipped with distillation apparatus. Add pyroligneous acid and finally sulfuric acid (66°Be) slowly with agitation, maintaining the final temperature *below* 40–50°C. The mixture is then distilled under atmospheric pressure; the fraction distilling between 60° and 100°C is collected. Finally, the collected fraction undergoes rectification. The rectified fraction exhibits a boiling range between 65 and 87°C. Average yield is 98% based on the amount of ethanol used.

Sometimes the distillate is further divided into two additional fractions—one more, and one less rich in acetaldehyde. The amounts of starting material employed vary between the following limits:

Ethanol (95%)	kg 12–25
Pyroligneous acid (12% acetic acid)	kg 10–16
Sulfuric acid (66°Be)	kg 3–8
Manganese dioxide	kg 2–5

A gas chromatographic analysis of rum ether has led to the identification of 22 components in varying concentrations (as low as 50 ppm).[6] Caramel is added to the rum ether for coloring purposes. In general, the addition of rum ether to the finished liquor does not exceed 2–3% for flavoring purposes.

Reported uses[3]

Non-alcoholic beverages	67 ppm
Alcoholic beverages	80–1,600 ppm
Ice cream, ices, etc.	110 ppm
Candy	320 ppm
Baked goods	230 ppm
Gelatins and puddings	1.7 ppm
Chewing gum	380 ppm

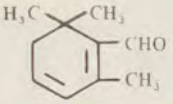
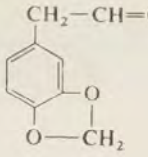
Regulatory status

FDA 121.1164; FEMA No. 2996

REFERENCES

For References 1–5, see end of Part III.

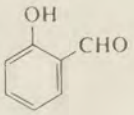
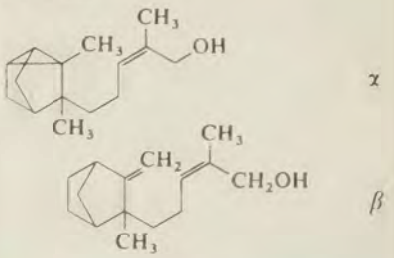
6. Fenaroli, Poy and Maroni, *Riv. Ital. EPPOS*, 9, 484, 495, 1965; 11, 593, 1965; 2, 75, 1966.

	Safranal	Safrole
Other names	2,6,6-Trimethylcyclohexa-1,3-dienyl methanal Dehydrocyclocitral	4-Allyl-1,2-methylenedioxybenzene *m*-Allylpyrocatechin methylene ether 3,4-Methylenedioxyallylbenzene
Empirical formula	$C_{10}H_{14}O$	$C_{10}H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellow oil	Colorless to slightly yellow, oily liquid
Molecular weight	150.09	162.18
Melting point		11°C
Boiling point	172°C 85–78°C at 12 mm Hg 70°C at 1 mm Hg	233–236°C
Congealing point		10.0 11.2°C[2]
Flash point		97 C
Specific gravity	0.9730 at 19°C	1.092–1.101 at 25 /25°C;[2] (1.100–1.107 at 15 C)
Refractive index	1.5281 at 19°C	1.5360–1.5385 at 20°C[2]
Optical rotation		−1° to +1°;[2] −0.30° to +0.30°
Solubility		1:3 in 90% alcohol;[2] insoluble in water; soluble in alcohol, ether, chloroform, and most common organic solvents
Organoleptic characteristics	Characteristic saffron-like odor and taste	Characteristic odor of sassafras
Synthesis	By acid hydrolysis of picrocrocin, the bitter principle in saffron;[6] by catalytic dehydrogenation of β-cyclocitral or α-cyclogeranic acid with selenium dioxide[8]	By distillation from the essential oils rich in safrole. An uneconomical synthesis starts with catechol methylene ether reacted with allyl chloride; also 4-allyl alcohol with methylene iodide
Natural occurrence	Occurring naturally as a glucoside (picrocrocin) in saffron[6]	Originally isolated in the oil from roots of *Sassafras officinale*; constituent of several essential oils, such as camphor, nutmeg, and cinnamon leaves. The essential oil from the rind of *Nemuaron humboldtii* contains up to 99% safrole;[6] Brazilian sassafras oil, up to 93%;[7] and American sassafras oil, up to 80%.[8]
Reported uses[3]	Candy 5.0 ppm Baked goods 10.0 ppm Condiments, pickles 5.0 ppm Preserves and spreads 10.0 ppm	
Regulatory status	FEMA No. 3389	Its use in foods is not permitted in USA.

REFERENCES

For References 1–5, see end of Part III.

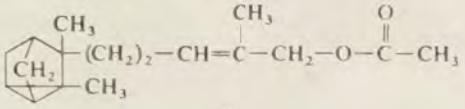
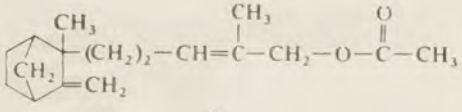
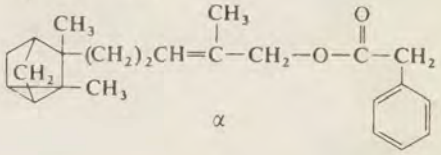
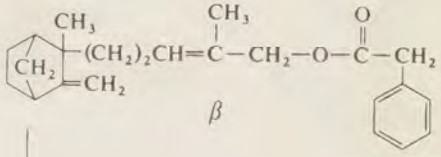
6. Kuhn and Winterstein, *Chem. Ber.*, 67, 354, 1934.
7. Kuhn and Wendt, *Chem. Ber.*, 69, 1546, 1936.
8. Bachli and Karrer, *Helv. Chim. Acta*, 38, 1863, 1955.
9. Chabeau, *Chem. Zentralbl.*, 1, 3747, 1939.
10. De Souza, *Chem. Zentralbl.*, p. 2765, 1952.
11. Hickey, *J. Org. Chem.*, 13, 443, 1948.

	Salicylaldehyde	Santalol, α and β
Other names	2-Hydroxybenzaldehyde *o*-Hydroxybenzaldehyde Salicylic aldehyde	"Argeol" "Arheol" *d*-α-Santalol *l*-β-Santalol
Empirical formula	$C_7H_6O_2$	$C_{15}H_{24}O$
Structure		 α β
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid; solidifies when cold	Colorless to slightly yellow, viscous liquid
Assay		95% min[2] (98% min)
Molecular weight	122.12	220.34
Melting point	2°C	
Boiling point	93°C (196°C) at 25 mm Hg	α, 129°C at 1 mm Hg; 302°C β, 133°C at 1 mm Hg; 309°C
Congealing point	1.6°C	
Specific gravity	1.1690 (1.17) at 20°C	0.965–0.975 at 25°/25°C;[2] 0.9769 at 20°C; 0.9750 at 20°C; 0.970–0.974
Refractive index	1.5740 at 19.7°C	1.5060–1.5090 at 20°C;[2] 1.5050–1.5080; α, 1.5023; β, 1.5115
Optical rotation		−11° to −19°;[2] −14° to −19°; α, +17.0° at 20°C; β, −90.5° at 20°C
Solubility	Soluble in most organic solvents; slightly soluble in water	1:4 in 70% alcohol;[2] insoluble in water; soluble in most common organic solvents
Organoleptic characteristics	Pungent, irritating odor similar to benzaldehyde, acetophenone, and nitrobenzene, but with phenolic notes; nut-like, coumarin flavor at low levels	Sweet, sandalwood odor
Synthesis	From phenol, chloroform, and alkali according to Reimer-Tiemann method (1876); starting material for the manufacture of coumarin	The commercial product is generally a mixture of α- and β-santalol obtained by fractional distillation of sandalwood oil. Non-commercial syntheses are known.
Natural occurrence	Occurs rather frequently in nature; in the flowers of *Spirea ulmaria* and other *Spireae*, in the roots of *Crepis foetida* L., in the fruits of *Pinus avium*, in the rind of *Rauwolfia caffra*, in the leaves of *Ceanothus velutinus*, and in the essential oils of *Cinnamomum cassia* and of tobacco leaves[6]	The stereochemistry of santalols has been discussed by Brieger.[6] Santalols are found among the constituents of various sandalwood species (*Santalum album* L., *S. spicatum*, *S. autrocaledonicum*). The α- and β-isomers are present in varying ratios, with the α-isomer usually more abundant.
Reported uses[3]	Non-alcoholic beverages 0.55 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 1.1 ppm Candy 1.8 ppm Baked goods 6.3 ppm Chewing gum 11–18 ppm Condiments 2.0 ppm	Non-alcoholic beverages 0.06–2.0 ppm Ice cream, ices, etc. 0.35–2.0 ppm Candy 1.0–1.0 ppm Baked goods 1.0–8.0 ppm Chewing gum 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 3004	FDA 121.1164; FEMA No. 3006

REFERENCES

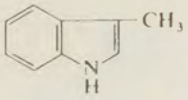
For References 1–5, see end of Part III.

6. Onishi and Yamamoto, *Chem. Abstr.*, 50, 15028, 1956.

	Santalyl acetate, α- and β-	Santalyl phenylacetate, α and β
Other names	α-Santalol, acetate β-Santalol, acetate	α-Santalyl α-toluate β-Santalyl α-toluate
Empirical formula	$C_{17}H_{26}O_2$	$C_{23}H_{30}O_2$
Structure	 α  β	 α  β
Physical/chemical characteristics[5]		
Appearance	Colorless to yellowish liquid	Colorless liquid
Assay	95% min	
Molecular weight	262.40	338.49
Boiling point	Approx 20.8°C at 3 mm Hg	
Specific gravity	0.9884–0.9900 at 15°C; 0.981–0.985 at 25°C	1.024–1.026 at 25°/25°C
Refractive index	1.4894–1.4901 (1.4880–1.4910) at 20°C	
Optical rotation	Approx −16°	
Acid value		1 max
Solubility	1:1 in 90% alcohol; 1:9–11.5 in 80% alcohol; soluble in most common organic solvents	Slightly soluble in alcohol; soluble in benzyl benzoate and in diethyl phthalate
Organoleptic characteristics	Characteristic, sandalwood-like odor; pleasant bittersweet taste with an apricot-like undertone	Sandalwood-like odor; characteristic flavor with a fruity and honey-like undertone
Synthesis	By acetylation of santalol obtained from sandalwood oil that contains the two stereoisomer forms (α and β) of the alcohol. Therefore, the resulting ester is a mixture of the α- and β-isomers.	The commerical product consists of a mixture of the α- and β-isomers
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.53 ppm Ice cream, ices, etc. 0.78 ppm Candy 2.0 ppm Baked goods 2.0 ppm Chewing gum 2.3 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 0.95 ppm Candy 2.0 ppm Baked goods 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3007	FDA 121.1164; FEMA No. 3008

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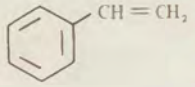
For References 1–5, see end of Part III.

	Skatole
Other names	3-Methylindole β-Methylindole
Empirical formula	C_9H_9N
Structure	
Physical/chemical characteristics[5]	
Appearance	White scales or powder (from pet ether); tends to darken on exposure to air
Molecular weight	121.18
Melting point	96°C (93 96°C)
Boiling point	265–266°C
Solubility	Soluble in boiling water; soluble in alcohol and other common organic solvents
Organoleptic characteristics	Characteristic fecal odor at high levels, becoming pleasant, sweet, and warm at very low levels; warm, over-ripe, fruity flavor below 0.1 ppm
Synthesis	Synthesized by Fischer and German[6] by heating glycerol and aniline in the presence of $ZnCl_2$; also by treating the phenylhydrazone of propionic aldehyde with a calculated amount of $ZnCl_2$ in an oil bath at 180°C;[7] or by fusing egg albumin with KOH
Natural occurrence	Reported as a constituent of feces,[8] nectandra wood, and civet
Reported uses[3]	Non-alcoholic beverages 0.75 ppm Ice cream, ices, etc. 1.0 ppm Candy 0.78 ppm Baked goods 0.80 ppm Gelatins and puddings 0.01 ppm Chewing gum 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 3019

REFERENCES

For References 1–5, see end of Part III.

6. Fischer and German, *Ber. Dtsch. Chem. Ges.*, 16, 710, 1883.
7. Fischer, *Ber. Dtsch. Chem. Ges.*, 12, 1566, 1879.
8. Brieger, *Ber. Dtsch. Chem. Ges.*, 12, 1985, 1879.

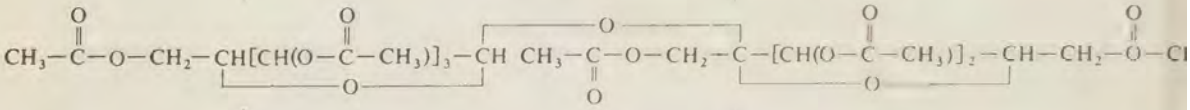
	Styrene
Other names	Styrol Phenylethylene Vinylbenzene
Empirical formula	C_8H_8
Structure	
Physical/chemical characteristics	
Appearance	Colorless to yellowish oily liquid
Molecular weight	104.14
Melting point	33°C
Boiling point	145–146°C 48°C at 20 mm Hg
Flash point	38°C
Specific gravity	0.9090 at 20°C 0.9045 at 25°C
Refractive index	1.5463 at 20°C
Solubility	Soluble in alcohol, ether, acetone, and carbon disulfide; sparingly soluble in water
Organoleptic characteristics	Characteristic sweet, balsamic, almost floral odor, extremely penetrating
Synthesis	From ethylbenzene or from phenylethanol[a]
Natural occurrence	In cranberry and bilberry,[7] currants,[8-10] grape,[11,12] vinegar,[13] parsley,[14] milk and dairy products,[15] whisky,[16,17] cocoa,[18,19] coffee,[20-22] tea,[20] roasted filberts,[23] and roasted peanuts[24]
Reported uses[3]	Ice cream, ices, etc. 0.20 ppm Candy 0.20 ppm Baked goods 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 3234

REFERENCES

For References 1–5, see end of Part III.

6. Wilen et al., *J. Chem. Educ.*, 38, 304, 1961.
7. Sydow et al., *Lebensm. Wiss. Technol.*, 2, 78, 1969; 3, 11, 1970.
8. Andersson et al., *Acta Chem. Scand.*, 20, 522, 1966.
9. Nursten et al., *Chem. Ind.* (London), p. 487, 1967; *J. Sci. Food Agric.*, 20, 613, 1969.
10. Sydow et al., *Lebensm. Wiss. Technol.*, 4, 54, 1971.
11. Stevens et al., *J. Agric. Food Chem.*, 14, 249, 1966.
12. Stern et al., *J. Agric. Food Chem.*, 15, 1100, 1967.
13. Kahn et al., *J. Agric. Food Chem.*, 20, 214, 1972.
14. Kasting et al., *Phytochemistry*, 11, 2277, 1972.
15. Siek et al., *J. Dairy Sci.*, 51, 1887, 1968.
16. Kahn et al., *J. Food Sci.*, 33, 395, 1968; *J. Assoc. Of. Agric. Chem.*, 52, 1166, 1969; *J. Food Sci.*, 34, 587, 1969.
17. Williams et al., *J. Sci. Food Agric.*, 23, 1, 1972.
18. Van de Wal et al., *Recl. Trav. Chim. Pays-Bas*, 87, 238, 1968; *J. Agric. Food Chem.*, 19, 276, 1971.
19. Rohan, *Food Process. Mark.*, 38, 12, 1969.
20. Heins et al., *J. Gas Chromatogr.*, 4, 395, 1966.
21. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.
22. Goldmann et al., *Helv. Chim. Acta*, 50, 694, 1967.
23. Walter et al., *Z. Ernährungswiss.*, 9, 123, 1969.
24. Kinlin et al., *J. Agric. Food Chem.*, 20, 1021, 1972.

	Sucrose octaacetate	Tartaric acid
Other names	Octoacetyl sucrose	*l*-2,3-Dihydroxy butanedioic acid *d*-α-β-Dihydroxysuccinic acid *l*-Tartaric acid
Empirical formula	$C_{28}H_{38}O_{19}$	$C_4H_6O_6$
Structure	See below.	

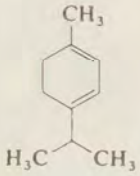
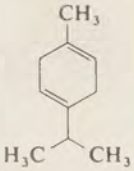


Physical/chemical characteristics[5]		
Appearance	Needles from alcohol	Colorless crystals
Molecular weight	678.61	150.09
Melting point	84°C	*d*, 168–170°C; *dl*, 206°C; *meso*-, 165–166°C
Specific gravity		*d*, 1.7598 at 20°C; *dl*, 1.697 at 20°C
Optical rotation	+56.6° at 20°C (in chloroform)	*d*, +11.98°C
Solubility	0.1% in water; 9% in alcohol	Soluble in water and alcohol; slightly soluble in chloroform and ether
Organoleptic characteristics	Odorless; intensely bitter flavor influenced by food acids	Odorless; characteristic acid taste
Synthesis	By heating sucrose, acetamide, and sodium acetate;[7] or by acetylation of sucrose using acetic anhydride, zinc chloride, and acetic acid	*dl*-Tartaric acid can be produced by oxidation of fumaric and maleic acids; also from glyoxal and hydrocyanic acid, followed by acid hydrolysis
Reported uses	Non-alcoholic beverages, such as ginger ale, "quinine bitters," and others: 0.35–20 ppm	*d*-Tartaric acid occurs in many fruits or other parts of plants, free or combined with potassium, calcium, or magnesium. Produced from argols or wine-lees, which are formed in the manufacture of wine by extracting the potassium acid tartrate, transforming this into the calcium salt, and then acidifying with dilute sulfuric acid. Also by oxidation of *d*-glucose with nitric acid. The *dl*-tartaric acid is obtained by boiling the *d*-tartaric acid with an aqueous solution of NaOH or by oxidation of fumaric acid. The *l* and the *meso*-tartaric acid are also known but are less important. Non-alcoholic beverages 960 ppm Ice cream, ices, etc. 570 ppm Candy 5,400 ppm Baked goods 1,300 ppm Gelatins and puddings 60 ppm Chewing gum 3,700 ppm Condiments 10,000 ppm
Regulatory status	FDA 121.1164; FEMA No. 3038	FDA GRAS (general); FEMA No. 3044

REFERENCES

For References 1–5, see end of Part III.

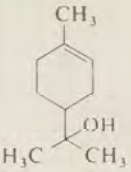
6. Herzfeld, *Chem. Zentralbl.*, p. 749, 1887.

	α-Terpinene	α-Terpineol
Other names	*p*-Menthadiene-1,3 1,3-*p*-Menthadiene 1-Methyl-4-isopropyl-1,3-cyclohexadiene 1-Methyl-4-isopropylcyclohexadiene-1,3	1,4-*p*-Menthadiene 1-Methyl-4-isopropyl-1,4-cyclohexadiene
Empirical formula	$C_{10}H_{16}$	$C_{10}H_{16}$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless, oily liquid
Molecular weight	136.23	136.23
Boiling point	173.5–174.8°C (176°C)	183°C
Specific gravity	0.8375 at 19.6 C	0.849 at 20°C
Refractive index	1.477 at 19.7°C	1.4765 at 14.5°C
Solubility	Miscible with alcohol and ether; insoluble in water	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic lemon odor, lemony flavor, becoming bitter at high levels	Characteristic lemon odor (not as lemony as the α-isomer, but warmer); slightly bitter, herbaceous, citrus-like flavor
Synthesis	By isolation from the terpene fraction of sweet orange oil or orange terpenes (8–10% of the total monoterpenes); by isolation from fractions of American turpentine oil; from 1-methyl-4-isopropylcyclohexadien-1,3-one-2; also from terpinene dihydrochloride with aniline	Isolated from the essential oil of *Lantana camara*; also from *p*-cymene by the action of sodium and alcohol in liquid ammonia
Natural occurrence	Originally reported found in cardamom essential oil; also in orange, coriander, wormseed, *Eucalyptus australiana*, and in approximately 20 additional essential oils.	Reported found in several essential oils: *Mosla japonica*, *Eucalyptus dives*. *Orthodon perforatum* and other *Orthodon* species, lemon, pine, and others, often in mixture with the α-isomer; primarily in *Lantana camara*
Regulatory status	FDA 121.1164	FDA 121.1164

REFERENCES

For References 1–5, see end of Part III.
For further information on γ-terpinene see the following.
Marot, *Bull. Inst. Pin*, 38, 61, 1933.
Richter and Wolff, *Ber. Dtsch. Chem. Ges.*, 60, 477, 1927; 63, 1714, 1930.

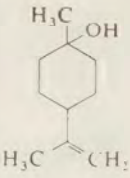
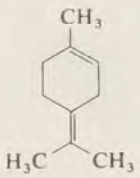
α-Terpineol

Other names	*p*-Menth-1-en-8-ol 1-Methyl-4-isopropyl-1-cyclohexen-8-ol
Empirical formula	$C_{10}H_{18}O$
Structure	
Physical chemical characteristics[5]	
Appearance	Colorless liquid, viscous at room temperature; the pure α-isomer is a white, crystalline powder
Assay	Commercial terpineol is a mixture of α- and β-isomers with possibly some γ- and other alcohols.[2] A good grade of α-terpineol contains about 3–5% β-isomer
Molecular weight	154.24
Melting point	*d*, 40–41°C; *l*, 37–38°C; *dl*, 35°C
Boiling point	214–224°C;[2] *d*, 115–116°C at 25 mm Hg; *l*, 219–221°C; *dl*, 218–219°C
Congealing point	+2°C[2]
Flash point	91°C
Specific gravity	0.930–0.936 at 25°/25°C;[2] *d*, 0.940 at 15°C; *dl*, 0.935–0.940 at 15°C
Refractive index	1.4825–1.4850 at 20°C;[2] *d*, 1.48322 at 18°C; *dl*, 1.48131 at 20°C; *dl*, 1.48084 at 20°C
Optical rotation	−0°10′ to +0°10′;[2] *d*, −95°9′; *l*, 106°
Solubility	1:8 or more in 50% alcohol;[2] soluble in propylene glycol; very slightly soluble in water
Organoleptic characteristics	Characteristic lilac odor; sweet taste reminiscent of peach on dilution
Synthesis	Obtained from terpin hydrate by splitting off water;[2] from pentane tricarboxylic acid by cyclization, followed by esterification to the hydroxy ester, then the unsaturated ester and Grignard to terpineol; also from isoprene and methyl vinyl ketone, using methyl magnesium iodide
Natural occurrence	Reported found in more than 150 derivatives from leaves, herbs, and flowers. The *d*-, *l*-, and *dl*-isomers are known. The *d*-form is found in the essential oils from *Cupressaceae* in general; also in the oils of *Elettaria cardamomum*, star anise, marjoram, clary sage, neroli, and others. The *l*-form is found in *Satureia montana*, lavandin, cajeput, lime, lemon, cinnamon leaves, and the distillates from *Pinaceae* (with the exception of *Pinus silvestris*, which contains *d*-terpineol together with the racemic form); likewise, *Nectandra elaiophora* (wood) and petitgrain bigarade. The racemic form is found in cajenne linalool, *Thymus caespititius*, cajeput, *Eucalyptus globulus*; mixed with the *l*-form it is found in petitgrain.[6] A non-defined form of terpineol has been reported in bitter orange.[7]
Reported uses[3]	Non-alcoholic beverages 5.4 ppm Ice cream, ices, etc. 16 ppm Candy 14 ppm Baked goods 19 ppm Gelatins and puddings 12–16 ppm Chewing gum 40 ppm Condiments 38 ppm
Regulatory status	FDA 121.1164; FEMA No. 3045

REFERENCES

For References 1–5, see end of Part III.

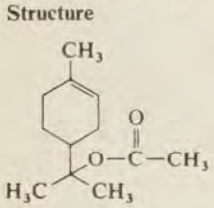
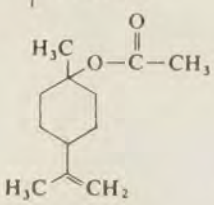
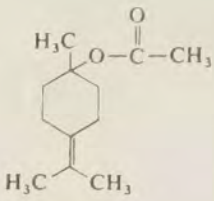
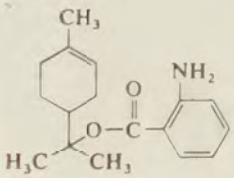
6. Peyron, *Fr. Ses Parfums*, 6(1), 17, 1958.
7. Mehlitz and Minas, *Ind. Obst Gemueseverwert.*, 50, 861, 1965.

	β-Terpineol	Terpinolene
Other names	*p*-Menth-8-en-1-ol Δ-8,9-*p*-Menthenol-1 1-Methyl-4-isopropenylcyclohexan-1-ol *Note*: the *trans*-β-form is the most common.	*p*-Menth-1,4(8)-diene 1-Methyl-4-isopropylidene-1-cyclohexene 1,4(8)-Terpadiene
Empirical formula	$C_{10}H_{18}O$	$C_{10}H_{16}$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to very pale, straw-yellow, oily liquid; polymerizes readily
Molecular weight	154.24	136.23
Melting point	*cis*-, 36 C; *trans*-, 32–33 C	
Boiling point	*cis*-, 78°C at 1.5 mm Hg; *trans*-, 90°C at 10 mm Hg; 210°C	183–185°C
Specific gravity	*cis*-, 0.9258 at 20°C; *trans*-, 0.923 at 15 C	0.8620 at 20°C
Refractive index	*cis*-, 1.4793 at 20 C; *trans*-, 1.4747 at 20 C	1.4900 at 20°C
Solubility	Very slightly soluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Pungent or earthy, woody odor	Sweet, pine odor; somewhat sweet, citrus flavor
Synthesis	From steam-distilled fractions of pine oil; from foreruns of the rectification of terpineol obtained from α-pinene and terpin hydrate; by reduction of limonene epoxide	The pure product was isolated and structurally identified by Baeyer;[6] by alcoholic H_2SO_4 treatment of pinene
Natural occurrence	In strawberry, raspberry, and blackberry	Reported found as a constituent of a few essential oils in small amounts: *Manilla elemi*, a few pine and fir varieties, *Neetandra elatiophora*, *Dacrydium colensoi*, and a few others
Reported uses[3]		Non-alcoholic beverages 16 ppm Ice cream, ices, etc. 64 ppm Candy 0.12–48 ppm Baked goods 49 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 3046

REFERENCES

For References 1–5, see end of Part III.

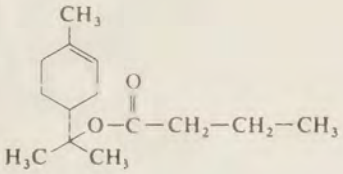
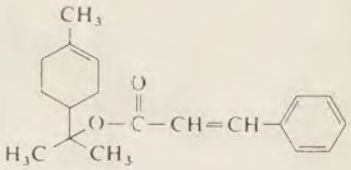
6. Baeyer, *Ber. Dtsch. Chem. Ges.*, 27, 443, 1894.

	Terpinyl acetate	Terpinyl anthranilate
Other names	*p*-Menth-1-en-8-yl acetate	*p*-Menth-1-en-8-yl anthranilate Terpinyl-2-aminobenzoate Terpinyl-*o*-aminobenzoate
Empirical formula	$C_{12}H_{20}O_2$	$C_{17}H_{23}NO_2$
Structure	 α  β  γ	
Physical/chemical characteristics[5]		
Appearance	Clear, colorless liquid	
Assay	97% min[2]	
Molecular weight	196.29	273.38
Boiling point	α, 105°C at 11 mm Hg; α, *dl*-, 220°C	365°C
Flash point	α, *dl*-, 85°C; α, 100°C	
Specific gravity	0.953–0.962 at 25°/25°C;[2] α, *dl*-, 0.9704 at 15°C	1.055 at 15.5°C
Refractive index	1.4640–1.4670 at 20°C;[2] α, *dl*-, 1.4689 at 21°C	1.4830 at 20°C
Optical rotation	+9° to −9°[2]	
Solubility	1:5 in 70% alcohol;[2] soluble in essential oils and most common organic solvents	
Organoleptic characteristics	Lavender- and bergamot-like character; characteristic flavor—first slightly pungent, then slightly sweet—similar to currant	Complex fruity odor and bitter taste
Synthesis	Usually prepared by acetylation of α-terpineol or mixed isomeric terpineols, using acetic anhydride and anhydrous sodium acetate. The first synthesis dates back to 1888.[6] Another synthetic route starts with 1,8-cineol.[7] α-Terpinyl acetate is also the starting material for the synthesis of carvone.[8]	By esterification of anthranilic acid with terpineol[10]
Natural occurrence	Reported in the essential oils of cypress, Malabar cardamom, cajeput, niaouli, Siberian pine needles, pine, *Melaleuca trichostachya*, *Melaleuca pauciflora*, and others; also identified in the essential oil of bitter orange.[9]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.5 ppm Ice cream, ices, etc. 3.2 ppm Candy 9.9 ppm Baked goods 1.5 ppm Chewing gum 14–260 ppm Condiments 15 ppm Meats 1.7–40 ppm	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 1.5–2.6 ppm Candy 6.3 ppm Baked goods 6.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3047	FDA 121.1164; FEMA No. 3048

REFERENCES

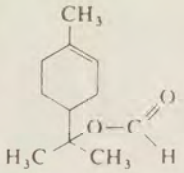
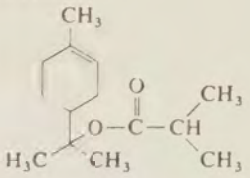
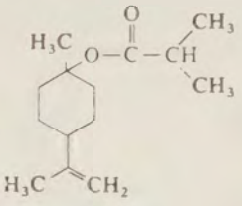
For References 1–5, see end of Part III.

6. Lafont, *Ann. Chim. Paris*, 15, 153, 1888.
7. Matsuura et al., *Militizer Ber.*, p. 34, 1956.
8. Suga, *Bull. Chem. Soc. Jap.*, 7, 569, 1958.
9. Mehlitz and Minas, *Ind. Obst Gemueseverwert.*, 50, 861, 1965.
10. Wagner, *Chem. Ztg.*, 51, 855, 1927.

	Terpinyl butyrate	Terpinyl cinnamate
Other names	*p*-Menth-1-en-8-yl butyrate	*p*-Menth-1-en-8-yl cinnamate Terpinyl β-phenacrylate Terpinyl-3-phenyl propenoate
Empirical formula	$C_{14}H_{24}O_2$	$C_{19}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless to straw-yellow, viscous liquid
Molecular weight	224.34	284.40
Boiling point	244°C	360°C
Specific gravity	0.965 at 15.5°C	1.030 at 15.5°C
Refractive index	1.4656 at 20°C	1.5500 at 20°C
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic, rosemary-like, acrid, fruity odor with a balsamic undertone; bittersweet taste reminiscent of plum	Persistent, sweet, balsamic odor reminiscent of wine moscato; heavy, fruity, somewhat spicy taste
Synthesis		By esterification from terpineol and cinnamic acid; also from methyl cinnamate, sodium terpineol, and terpinyl formate
Natural occurrence	Reported found in the essential oils of niaouli, cypress, and *Eucalyptus diversicolor*	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 6.4 ppm Ice cream, ices, etc. 9.2 ppm Candy 11 ppm Baked goods 9.5 ppm Chewing gum 210 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 2.6 ppm Candy 6.0 ppm Baked goods 6.0 ppm
Regulatory status	FEMA No. 3049	FDA 121.1164; FEMA No. 3051

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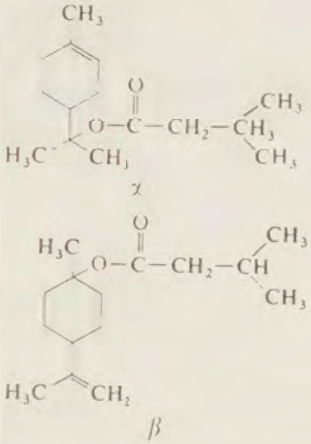
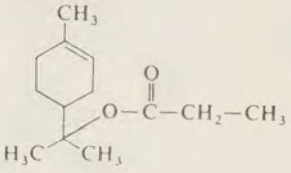
For References 1–5, see end of Part III.

	Terpinyl formate	Terpinyl isobutyrate
Other names	*p*-Menth-1-en-8-yl formate	*p*-Menth-1-en-8-yl isobutyrate
Empirical formula	$C_{11}H_{18}O_2$	$C_{14}H_{24}O_2$
Structure		 α  β
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Molecular weight	182.26	224.34
Boiling point	*d*-α, 133–136°C; *l*-α, 135–138°C;[8] 225°C (commercial product)	Approx 242°C
Specific gravity	*d*-α, 0.971 at 36°C; *l*-α, 0.9986;[8] 0.990 at 15.5°C (commercial product)	0.93
Refractive index	*d*-α, 1.4712 at 20°C; 1.4700 at 20°C (commercial product)	
Optical rotation	*d*-α, undiluted, +88.32°; *l*-α, −69.25°[8]	
Solubility	1:6 in 60% alcohol; very slightly soluble in water	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Pleasant, floral, citrus odor; bitter taste at high levels, becoming dry and fruity at lower levels	Fruity, floral, herbaceous odor; heavy, fruity-type flavor
Synthesis	From *d*-α-terpineol and formic acetic anhydride;[6] the racemic α-terpineol is also obtained by an analogous synthesis.[7]	By esterification of terpineol with isobutyric acid
Natural occurrence	Probably occurring in Ceylon cardamom essential oil	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.50–3.0 ppm Alcoholic beverages 1.0 ppm Ice cream, ices, etc. 2.6–5.0 ppm Candy 6.0–10 ppm Baked goods 6.0–10 ppm	Non-alcoholic beverages 0.90–2.4 ppm Ice cream, ices, etc. 5.0 ppm Candy 4.0–15 ppm Baked goods 5.0–15 ppm
Regulatory status	FDA 121.1164; FEMA No. 3052	FDA 121.1164; FEMA No. 3050

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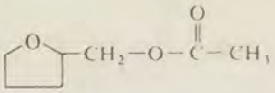
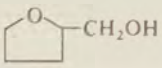
For References 1–5, see end of Part III.

6. Fuller and Kenyon, *J. Chem. Soc.* (London), 125, 2306, 1924.
7. Robert, *Chem. Zentralbl.*, 2, 2295, 1927.
8. Lafont, *Bull. Soc. Chim. Fr.*, 2(49), 325, 1888; *Ann. Chim. Paris*, 6(15), 185, 1888.

	Terpinyl isovalerate	Terpinyl propionate
Other names	*p*-Menth-1-en-8-yl isovalerate *p*-Menth-1-en-8-yl-β-methylbutyrate	*p*-Menth-1-en-8-yl propionate
Empirical formula	$C_{15}H_{26}O_2$	$C_{13}H_{22}O_2$
Structure	 α β	
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless to slightly yellow liquid
Assay		95% min[2]
Molecular weight	238.37	210.31
Boiling point	248 C	
Flash point		>100°C
Specific gravity	0.93	0.944–0.949 at 25°/25°C[2]
Refractive index		1.4620–1.4660 at 20°C[2]
Acid value		1 max[2]
Solubility	Almost insoluble in water; soluble in alcohol	1:2 in 80% alcohol[2]
Organoleptic characteristics	Peculiar, floral odor with a sweet, pine, incense, and orange undertone; bittersweet flavor reminiscent of apple	Somewhat floral, lavender note; bitter flavor
Synthesis	By esterification of terpineol with isovaleric acid	Usually prepared by esterification of terpineols[2]
Natural occurrence	Not reported found in nature	Reported found in citrus fruits and celery; also, the racemic form (*dl*) has been identified in cajeput
Reported uses[3]	Non-alcoholic beverages 0.50–5.0 ppm Ice cream, ices, etc. 2.6–5.0 ppm Candy 6.0–10 ppm Baked goods 6.0–10 ppm	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 2.6–3.0 ppm Candy 6.0–10 ppm Baked goods 6.0–10 ppm
Regulatory status	FDA 121.1164; FEMA No. 3054	FDA 121.1164; FEMA No. 3053

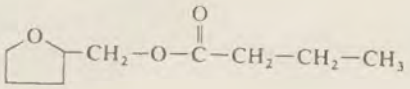
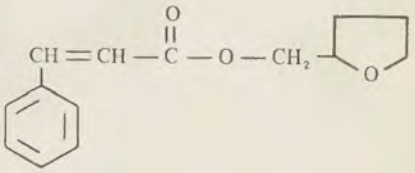
REFERENCES

For References 1–5, see end of Part III.

	Tetrahydrofurfuryl acetate	Tetrahydrofurfuryl alcohol
Other names	Tetrahydro-2-furyl methylacetate	Tetrahydro-2-furancarbinol Tetrahydro-2-furanmethanol Tetrahydro-2-furylmethanol THFA
Empirical formula	$C_7H_{12}O_3$	$C_5H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	144.17	102.13
Boiling point	194–196°C	178–179°C
Specific gravity	1.061 at 20°/20°C (1.005 at 15.5°C)	1.0495 at 20°C
Refractive index	1.4475 at 20°C	1.4505 at 20°C
Solubility	Completely miscible with water, alcohol, ether, and chloroform	Completely miscible with water, alcohol, and ether
Organoleptic characteristics	Faint, fruity, ethereal odor, somewhat similar to acetic acid (reminiscent of methyl formate); sweet, ethereal, deep, fruit-like flavor	Faint, warm, oily, caramellic odor; coffee and nut-like flavor at very low levels (0.03–1 ppm)
Synthesis	By acetylation of the corresponding alcohol with acetic anhydride, acetyl chloride, or acetic acid and mineral acids	By catalytic reduction of furfural with Raney-Nickel; also by the destructive hydrogenation of lignin
Natural occurrence		
Reported uses[3]	Non-alcoholic beverages 1.3–2.0 ppm Ice cream, ices, etc. 8.0 ppm Candy 1.0–20 ppm Baked goods 1.0–20 ppm	Non-alcoholic beverages 0.03–14 ppm Ice cream, ices, etc. 0.03 ppm Candy 0.03–18 ppm Baked goods 0.04 ppm
Regulatory status	FDA 121.1164; FEMA No. 3055	FDA 121.1164; FEMA No. 3056

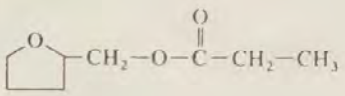
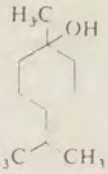
REFERENCES

For References 1–5, see end of Part III.

	Tetrahydrofurfuryl butyrate	Tetrahydrofurfuryl cinnamate
Other names	Tetrahydrofu-furyl-*n*-butyrate Tetrahydro-2-furylmethyl-*n*-butanoate	Cinnamic acid, tetrahydrofurfuryl ester
Empirical formula	$C_9H_{16}O_3$	$C_{14}H_{16}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, slightly viscous liquid
Molecular weight	172.23	232.28
Boiling point	227 C	>300° C
Specific gravity	1.01	1.11
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Heavy, sweet odor reminiscent of apricot and pineapple; sweet, fruity flavor at low levels, becoming pungent at higher levels	Sweet, persistent, balmy-vinous odor
Synthesis	By esterification of the alcohol with *n*-butyric acid	By azeotropic esterification of the corresponding acid
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 0.90 ppm Ice cream, ices, etc. 6.0 ppm Candy 15 ppm Baked goods 15 ppm	Non-alcoholic beverages 20.0 ppm Ice cream, ices, etc. 20.0 ppm Baked goods 20.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3057	FEMA No. 3320

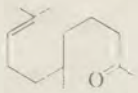
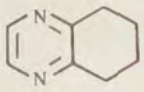
REFERENCES

For References 1–5, see end of Part III.

	Tetrahydrofurfuryl propionate	Tetrahydrolinalool
Other names	Tetrahydro-2-furylmethylpropionate	3,7-Dimethyloctan-3-ol 3,7-Dimethyloctanol-3
Empirical formula	$C_8H_{14}O_3$	$C_{10}H_{22}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Assay		98% min
Molecular weight	158.20	158.29
Boiling point	64–68°C (207°) at 3 mm Hg	87–88°C at 10 mm Hg; *l*, 89°C at 15 mm Hg
Flash point		Approx. 84°C
Specific gravity	1.04	0.825–0.830 at 25/25°C; 0.8280; *l*, 0.8327 at 16°C
Refractive index	1.4370 at 23°C	1.4320–1.4360 (1.4335) at 20°C
Optical rotation		±1; *l*, −0.78°
Solubility	Slightly soluble in water; soluble in alcohol	Very slightly soluble in water; soluble in alcohols and other organic solvents; 1:2 in 70% ethanol
Organoleptic characteristics	Sweet, caramellic, fruity odor; sweet flavor, apricot and chocolate-like	Sweet, oily, floral odor (more so than linalool); citrus, floral taste
Synthesis	Synthetically prepared by esterification of the corresponding alcohol with acetic anhydride and melted sodium acetate	By hydrogenation of *dl*-linalool in the presence of platinum black according to Barbier and Lacquin. Also from magnesium ethyl bromide and isoamylketone, or by hydrogenation of 2,6-dimethyl-2-octen-6-ol in the presence of nickel at 100°C. Optically active and racemic forms are expected because of the structure of this product
Natural occurrence	Not reported found in nature	Not reported found among the natural constituents of essential oils
Reported uses[3]	Non-alcoholic beverages 1.3–2.0 ppm Ice cream, ices, etc. 8.0 ppm Candy 1.0–20 ppm Baked goods 1.0–20 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 2.7 ppm Candy 5.6 ppm Baked goods 5.6 ppm
Regulatory status	FDA 121.1164; FEMA No. 3058	FDA 121.1164; FEMA No. 3060

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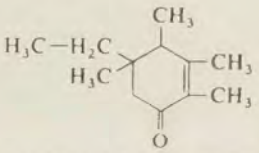
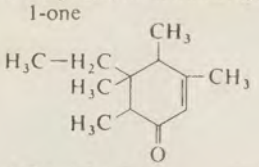
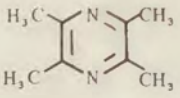
For References 1–5, see end of Part III.

	Tetrahydro-pseudoionone	5,6,7,8-Tetrahydroquinoxaline
Other names	Dihydrogeranyl acetone 6,10-Dimethyl-9-undecen-2-one	Cyclohexapyrazine Tetrahydroquinoxaline
Empirical formula	$C_{13}H_{24}O$	$C_8H_{10}N_2$
Structure		
Physical/chemical characteristics		
Appearance	Pale straw-yellow or colorless, oily liquid	
Assay		C: 71.61%; H: 7.51%; N: 20.88%
Molecular weight	196.33	134.18
Melting point		29–30°C
Boiling point	126–127°C (234°C) at 14 mm Hg	108–111°C
Mass spectra[5]		134(100), 133(46), 106(18), 52(17), 39(14), 119(14), 41(11)
IR spectra[5]		3040, 3000, 1475, 1445, 1405, 1165, 1120, 1070, 850, 755 cm^{-1}
UV spectra[5]		λ_{max} (MeOH): 273 mm, 278 nm ($\epsilon = 9.2 \times 10^{-3}$), 302 nm
NMR spectra[6]		($CDCl_3$) δ 7.6 (5,2, pyrazinyl–H) 2.4 (1,4, $CH_2-CH_2-CH_2-CH_2$) 1.4 (4,–$CH_2-CH_2-CH_2-CH_2$)
Specific gravity	0.87	1.1334 at 48°C
Refractive index		1.6231 at 48°C
Solubility	Almost insoluble in water; soluble in alcohol	
Organoleptic characteristics	Sweet, floral, balsamic odor with a rose to woody quality; sweet, fruity flavor, somewhat apple- and peach-like	
Synthesis	By hydrogenation of pseudoionone with colloidal palladium; this reaction leads to a product with considerable mixture. Also from linalool plus acetic anhydride and sodium ethoxide, followed by hydrogenation. Another method starts with geraniol via the acid chloride.	Condensation of an alicyclic α,β-diketone with an α,β-diamine;[8] condensation of an alicyclic α,β-diamine with an α,β-dicarbonyl[8]
Natural occurrence		Reported present in filberts and peanuts[7]
Reported uses[3]	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.60–2.4 ppm Candy 14 ppm Baked goods 14 ppm	Non-alcoholic beverages 5.0 ppm Candy 5.0 ppm Gelatins and puddings 5.0 ppm Baked goods 2.0 ppm Condiments 2.0 ppm Meat, meat sauces, soups 2.0 ppm Milk, dairy products 1.0 ppm Cereals 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3059	FEMA No. 3321

REFERENCES

For References 1–5, see end of Part III.

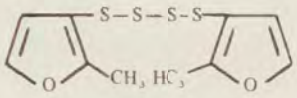
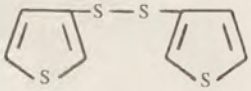
6. **Walradt et al.,** *J. Agric. Food Chem.*, 19, 972, 1971.
7. **Maga and Sizer,** *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
8. **Pittet et al.,** *J. Agric. Food Chem.*, 22(2), 273, 1974.

	Tetramethyl ethylcyclohexenone	2,3,5,6-Tetramethylpyrazine
Other names	Mixture of 5-ethyl-2,3,4,5-tetramethyl-2-cyclohexen-1-one and 5-ethyl-3,4,5-6-tetramethyl-2-cyclohexen-1-one	Tetramethylpyrazine
Empirical formula	$C_{12}H_{20}O$	$C_8H_{12}N_2$
Structure	 5-Ethyl-2,3,4,5-tetramethyl-2-cyclohexen-1-one  5-Ethyl-3,4,5,6-tetramethyl-2-cyclohexen-1-one	
Physical/chemical characteristics		
Appearance	Almost colorless, oily liquid	
Assay	Approx. 30% 5-ethyl-2,3,4,5 and 70% 5-ethyl-3,4,5,6	C: 70.55%; H: 8.88%; N: 20.57%
Molecular weight	180.29	136.20
Mass spectra[6]		39(20), 42(37), 53(23), 54(100), 66(2), 68(2), 80(3), 94(3), 95(6), 121(3), 135(7), 136(85)
IR spectra[6]		7.06, 6.91, 10.08, 8.17, 3.42, 8.46, 8.32 μ
Solubility	Very slightly soluble in water; soluble in alcohol	
Organoleptic characteristics	Warm, caramellic, fruity, spicy odor; pleasant, creamy, caramellic, fruity flavor	Odor threshold: 10,000 ppb in H_2O[8]
Synthesis		From 2,5-dimethylpyrazine by ring alkylation with MeLi;[9] also by condensation of 2,3-butanedione with 2,3-butanediamine
Natural occurrence		Reported present in cocoa products, coffee, dairy products, galbanum oil, meats, peanuts, filberts, rum, whisky, and soy products[7]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 30 ppm Candy 30 ppm Baked goods 30 ppm	Non-alcoholic beverages 5.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Condiments 10.0 ppm Meat, meat sauces, soups 10.0 ppm Milk, dairy products 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3061	FEMA No. 3237

REFERENCES

For References 1–5, see end of Part III.

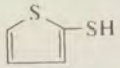
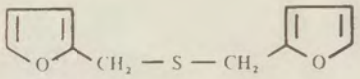
6. Friedel et al., *J. Agric. Food Chem.*, 19, 530, 1971.
7. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
8. Koehler et al., *J. Food Sci.*, 30, 816, 1971.
9. Rizzi, *J. Org. Chem.*, 33(4), 1333, 1968.

	3,3′-Tetrathio-bis(2-methylfuran)		2-Thienyl disulfide	
Other names	Bis(2-methyl-3-furyl) tetrasulfide 2-Methyl-3-furyl tetrasulfide		2,2′-Dithiodithiophene	
Empirical formula			$C_8H_6S_4$	
Structure				
Physical/chemical characteristics				
Molecular weight	290.44		230.39	
Melting point			55–60°C	
Boiling point			115–45°C at 0.02 mm Hg	
Synthesis			By reduction of the corresponding sulfonyl chloride by red phosphorus in the presence of iodine as a catalyst;[6] by reduction of 2-thiocyano thiophene with $NaBH_4$ in methanol[7,8]	
Reported uses[3]	Baked goods	0.1 ppm	Baked goods	0.15 ppm
	Condiments, pickles	0.1 ppm	Condiments, pickles	0.15 ppm
	Meat, meat sauces, soups	0.1 ppm	Meat, meat sauces, soups	0.15 ppm
	Milk, dairy products	0.1 ppm	Cereals	0.15 ppm
	Cereals	0.1 ppm		
Regulatory status	FEMA No. 3260		FEMA No. 3323	

REFERENCES

For References 1–5, see end of Part III.

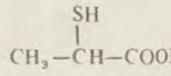
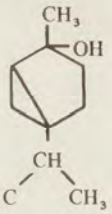
6. **Kiyoski and Kawahara,** *Yakugaki Zasshi*, 77, 963, 1957.
7. **Fedorov and Stoyanovich,** *Zh. Obshch. Khim.*, 32, 1518, 1962; *Chem. Abstr.*, 58, 4495h, 1963.
8. **Stoyanovich et al.,** *Izv. Akad. Nauk, SSSR Ser. Khim.*,(2), 387, 1969.

	2-Thienyl mercaptan	2,2'-(Thiodimethylene)-difuran
Other names	2-Mercapto-thiophene 2-Thienylthiol	2-Furfuryl monosulfide Difurfurylsulfide
Empirical formula	$C_4H_4S_2$	$C_{10}H_{10}O_2S$
Structure		
Physical/chemical characteristics		
Appearance	Oily, yellowish, or colorless liquid; tends to oxidize in air	
Molecular weight	116.21	194.25
Melting point		31–32°C
Boiling point	166°C	135–143°C at 14 mm Hg
Solubility	Very slightly soluble in water; soluble in alcohol	
Organoleptic characteristics	Very unpleasant, burnt caramellic and sulfuraceous odor; similar flavor	
Synthesis	By heating sodium sulfosuccinate with phosphorous trichloride;[6] also by reduction of thiophene-2-sulfonyl chloride	By reflexing a mixture of 2-furylmethanethiol in ethanolic KOH and furfuryl bromide in ether[7]
Natural occurrence	Not reported found in nature	In coffee[7–9]
Reported uses[3]	Candy 0.10 ppm Baked goods 0.10 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm Gelatins and puddings 1.0 ppm Chewing gum 1.0 ppm Condiments 1.0 ppm Meat, meat sauces, soups 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3062	FEMA No. 3238

REFERENCES

For References 1–5, see end of Part III.

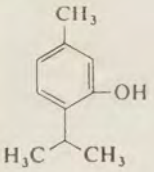
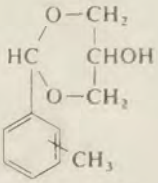
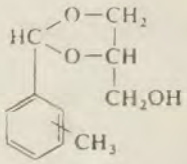
6. Meyer and Neure, *Ber. Dtsch. Chem. Ges.*, 20, 1756, 1887.
7. Stoll et al., *Helv. Chim. Acta*, 50, 688, 1967.
8. Gautschi et al., *J. Agric. Food Chem.*, 15, 15, 1967.
9. Walter et al., *Z. Ernährungswiss.*, 9, 123, 1969.

	Thiolactic acid	Thujan-4-ol
Other names	2-Mercaptopropionic acid α-Thiolpropionic acid	Sabina hydrate Sabinene hydrate
Empirical formula	$C_3H_6O_2S$	$C_{10}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	White crystals
Molecular weight	106	154.24
Melting point	10°C	*trans*-, 60–61°C *cis*-, 36.5–37.2°C
Boiling point	*d*-, 95–100°C at 16 mm Hg *dl*-, 98.5–99.0°C at 14 mm Hg	*trans*-, 193–198°C *cis*-, 195–200°C
Specific gravity	*l*-, 1.193 at 19.2°C	
Refractive index	*dl*-, 1.4823	*trans*-, 1.4430 at 60°C *cis*-, 1.4489 at 60°C *cis*-, 1.4632 at 25°C
Optical rotation	+38.32°C at 20°C −45.47	*trans*-, +47.2° at 25°C (natural source)
Solubility	Soluble in water, alcohol, and ether	
Organoleptic characteristics		Odor reminiscent of terpineol
Synthesis	By electrolysis of the corresponding sulfide, $S(SCHMeCO_2H)_2$[6]	The Grignard reaction with sabina ketone yields two isomers, of which one is identical to an alcohol isolated from American peppermint oil;[7] synthetic routes for the preparation of both the *cis*- and *trans*-form are also available[8]
Natural occurrence		Reported found in peppermint oil (*trans*-form)
Reported uses[3]	Meat, meat sauces, soups 50.0 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm
Regulatory status	FEMA No. 3180	FEMA No. 3239

REFERENCES

For References 1–5, see end of Part III.

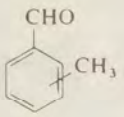
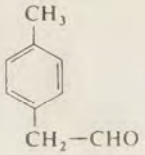
6. **Parsonn,** *Chem. Abstr.*, 22, 4470, 1928.
7. **Daly, Green and Eastman,** *J. Am. Chem. Soc.*, 80, 6330, 1958.
8. **Fanta and Eastman,** *J. Org. Chem.*, 33, 1656, 1968.

	Thymol	Tolualdehyde glyceryl acetal, mixed *o-*, *m-*, *p-*
Other names	3-*p*-Cymenol 3-Hydroxy-*p*-cymene *p*-Isopropyl-*m*-cresol 1-Methyl-3-hydroxy-4-isopropylbenzene 3-Methyl-6-isopropylphenol "Thyme camphor" *m*-Thymol	2-(*o-*,*m-*,*p*-Cresyl)-5-hydroxydioxan 2-(*o-*,*m-*,*p*-Cresyl)-5-hydroxymethyldioxolan 2-(Methylphenyl)-1,3-dioxan-5-ol, mixed *o-*, *m-*,*p-* "Tolyl glycerin"
Empirical formula	$C_{10}H_{14}O$	$C_{11}H_{14}O_3$
Structure		  Approx. 40% Approx. 60%
Physical/chemical characteristics[5]		
Appearance	White crystals	Colorless, slightly viscous liquid
Assay		Commercial products are about 60% of the dioxolans and 40% dioxans.
Molecular weight	150.22	194.23
Melting point	48–51°C	
Boiling point	233°C	292°C
Specific gravity	0.972–0.979	1.14
Refractive index	1.523 at 20 C	
Solubility	Very slightly soluble in water (0.1%) and glycerol; soluble in alcohol, various organic solvents, and glacial acetic acid	Slightly soluble in water (decomposes slowly, especially under acidic conditions); soluble in alcohol
Organoleptic characteristics	Characteristic phenol-like, aromatic odor; sweet, medicinal, spicy flavor	Fresh material is almost odorless; mild, bitter-almond flavor
Synthesis	By action of potassium nitrite on thymyl amine in acetic acid solution and subsequent heating of the diazonium salt to boiling;[6] also by boiling 1 mole of 2,4-dibromomenthone with 6 moles of quinoline (Beckmann); from *m*-cresol and isopropyl chloride at −10°C according to Friedel-Crafts condensation.	From mixed tolylaldehydes and glycerol with phosphoric acid, finishing with an azeotropic distillation to remove water
Natural occurrence	Reported in the essential oils of *Monarda punctata*,[7] *Satureia thymera*,[8] *Origanum floribundum*, *Ocimum viride*, *Ocimum gratissimum*, and particularly in thyme (*Thymus vulgaris* L., *T. capitatus*, *T. serpillum* L.), where it is contained up to 50%	
Reported uses[3]	Non-alcoholic beverages 2.5–11 ppm Ice cream, ices, etc. 44 ppm Candy 9.4 ppm Baked goods 5.0–6.5 ppm Chewing gum 100 ppm	Non-alcoholic beverages 0.08–6.0 ppm Ice cream, ices, etc. 6.0–8.0 ppm Candy 12–15 ppm Baked goods 12–15 ppm
Regulatory status	FDA 121.1164; FEMA No. 3066	FDA 121.1164; FEMA No. 3067

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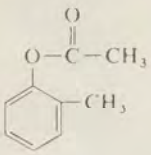
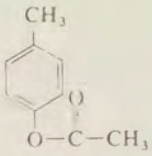
For References 1–5, see end of Part III.

6. Widmann, *Ber. Dtsch. Chem. Ges.*, 15, 170, 1882.
7. *Schimmel Ber.*, p. 20, September 1885.
8. *Schimmel Ber.*, pp. 55, October 1889.

	Tolualdehydes, mixed *o*-,*m*-,*p*-	*p*-Tolylacetaldehyde
Other names	Methyl benzaldehydes, mixed *o*-,*m*-,*p*- Tolyl aldehydes, mixed *o*-,*m*-,*p*-	*p*-Methyl phenylacetaldehyde Syringa aldehyde
Empirical formula	C_8H_8O	$C_9H_{10}O$
Structure		
Physical/chemical characteristics[5]	The commercial product is a mixture of the three isomers	
Appearance	Colorless liquid	Colorless, oily liquid
Assay		95% min
Molecular weight	120.14	134.17
Boiling point	*m*-, 199°C; *o*-, 200°C; *p*-, 204°C	210°C
Flash point		70°C
Specific gravity	*m*-, 1.019 at 20°C; *o*-, 1.0386 at 19°C; *p*-, 1.015 at 15.5°C	1.010–1.016 at 25°C
Refractive index	*m*-, 1.5407 at 21.4°C; *o*-, 1.549 at 19°C; *p*-, 1.5469 at 16.6°C	1.5300–1.5350 at 20°C
Solubility	Slightly soluble in water; soluble in alcohol and ether	1:1 in 80% alcohol; soluble in most common organic solvents; insoluble in alcohol
Organoleptic characteristics	Odor reminiscent of bitter almond	Characteristic odor reminiscent of bitter almond and corresponding flavor
Synthesis	By oxidation of *o*-, *m*-, or *p*-xylene (chemical or electrolytical oxidation)	From *p*-methylbenzaldehyde; also from *p*-methylbenzyl chloride and hexamethylene tetramine
Natural occurrence	Reported found in roasted nuts[6]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 16 ppm Candy 25 ppm Baked goods 28 ppm Gelatins and puddings 8.3 ppm Chewing gum 430 ppm Maraschino cherries 100 ppm	Ice cream, ices, etc. 2.0 ppm Candy 0.03–2.0 ppm Baked goods 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3068	FDA 121.1164; FEMA No. 3071

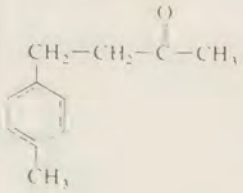
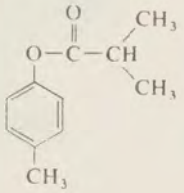
REFERENCES

For References 1–5, see end of Part III.
6. *J. Agric. Food Sci.*, 20, 5, 1972.

	o-Tolyl acetate	*p*-Tolyl acetate
Other names	Acetyl *o*-cresol *o*-Cresyl acetate *o*-Cresylic acetate	Acetyl-*p*-cresol *p*-Cresyl acetate (true name) *Note*: this compound title is *not* true *p*-tolyl acetate.
Empirical formula	$C_9H_{10}O_2$	$C_9H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Clear, colorless liquid
Assay		98% min[2]
Molecular weight	150.18	150.18
Boiling point	Approx 208°C (approx 87°C at 12 mm Hg)	208–209 C
Flash point		95 C
Specific gravity		1.044–1.050 at 25°/25°C;[2] 1.056 at 15.5°C; 1.0512 at 4°C
Refractive index		1.4990–1.5020[2] (1.5035) at 20°C
Acid value		1.0 max[2]
Free cresol		1% max[2]
Solubility	Almost insoluble in cold water; slightly soluble in hot water, essential oils, and most common organic solvents	1:2 in 70% alcohol;[2] 1:9–12 in 60% alcohol; soluble in most common organic solvents
Organoleptic characteristics	Powerful, fruity, medicinal odor that becomes sweet and floral on dilution; sweet and fruity flavor at low levels	Strong, floral odor (narcissus); characteristic honey-like flavor
Synthesis	From sodium *o*-cresol and acetic anhydride	Synthetically prepared by suitable acetylation of *p*-cresol
Natural occurrence	Not reported found in nature	Reported as a constituent of the essential oils of wallflower, cananga, and ylang-ylang
Reported uses[3]	Non-alcoholic beverages 2.8 ppm Ice cream, ices, etc. 2.6 ppm Candy 11 ppm Baked goods 9.0–10 ppm Gelatins and puddings 1.0 ppm Chewing gum 0.30–220 ppm	Non-alcoholic beverages 0.50–1.0 ppm Ice cream, ices, etc. 1.3 ppm Candy 4.3 ppm Baked goods 4.4 ppm Chewing gum 0.30–220 ppm Condiments 10 ppm
Regulatory status	FDA 121.1164; FEMA No. 3072	FDA 121.1164; FEMA No. 3073

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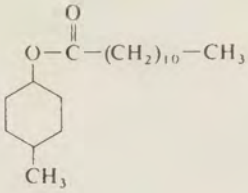
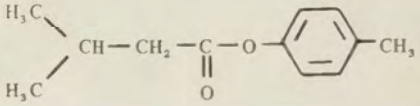
For References 1–5, see end of Part III.

	4-(*p*-Tolyl)-2-butanone	*p*-Tolyl isobutyrate
Other names	*p*-Methylbenzylacetone	*p*-Cresyl isobutyrate (true name)
Empirical formula	$C_{11}H_{14}O$	$C_{11}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Assay		95% min[2]
Molecular weight	162.23	178.23
Boiling point		237°C
Flash point		> 100°C
Specific gravity		0.991–0.996 at 25°/25°C;[2] 1.005 at 25°C
Refractive index		1.4860–1.4890[2] (1.4840) at 20°C
Acid value		1.0 max[2]
Free cresol		1.0% max[2]
Solubility	Very slightly soluble in water; soluble in alcohol	1:2 in 80% alcohol;[2] 1:7 in 70% alcohol; insoluble in water
Organoleptic characteristics	Very sweet, fruity, floral odor, with raspberry, plum, and gardenia notes; intense, sweet, deep fruit flavor	Very strong, lily-narcissus odor
Synthesis	By condensation of *p*-tolylaldehyde with acetone followed by hydrogenation	By esterification of *p*-cresol with isobutyric acid
Natural occurrence	Not reported found in nature. Its use as an insect attractant has been studied[6]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.5 ppm Candy 6.0 ppm Baked goods 6.0 ppm	Non-alcoholic beverages 0.10–4.0 ppm Ice cream, ices, etc. 0.05 ppm Candy 0.12–6.0 ppm Baked goods 0.12–7.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3074	FDA 121.1164; FEMA No. 3075

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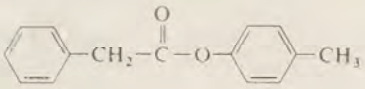
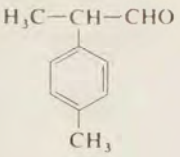
For References 1–5, see end of Part III.

6. *J. Agric. Food Chem.*, 10, 270, 1962.

	p-Tolyl laurate	*p*-Tolyl-3-methyl butyrate
Other names	*p*-Cresyl dodecanoate (true name) *p*-Cresyl laurate *p*-Tolyl dodecanoate *p*-Tolyl dodecylate	*p*-Cresyl isovalerate
Empirical formula	$C_{19}H_{30}O_2$	$C_{12}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	
Molecular weight	290.45	192.25
Solubility	Insoluble in water; soluble in alcohol	
Organoleptic characteristics	Mild, nondescript, floral, sweet odor and flavor	
Synthesis	From sodium *p*-cresol and lauryl chloride	
Natural occurrence	Not reported found in nature	Naturally occurring in passion fruit, raspberry, rum, whisky, coffee, tea, and soybean.
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Baked goods 2.0 ppm Gelatins and puddings 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3076	FEMA No. 3387

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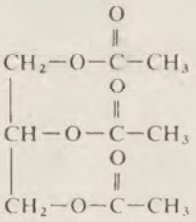
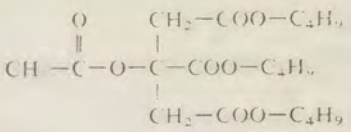
For References 1–5, see end of Part III.

	p-Tolyl phenylacetate	2-(*p*-Tolyl)-propionaldehyde
Other names	*p*-Cresyl phenylacetate (true name) *p*-Tolyl α-toluate	*p*-Methylhydratropic aldehyde 2-(*p*-Methylphenyl)-propionaldehyde
Empirical formula	$C_{15}H_{14}O_2$	$C_{10}H_{12}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	White crystals	Colorless to slightly yellow liquid
Assay	98% min[2]	95% min
Molecular weight	226.28	148.20
Melting point	74–75°C	
Boiling point	310°C	222–224°C
Flash point		89°C
Specific gravity		0.979–0.985 at 25°C; 0.9941 at 13°C
Refractive index		1.5140–1.5160 at 20°C
Congealing point	73.5 C[2] (73.7°C)	
Acid value	1.0 max[2]	5 max
Solubility	1 gm in 45 ml of 95% alcohol;[2] insoluble in water; poorly soluble in propylene glycol	Insoluble in water; readily soluble in alcohol and ether
Organoleptic characteristics	Faint but tenacious lily, hyacinth, narcissus odor; sweet, honey-like flavor	Intense, sweet, refreshing odor similar to peppermint
Synthesis	From *p*-cresol and phenylacetic acid by esterification, or by heating phenylacetyl chloride with freshly distilled *p*-cresol[6]	By reaction of α-terpinene and chromyl chloride in carbon disulfide and subsequent hydrolysis of the resulting cymene-chromyl chloride addition product; also by heating *p*-tolyl glycidic acid and water
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 1.6 ppm Ice cream, ices, etc. 0.87 ppm Candy 4.8 ppm Baked goods 5.4 ppm	Non-alcoholic beverages 0.13 ppm Alcoholic beverages 0.005 ppm Ice cream, ices, etc. 0.13 ppm Candy 0.13 ppm Baked goods 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 3077	FDA 121.1164; FEMA No. 3078

REFERENCES

For References 1–5, see end of Part III.

6. **Raiford and Hildebrand,** *Am. J. Pharm.*, 101, 471, 1929.

	Triacetin	Tributyl acetylcitrate
Other names	"Acetin" "Enzactin" Glyceryl triacetate "Vanay"	Acetyl tributylcitrate Citroflex A-4 (Pfizer)
Empirical formula	$C_9H_{14}O_6$	$C_{20}H_{34}O_8$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid; solidifies at low temperature	Colorless, slightly viscous liquid
Molecular weight	218.20	402.46
Melting point	3.2°C	
Boiling point	130.5°C at 7 mm Hg (260°C)	172–174°C (~300°C) at 1 mm Hg
Flash point	138°C	
Specific gravity	1.1596 at 20°C	1.14
Refractive index	1.4306 at 20°C	
Solubility	7% soluble in water; soluble in alcohol and most common organic solvents	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Very faint, fruity odor; mild, sweet taste, bitter above 0.05%	Very faint, sweet, herbaceous odor; at high levels (e.g., 1000 ppm emulsion in water) mild, fruity, non-descript flavor
Synthesis	By direct reaction of glycerol with acetic acid in the presence of Twitchell reagent;[6] or in benzene solution of glycerol and boiling acetic acid in the presence of a cationic resin (Zeo-Karb H) pretreated with diluted H_2SO_4[7]	From citric acid via the tributyl ester followed by acetylation
Natural occurrence	Reported found in several natural products	Non-alcoholic beverages 0.40 ppm (probably 20–40 ppm and higher)
Reported uses[3]	Non-alcoholic beverages 190 ppm Ice cream, ices, etc. 60–2,000 ppm Candy 560 ppm Baked goods 1,000 ppm Chewing gum 4,100 ppm	
Regulatory status	FDA GRAS (general); FEMA No. 2007	FDA 121.1164; FEMA No. 3080

REFERENCES

For References 1–5, see end of Part III.

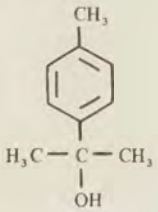
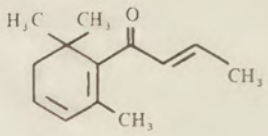
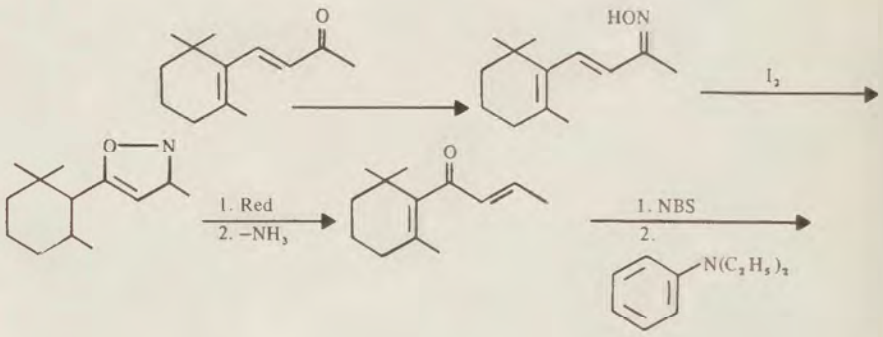
6. Zaganiaris and Varvoglis, *Ber. Dtsch. Chem. Ges.*, 69, 2279, 1936.
7. Sussman, *Ind. Eng. Chem.*, 38, 1229, 1946.

	2-Tridecenal	Trimethylamine
Other names	3-Decylacrolein Tridecen-2-al-1	
Empirical formula	$C_{13}H_{24}O$	C_3H_9N
Structure	$CH_3-(CH_2)_9-CH=CH-C(=O)H$	$N(CH_3)_3$
Physical chemical characteristics[2]		
Appearance	Colorless, oily liquid	
Molecular weight	196.33	59.1
Boiling point	106–108 C at 0.28 mm Hg; 115–118 C at 10 mm Hg; (232 C)	3.8°C
Melting point		124 C
Specific gravity	0.8476 at 19 C	0.6709 at 0°C
Refractive index	1.4582 at 19 C	
Solubility	Almost insoluble in water; soluble in alcohol	Miscible with water and alcohol; soluble in ether, benzene, and chloroform
Organoleptic characteristics	Very strong, citrus-peel waxy odor; bittersweet taste	Pungent fishy odor
Synthesis	From undecyl aldehyde by condensation with acetic aldehyde using sodamide in ether	From paraformaldehyde and ammonium chloride;[6] by the action of formaldehyde and formic acid on ammonia[7]
Natural occurrence	Identified in sunguli oil from Turkmenistan;[22] studied by Stoll[23]	In cheese,[8,9] caviar,[10] fish (also as the N-oxide),[11–15] beer,[16] whisky,[17] cocoa,[18–20] and coffee[21]
Reported uses[3]	Non-alcoholic beverages 0.10–0.30 ppm Ice cream, ices, etc. 1.6–6.0 ppm Candy 4.0–6.0 ppm Baked goods 4.0–6.0 ppm Chewing gum 0.10 ppm	Soups 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3082	FEMA No. 3241

REFERENCES

For References 1–5, see end of Part III

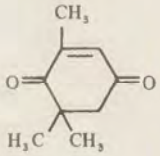
6. Adams et al., *Organic Syntheses*, Coll. Vol. 1, Gilman, H. and Blatt, A. H., Eds., Wiley & Sons, New York, 1941, 58.
7. Sommelet et al., *Bull. Soc. Chim.*, [4]35, 446, 1924.
8. Golovnja et al., *J. Anal. Chem. U.S.S.R.*, 23, 766, 1968.
9. Panouse et al., *Ind. Aliment. Agric.*, p. 133, 1972.
10. Golovnja et al., *J. Anal. Chem. U.S.S.R.*, 22, 612, 956, 1967.
11. Herrit et al., 142nd National Meeting of the American Chemical Society, 1962.
12. Jones, 4th Symposium on Food, Oregon State University, 1965, Oregon State University Press, Corvallis, 1967, 267.
13. Wong et al., *J. Assoc. Of. Agric. Chem.*, 50, 8, 1967.
14. Hard et al., *Naeringsmiddelindustrien*, 1/2, 46, 1970.
15. Weurman et al., *J. Food Sci.*, 26, 239, 1961.
16. Slaughter et al., *J. Inst. Brew.*, 77, 446, 1971.
17. Kahn, *J. Assoc. Of. Agric. Chem.*, 52, 1166, 1969.
18. Weurman et al., *J. Food Sci.*, 26, 239, 1961.
19. Marion et al., *Helv. Chim. Acta*, **50, 1509, 1967.**
20. Rohan, *Food Process. Mark.*, 38, 12, 1969.
21. Walter et al., *Z. Ernährungswiss.*, 9, 123, 1969.
22. Isskenderow, *Chem. Zentralbl.*, 1, 1892, 1938.
23. Stoll, *Helv. Chim. Acta*, 30:995, 1947.

	p,α,α-Trimethylbenzylalcohol	4-(2,6,6-Trimethyl-cyclohexa-1,3-dienyl)but-2-en-4-o
Other names	*p*-Cymen-8-ol Dimethyl-*p*-tolylcarbinol	(2,6,6-Trimethyl-1,3-cylcohexadien-1-yl)-2-buten-one *trans*-Damascenone β-Damascenone
Empirical formula	$C_{10}H_{14}O$	$C_{13}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Molecular weight	166.22	190.28
Synthesis		By treating the corresponding ethyl safranate with allyl lithium, followed by catalytic isomerization of the reaction product;[17] also from the oxirane derivative of β-damascone by an acid-catalyzed reaction[18] also[22]
		 Ger. Pat. 2,315,639 (dos)
Natural occurrence	In citrus fruits,[6] cranberry and bilberry,[7] currants,[8-12] mint,[13,14] and pepper[15,16]	Reported found in raspberry oil,[19] in Burley tobacco,[20] and in apple[21]
Reported uses[3]	Non-alcoholic beverages 0.20 ppm Candy 2.8 ppm Gelatins and puddings 1.0 ppm	Non-alcoholic beverages 0.2 ppm Ice cream, ices, etc. 0.2 ppm Candy 0.2 ppm Baked goods 0.2 ppm Gelatins and puddings 0.2 ppm Condiments, pickles 0.2 ppm Jellies, preserves, spreads 0.2 ppm
Regulatory status	FEMA No. 3242	FEMA No. 3420

REFERENCES

For References 1–5, see end of Part III.

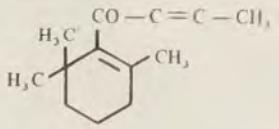
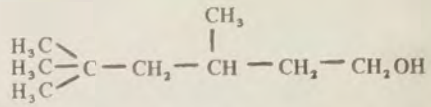
6. Moshonas et al., *J. Agric. Food Chem.*, 20, 751, 1029, 1972.
7. Anjou et al., *Acta Chem. Scand.*, 21, 945, 1967.
8. Andersson et al., *Acta Chem. Scand.*, 20, 529, 1966.
9. Nursten et al., *Chem. Ind.* (London), p. 426, 1967.
10. Giesschner et al., *Riechst. Aromen*, 18, 3, 37, 94, 134, 179, 220, 322, 1968.
11. Nursten et al., *J. Sci. Food Agric.*, 20, 91, 613, 1969.
12. Sydow et al., *Lebensm. Wiss. Technol.*, 4, 54, 1971.
13. Schnelle et al., *Planta Med.*, 16, 48, 1968.
14. Canova, 5th International Congress on Essential Oils, Sao Paulo, 1971.
15. Russell et al., *J. Agric. Food Chem.*, 17, 1107, 1969.
16. Richard et al., *J. Food Sci.*, 36, 584, 1971.
17. Buchi et al., *Helv. Chim. Acta*, 54, 1767, 1971.
18. Schulte-Elte et al., *Helv. Chim. Acta*, 54, 1899, 1971.
19. Winter et al., *Helv. Chim. Acta*, 54, 1891, 1971.
20. Demole et al., *Helv. Chim. Acta*, 54, 681, 1971; 55, 1866, 1972.
21. Narsten and Woolfe, *J. Sci. Food Agric.*, 23, 803, 1972.
22. German Patent 2,315,639.

	2,6,6-Trimethylcyclohexa-1,3-dienyl methanal		2,6,6-Trimethylcyclohex-2-ene-1,4-dione	
Other names	2,6,6-Trimethyl-1-carboxy-1,3-cyclohexadiene		3,5,5-Trimethyl-2-cyclohexene-1,4-dione	
Empirical formula	$C_9H_{14}O$		$C_9H_{12}O_2$	
Structure				
Physical/chemical characteristics[5]				
Molecular weight	138.20		152.19	
Natural occurrence			Reported found among the volatile components in saffron[6] and in cigarette smoke[7]	
Reported uses[3]	Candy	5.0 ppm	Non-alcoholic beverages	1.0 ppm
	Baked goods	10.0 ppm	Candy	5.0 ppm
	Condiments, pickles	5.0 ppm		
	Preserves and spreads	10.0 ppm		
Regulatory status	FEMA No. 3389		FEMA No. 3421	

REFERENCES

For References 1–5, see end of Part III.

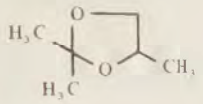
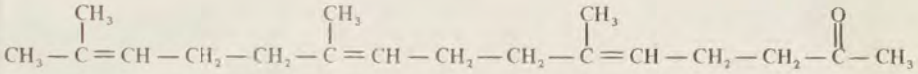
6. Zarghami et al., *Photochemistry*, p. 2755, 1971.
7. Neurath et al., *Beitr. Tabakforsch.*, (6)12, 1971.

	4-[(2,6,6)-Trimethyl-cyclohex-1-enyl]-but-2-en-4-one		3,5,5-Trimethyl-1-hexanol	
Other names	1-[(2,6,6)-Trimethyl-cyclohex-1-enyl]-but-2-en-1-one β-Damascone Dorinone® (Firmenich)		Isononyl alcohol *tert*-Butyl isopentanol Trimethyl hexyl alcohol	
Empirical formula	$C_{13}H_{20}O$		$C_9H_{20}O$	
Structure				
Physical/chemical characteristics				
Appearance			Colorless oily liquid	
Molecular weight	192.30		144.26	
Boiling point	*trans*-, 55°C at 0.001 mm Hg[6] *cis*-, 52°C at 0.001 mm Hg[6]		142°C at 150 mm Hg 62°C at 14 mm Hg	
Specific gravity	*trans*-, 0.934 at 20°C[6] *cis*-, 0.930 at 20°C[6]		0.8350 at 20°C	
Refractive index	*trans*-, 1.4980 at 20°C[6] *cis*-, 1.4957 at 20°C[6]		1.4352 at 20°C 1.4300 at 25°C	
Solubility			Almost insoluble in water; soluble in alcohol, acetone, and ether	
Organoleptic characteristics			Strong, oily-herbaceous odor; becomes sweet on dilution	
Synthesis	Various methods;[6] recently from ionone izoxazoles;[7] also from 7,8-dehydro-β-ionole;[9] see various patents.[8]		By oxo-reaction of diisobutylene to the corresponding aldehyde, from which the alcohol is prepared by hydrogenation[12]	
Natural occurrence	In Burley tobacco oil;[10] in volatile fractions from leaves of *Carphephorus corymbosus* and *C. paniculatus*[11]			
Reported uses[3]	Non-alcoholic beverages	10.0 ppm	Baked goods	30.0 ppm
	Ice cream, ices, etc.	10.0 ppm	Condiments, pickles	30.0 ppm
	Candy	10.0 ppm		
	Baked goods	10.0 ppm		
	Gelatins and puddings	10.0 ppm		
	Chewing gum	10.0 ppm		
Regulatory status	FEMA No. 3243		FEMA No. 3324	

REFERENCES

For References 1–5, see end of Part III.

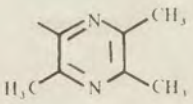
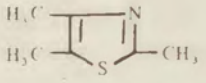
6. Demole et al., *Helv. Chim. Acta*, 53, 541, 1970.
7. Schulte-Elte et al., *Helv. Chim. Acta*, 56, 310, 1973.
8. German Patent 2,242,751; *Chem. Abstr.*, 79, 5053, 1972. German Patent 2,065,324; *Chem. Abstr.*, 79, 18207p, 1972. German Patent, 2,065,322; *Chem. Abstr.*, 18208g, 1972. German Patent 2,065,323; *Chem. Abstr.*, 79, 31582f, 1972. Swiss Patent 53,752; *Chem. Abstr.*, 79, 104808s, 1972. German Patent 2,305,140; *Chem. Abstr.*, 79, 115743t, 1972.
9. Ohloff, *Helv. Chim. Acta*, 56, 1503, 1973.
10. Demole et al., *Helv. Chim. Acta*, 54, 681, 1971.
11. Karlsson et al., *Acta Chem. Scand.*, 26, 3839, 1972.
12. Keulmans, Kwantes and Van Bavel, *Recl. Trav. Chim.*, 67, 298, 1948.

	2,2,4,-Trimethyl-1,3-oxacyclopentane		2,6,10-Trimethyl-2,6,10-pentadecatrien-14-one	
Other names	2,2,4-Trimethyl-1,3-dioxolane Propylene glycol acetone ketal		6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one Farnesyl acetone	
Empirical formula	$C_6H_{12}O_2$		$C_{18}H_{30}O$	
Structure				
Physical/chemical characteristics				
Molecular weight	116.16		262.44	
Boiling point	98–99°C		147–148°C at 0.5 mm Hg	
Specific gravity	0.909 at 18.5°C		0.8900 at 20°C	
Refractive index	1.4019 at 18.5°C		1.4812 at 20°C	
Synthesis	From acetone and propylene glycol[6]		By treating farnesyl bromide with sodium acetate, followed by treating with methanolic KOH[7,8]	
Natural occurrence			In tomato[9,10]	
Reported uses[3]	Non-alcoholic beverages	4.0 ppm	Non-alcoholic beverages	2.0 ppm
	Alcoholic beverages	1.0 ppm	Ice cream, ices, etc.	2.0 ppm
	Ice cream, ices, etc.	4.0 ppm	Candy	3.0 ppm
	Candy	6.0 ppm	Gelatins and puddings	2.0 ppm
	Gelatins and puddings	4.0 ppm	Condiments	1.0 ppm
	Condiments	4.0 ppm	Jellies, preserves, spreads	1.0 ppm
	Jellies, preserves, spreads	4.0 ppm		
Regulatory status	FEMA No. 3441		FEMA No. 3442	

REFERENCES

For References 1–5, see end of Part III.

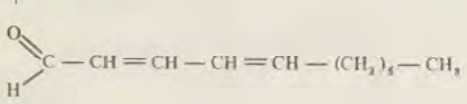
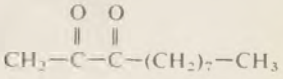
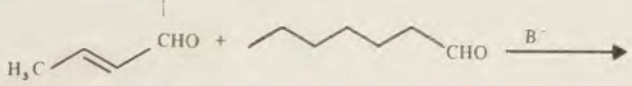
6. **Boseken et al.**, *Recl. Trav. Chim. Pays-Bas*, 42, 1105, 1923.
7. **Ruzička et al.**, *Helv. Chim. Acta*, 22, 394, 1949.
8. **Karrer et al.**, *Helv. Chim. Acta*, 27, 1299, 1944.
9. **Buttery et al.**, *Chem. Ind.* (London), p. 238, 1969; *J. Agric. Food Chem.*, 19, 524, 1971.
10. **Johnson et al.**, *Chem. Ind.* (London), p. 1212, 1971.

	2,3,5-Trimethylpyrazine	2,4,5-Trimethyl thiazole
Other names	Trimethylpyrazine	
Empirical formula	$C_7H_{10}N_2$	C_6H_9SN
Structure		
Physical/chemical characteristics		
Assay	C: 68.82%; H: 8.25%; N: 22.93%	
Molecular weight	122.17	127.21
Boiling point		167°C 65–67°C at 20 mm Hg
Mass spectra[7]	39 (27), 42 (100), 53 (8), 54 (12), 66 (1), 67 (2), 80 (5), 81 (22), 108 (2), 122 (81), 123 (8)	
IR spectra[7]	S (3.4, 6.8, 7.2, 7.3, 8.6, 10.6) M (7.8, 7.9, 9.8, 10.0, 11.2) W (5.6, 6.5, 9.2, 10.2, 12.0)	
UV spectra[7]	(277.5 nm)	
Organoleptic characteristics	Baked-potato or roasted-peanut aroma; odor threshold: 9,000 ppb in water[8]	
Synthesis	From 2,5-dimethylpyrazine by ring alkylation with MeLi;[9] by condensing propylenediamine with 2,3-butanedione[10]	By decarboxylation of 2,4-dimethylthiazole-5-acetic acid;[11] by reacting acetamide and phosphorous pentasulfide with methyl-α-bromoethyl ketone[12]
Natural occurrences	Reported to be present in the following foods: bakery products, roasted barley, cocoa products, coffee, dairy products, meat, peanuts, filberts, pecans, popcorn, potato products, rum and whisky, soy products[6]	
Reported uses[3]	Non-alcoholic beverages 5.0 to 10.0 ppm Candy 5.0 to 10.0 ppm Baked goods 5.0 to 10.0 ppm Condiments 2.0 ppm Meat, meat sauces, soups 2.0 ppm Milk, dairy products 1.0 ppm Cereals 2.0 ppm	Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Condiments, pickles 6.0 ppm Meat, meat sauces, soups 6.0 ppm
Regulatory status	FEMA No. 3244	FEMA No. 3325

REFERENCES

For References 1–5, see end of Part III.

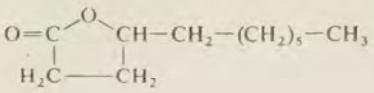
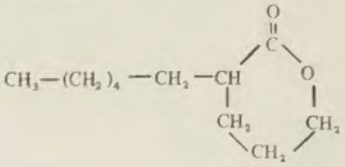
6. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
7. Bondarovich et al., *J. Agric. Food Chem.*, 15, 1093, 1967.
8. Koehler et al., *J. Food Sci.*, 36, 816, 1971.
9. Rizzi, *J. Org. Chem.*, 33(4), 1333, 1968.
10. Ishiguro and Matsumura, *Yakugaku Zasshi*, 78, 229, 1958.
11. Gregory and Wiggins, *J. Chem. Soc.*, p. 1400, 1947.
12. Kurkjy and Brown, *J. Am. Chem. Soc.*, 74, 5778, 1952.

	2,4-Undecadienal	2,3-Undecadione
Other names		Acetyl nonanoyl Acetyl nonyryl Acetyl pelargonyl
Empirical formula	$C_{11}H_{18}O$	$C_{11}H_{20}O_2$
Structure		
Physical/chemical characteristics		
Appearance	Colorless mobile oil	Oily, yellow liquid
Molecular weight	166.27	184.28
Boiling point		109–111 C at 10 mm Hg
Solubility	Insoluble in water, soluble in alcohol and oils[6]	Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Powerful green odor	Strong, sweet-cream, warm odor with a coconut-oil note; sweet-cream and coconut-milk taste
Synthesis		By reacting 3-bromo-2-undecanone with sodium azide in diluted methanol and then boiling the resulting solution with concentrated HCl;[8] also from methyl nonyl ketone via the monoxime of the title material
Natural occcurrence	Reported found in heated beef and in roasted peanuts[7]	Not reported found in nature
Reported uses[3]	Baked goods 1.0 ppm Meat, meat sauces, soups 1.0 ppm Cereals 1.0 ppm	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm
Regulatory status	FEMA No. 3422	FDA 121.1164; FEMA No. 3090

REFERENCES

For References 1–5, see end of Part III.

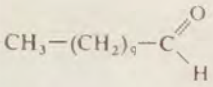
6. **Arctander,** *Perfume and Flavor Chemicals,* Montclair, N.J., 1969, No. 3022.
7. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Centraal Instituut vor Voedingsonderzoek, Zeist, Netherlands.
8. **I. G. Garbenindustrie,** German Patent 573,722, 1931.

	γ-Undecalactone	Δ-Undecalactone
Other names	"Aldehyde C-14" γ-Heptyl butyrolactone 4-Hydroxyundecanoic acid, γ-lactone Peach aldehyde Undecanolide-1,4	5-Hydroxyundecanoic acid, lactone α-*n*-Hexyl-δ-valerolactone Undecanolide-1,5
Empirical formula	$C_{11}H_{20}O_2$	$C_{11}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to very pale yellow, viscous liquid	Colorless, very viscous liquid
Assay	98% min[2]	
Molecular weight	184.28	184.28
Boiling point	297°C	152–155°C at 10.5 mm Hg
Flash point	137°C	
Specific gravity	0.942–0.945 at 25°/25°C[2]	0.96
Refractive index	1.4500–1.4540 at 20°C[2]	
Acid value	Not more than 5[2]	
Solubility	1:5 and more in 60% alcohol;[2] 1:2 in 70% alcohol; almost insoluble in water; soluble in most common organic solvents	Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Strong, fruity odor suggestive of peach (particularly on dilution); pungent and sweet flavor also similar to peach	Creamy, peachy, somewhat fatty aroma reminiscent of coconut
Synthesis	By the action of sulfuric acid on undecylenic acid;[2] also prepared starting from castor oil;[6] from octanol-1 plus methylacrylate with di-*tert*-butylperoxide; from heptylethylene oxide and sodiomalonic ester	By intramolecular Cannizzaro type rearrangement of 2-hexylglutaraldehyde[8]
Natural occurrence	Reported found in hydrolyzed soy protein,[7] butter, peach, apricot, and passion fruit	Reportedly occurring in coconut flavor[9]
Reported uses[3]	Non-alcoholic beverages 4.4 ppm Ice cream, ices, etc. 3.0 ppm Candy 11 ppm Baked goods 7.1 ppm Gelatins and puddings 90 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0 ppm Baked goods 25.0 ppm Meat, meat sauces, soups 1.0 ppm Milk, dairy products 10.0 ppm Cereals 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3091	FEMA No. 3294

REFERENCES

For References 1–5, see end of Part III.

6. Muller, *Riechstoffindustrie*, p. 39, 1927.
7. Manley et al., *J. Food Sci.*, 35(3), 286, 1970.
8. Meerwein, *Berichte*, 53, 1829, 1920.
9. Lin and Wilkens, *J. Food Sci.*, 35(5), 538, 1970.

	Undecanal
Other names	Aldehyde C_{11} (saturated) Hendecanal ω-Oxo-undecane *n*-Undecylic aldehyde
Empirical formula	$C_{11}H_{22}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless to slightly yellow liquid
Assay	92% min[2] (97%)
Molecular weight	170.30
Melting point	−4°C
Boiling point	118–120°C at 20 mm Hg
Flash point	96°C
Specific gravity	0.825–0.832 at 25°/25°C;[2] 0.8251 at 23°C; 0.8320–0.8350 at 15°C
Refractive index	1.430–1.435 at 20°C;[2] 1.4324 at 23°C; 1.4315–1.4330
Acid value	Not more than 10[2] (3.7)
Solubility	Insoluble in water; soluble in most common organic solvents; 1:1 in 80% alcohol; 1:5 in 70% alcohol
Organoleptic characteristics	Sweetish, fatty odor with an orange and rose undertone; characteristic flavor; tends to polymerize unless tightly sealed
Synthesis	Usually prepared by oxidation of the corresponding alcohol or reduction of the corresponding acid
Natural occurrence	Until a few years ago believed not to be found in nature. It has subsequently been identified in the essential oils of mandarin and lemon.[6]
Reported uses[3]	Non-alcoholic beverages 0.95 ppm Ice cream, ices, etc. 3.1 ppm Candy 2.0 ppm Baked goods 2.4 ppm Chewing gum 56 ppm
Regulatory status	FDA 121.1164; FEMA No. 3092

REFERENCES

For References 1–5, see end of Part III.

6. Riganenis and Calvarano, *Essenze Deriv. Agrum.*, 26, 167, 1956.

	Undecanoic acid	2-Undecanol
Other names	*n*-Undecylic acid Decane-α-carboxylic acid Hendecanoic acid	Methyl nonyl carbinol 2-Hendecanol *sec*-Undecyl alcohol
Empirical formula	$C_{11}H_{22}O_2$	$C_{11}H_{24}O$
Structure	$CH_3-(CH_2)_9-COOH$	$CH_3-(CH_2)_7-CH_2-\underset{\displaystyle OH}{\underset{\vert}{CH}}-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless crystals	Colorless liquid
Assay		
Molecular weight	186.30	172.31
Melting point	28–29°C 284°C	*dl*-, 0°C *d*-, 12°C
Boiling point	164.5°C at 15 mm Hg	*dl*-, 115°C at 10 mm Hg *d*-, 128°C at 20 mm Hg
Congealing point		*l*-, 231–233°C
Specific gravity	0.9948 at 20°C	*dl*-, 0.8263 at 19°C *d*-, 0.8270 at 20°C
Refractive index	1.4355 at 30°C 1.4294 at 45°C 1.4203 at 70°C	*d*-, 1.4369 at 20°C
Optical rotation		+10.29° at 20°C (c = 5.15 in benzene) +8.11° at 20°C (c = 5.11 in alcohol) −5.40° (from *Litsea odorifera;* l = 10 cm) −1.18° (from rue; l = 2.5 cm)
Solubility	Insoluble in water; very soluble in alcohol, chloroform, and acetone; soluble in benzene in all proportions	Insoluble in water; soluble in alcohol and ether
Organoleptic characteristics	Faint fatty, aldehydic odor	Fatty odor with a fruity note; a fruity taste is also detectable at low concentration
Synthesis	By reduction of undecylenic acid obtained from castor oil[6]	By reduction of methyl nonyl ketone with sodium metal in alcohol,[10] the *d*-form is isolated from the optically inactive material via the corresponding phthalate and its salt with strychnine and brucine[11]
Natural occurrence	Occurs naturally in butter[7] and in the oil of *Artemisia frigida* Willd; also reported found in the oils of *Chamaecyparis pisifera* Engl., wild thyme,[8] *Thymus marschollianus,* and coconut[9]	The *l*-form is reportedly found in rue oil[12] and in the essential oil of *Litsea odorifera;*[13] the *d*-form occurs in coconut[14]
Reported uses[3]	Baked goods 2.0 ppm	Baked goods 20.0 ppm
Regulatory status	FEMA No. 3245	FEMA No. 3246

REFERENCES

For References 1–5, see end of Part III.

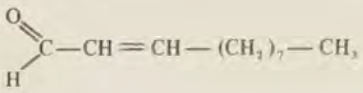
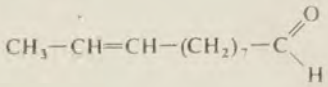
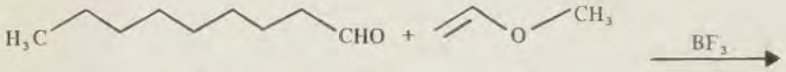
6. Rodd, *Chemistry of Carbon Compounds,* 2nd ed., Vol. 1, American Elsevier, New York, 1965, 137.
7. Martinenghi, *Olii, Grassi e Derivati,* 3rd ed., Hoepli.
8. Spiridonowa, *Chem. Zentralbl.,* 1, 1812, 1937.
9. Nobori, *Chem. Abstr.,* 42, 6140, 1948.
10. Mannich, *Ber. Dtsch. Chem. Ges.,* 35, 2144, 1902.
11. Pickard and Kempon, *J. Chem. Soc.* (London), 55, 70, 99, 1911; 103, 1957, 1913; 105, 850, 1914.
12. Power and Lees, *J. Chem. Soc.* (London), 81, 1585, 1902.
13. van Romburg, *Chem. Zentralbl.,* 2, 1863, 1911.
14. Haller and Lassieur, *Chem. Zentralbl.,* 2, 1913, 1910.

	2-Undecanone
Other names	Methyl nonyl ketone
Empirical formula	$C_{11}H_{22}O$
Structure	$CH_3-\overset{\overset{O}{\|}}{C}-(CH_2)_9-CH_3$
Physical/chemical characteristics[5]	
Appearance	Colorless to slightly yellowish liquid
Assay	95% min
Molecular weight	170.30
Melting point	12–13°C (13–15°C)
Boiling point	228–230°C; 105–107°C at 10 mm Hg
Specific gravity	0.8262 at 20°C; 0.822–0.826 at 25°C
Refractive index	1.4175 at 22°C; 1.4280–1.4330 at 20°C
Solubility	Insoluble in water; soluble in most common organic solvents; 1:3 in 70% alcohol
Organoleptic characteristics	Characteristic rue odor; sweet flavor reminiscent of peach (on dilution)
Synthesis	Can be isolated from natural oils by fractional distillation;[6] also by dry distillation of calcium acetate and calcium caprylate, or by boiling octylacetoacetic acid ethyl ester with an alcoholic KOH solution[7]
Natural occurrence	Originally reported found in the essential oil of *Ruta graveolens*;[8] subsequently was identified in the essential oils of *Citrus limetta* Risso., *Fagara xanthoxyloides* Lamm., and *Litsea odorifera* Val. (leaves). A method for the determination of methyl nonyl ketone in various rue species (*Ruta montana, Ruta bracteosa*) was devised.[9] It is also present in the essential oils of *Jaborandi* (leaves), *Hottuynia cordata, Phellodendron anaurense, Schizandar nigra* Maxim., and in coconut and palm oils. Also identified as the main constituent of the essential oil of the physiological variety of *Boronia ledifolia* Gai.[10] A 92% content level was reported in the essential oil of *Ruta chalepensis*.[11]
Reported uses[3]	Non-alcoholic beverages 2.8 ppm Ice cream, ices, etc. 0.54 ppm Candy 2.6 ppm Baked goods 3.1 ppm Gelatins and puddings 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3093

REFERENCES

For References 1–5, see end of Part III.

6. **Gorup et al.**, *Annalen*, 157, 275, 1871.
7. **Guthzeit**, *Annalen*, 204, 275, 1880.
8. **Williams**, *Annalen*, 107, 374, 1858.
9. **Roure-Bertrand fils**, *Chem. Zentralbl.*, 2, 139, 1911.
10. **Penfold and Morrison**, *Chem. Abstr.*, 43, 3148, 1949.
11. **Costa and do Vale**, *Chem. Abstr.*, 48, 11732, 1954.

	2-Undecenal	9-Undecenal
Other names	Undecen-2-al 3-Octylacrolein The commercial product is a mixture of several isomers of undecylenic aldehyde	Aldehyde C-11 undecylenic Hendecen-9-al 9-Undecen-1-al (correct name) Undecenoic aldehyde Undecylenic aldehyde
Empirical formula	$C_{11}H_{20}O$	$C_{11}H_{20}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless or very pale straw-colored liquid[5]	Colorless, pale yellow, oily liquid
Molecular weight	168.27	168.28
Boiling point	94°C at 2 mm Hg 229°C	
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics	Powerful fresh aldehydic odor	Orange peel-like, sweet odor; sweet, citrus flavor
Synthesis	By oxidation of 2-undecanol;[6] also	
		
Natural occurrence	Reported found among the volatile components in fish products;[8] also formed in the oxidative decomposition of heated lard;[9] its presence in nature has been reported in cranberry and bilberry, milk, cooked chicken, heated beef and pork, roasted filberts, roasted peanuts, pecans, and potato chips;[10] exhibits fungistatic activity[7]	
Reported uses[3]	Baked goods 0.05 ppm Condiments, pickles 0.02 ppm Meat, meat sauces, soups 0.05 ppm Milk, dairy products 0.05 ppm	Non-alcoholic beverages 4.8 ppm Ice cream, ices, etc. 4.2 ppm Candy 4.5 ppm Baked goods 4.6 ppm
Regulatory status	FEMA No. 3423	FDA 121.1164; FEMA No. 3094

REFERENCES

For References 1–5, see end of Part III.

6. Swift et al., *J. Am. Chem. Soc.*, 71, 1512, 1949.
7. Wyss et al., *Arch. Biochem.*, 7, 422, 1945.
8. Golovnya et al., *J. Chromatogr.*, 61, 65, 1971.
9. Watanabe et al., *Nippon Chikusan Gakkai-Ho*, 42, 393, 1971; *Chem. Abstr.*, 76, 57867m, 1972.
10. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Centraal Instituut voor Voedingsonderzoek, Zeist, Netherlands.
11. Arctander, *Perfume and Flavor Chemicals*, Montclair, N.J., 1969, No. 3033.

	10-Undecenal	10-Undecenoic acid
Other names	Aldehyde C-11 undecylenic Hendecenal Undecylenic aldehyde	10-Hendecenoic acid Undecylenic acid
Empirical formula	$C_{11}H_{20}O$	$C_{11}H_{20}O_2$
Structure	$CH_2{=}CH{-}(CH_2)_8{-}C(=O)H$	$CH_2{=}CH{-}(CH_2)_8{-}COOH$
Physical/chemical characteristics[2]		
Appearance	Colorless to light-yellow liquid	Colorless leaflets
Assay	90% min[2] (97%)	
Molecular weight	168.28	184.28
Melting point		24.5°C
Boiling point	103°C at 3 mm Hg; 101–103°C at 10 mm Hg	275°C 131°C at 1 mm Hg 165°C at 15 mm Hg
Flash point	92°C (100°C)	
Specific gravity	0.840–0.850 at 25/25°C;[2] 0.8496 at 21°C; 0.8470–0.8500 at 25°C	0.9072 at 24°C 0.910 at 15.5°C
Refractive index	1.4410–1.4470 at 20°C;[2] 1.4464 at 21°C; 1.4425–1.4440	1.4486 at 24°C
Acid value	6 max[2] (2.7)	
Iodine value		136–138
Solubility	1:1–2 in 80% alcohol;[2] insoluble in water; soluble in most common organic solvents	Insoluble in water; soluble in alcohol and ether
Organoleptic characteristics	Characteristic fatty, rose odor on dilution; unpleasant sweet, fatty taste; tends to polymerize	Characteristic pungent odor
Synthesis	By oxidation of the corresponding alcohol or reduction of the corresponding acid. By passing vapors of formic acid and undecylenic acid over TiO_2 at 250°C under pressure;[6] by passing vapors of undecylenic acid and methanol over a manganese dioxide based catalyst;[7] or by reduction of ethyl undecylenate with lithium hydride and sodium in tetrahydrofuran solution at very low temperature (−50°C)[8]	From malonic acid;[9] by pyrolysis of ricinoleic acid or castor oil[10,11]
Natural occurrence	Not reported found in nature	Reported found as a metabolite in *Rhodotorula glutinis* var. *lusitanica*,[11] naturally occurring in the essential oils of *Juniperus chinensis*[12] and *Thujopsis dolabrata*[13,14]
Reported uses[3]	Non-alcoholic beverages 0.05–1.0 ppm Ice cream, ices, etc. 0.20 ppm Candy 0.20 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50 ppm Baked goods 0.50 ppm
Regulatory status	FDA 121.1164; FEMA No. 3095	FEMA No. 3247

REFERENCES

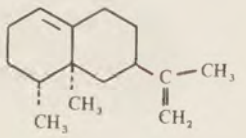
For References 1–5, see end of Part III.

6. Davies and Hodgson, *J. Chem. Soc.*, p. 86, 1943.
7. Kagon, Poljakova and Belov, *Oel Fettind.*, 19, 25, 1954.
8. Zakharkin et al., *Chem. Abstr.*, 61, 5505d, 1964.
9. Linstead et al., *J. Chem. Soc.*, p. 1971, 1937.
10. Vernon and Ross, *J. Am. Chem. Soc.*, 58, 2431, 1936.
11. Seher, *Fette and Seifen*, 58, 1077, 1956.
12. Prista, *Chem. Abstr.*, 49, 11075, 1952.
13. Uchida, *Chem. Zentralbl.*, 2, 2198, 1928.
14. Uchida, *Chem. Zentralbl.*, 1, 948, 1929.

	Undecen-1-ol	10-Undecen-1-yl acetate
Other names	Alcohol C-11 undecylenic 10-Undecen-1-ol Undecylenic alcohol	Acetate C-11 10-Hendecenyl acetate Undecenyl acetate Undecelynic acetate
Empirical formula	$C_{11}H_{22}O$	$C_{13}H_{24}O_2$
Structure	$CH_2=CH-(CH_2)_8-CH_2OH$	$CH_3-\overset{\overset{O}{\|}}{C}-O-(CH_2)_9-CH=CH_2$
Physical/chemical characteristics[5]		
Appearance	Clear, very mobile liquid	Colorless liquid
Assay	97–98.5% min	95% min
Molecular weight	170.30	212.33
Melting point	−3°C min	
Boiling point		272°C; 140–142°C at 15 mm Hg
Flash point	>82.5°C	
Specific gravity	0.8420–0.8460 at 25°C	0.876–0.880 at 25°C; 0.8808 at 20°C
Refractive index	1.4490–1.4540 at 20°C	1.4380–1.4420 (1.4389) at 20°C
Solubility	1:2 in 70% alcohol; insoluble in water; soluble in most common organic solvents	1:2 in 80% alcohol; soluble in most common organic solvents
Organoleptic characteristics	Fatty odor reminiscent of lemon; fatty, burning taste	Light, rose-like odor; fatty, somewhat agreeable flavor
Synthesis	Prepared from coconut fatty acids as starting material	By acetylation of the corresponding alcohol
Natural occurrence		Not reported found in nature
Reported uses[3]	Reported found in distilled essential oil from leaves of *Litsea odorifera* Valeton.	Non-alcoholic beverages 3.7 ppm Ice cream, ices, etc. 15 ppm Candy 12 ppm Baked goods 12 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 3096

REFERENCES

For References 1–5, see end of Part III.

	Undecyl alcohol	Valencene
Other names	Alcohol C-11 Hendecanol 1-Undecanol	1,2,3,5,6,7,8,8a-Octahydro-1,8a-dimethyl-7-(1-methylethenyl)- naphthalene
Empirical formula	$C_{11}H_{24}O$	$C_{15}H_{24}$
Structure	$CH_3-(CH_2)_9-CH_2OH$	
Physical/chemical characteristics		
Appearance	Colorless liquid at room temperature	
Assay	97–98.5% min	
Molecular weight	172.31	204.36
Melting point	15–19°C	
Boiling point		123°C at 11 mm Hg
Flash point	>82°C	
Specific gravity	0.828–0.834 at 25°C	
Refractive index	1.4370–1.4430 at 20°C	1.5075 at 20°C
Solubility	1:4 in 60% alcohol; insoluble in water; soluble in most common organic solvents	
Organoleptic characteristics	Floral, citrus-like odor; fatty flavor	
Synthesis	By reduction of the corresponding aldehyde	By a Wolf-Kishner reduction of nootkatone[6,7]
Natural occurrence	Reported found in nature (citrus fruits)	In citrus fruits[8–10] and in cocoa[11,12]
Reported uses[3]	Non-alcoholic beverages 2.9 ppm Ice cream, ices, etc. 15 ppm Candy 12 ppm Baked goods 12 ppm	Non-alcoholic beverages 0.9 ppm Alcoholic beverages 0.9 ppm Ice cream, ices, etc. 0.9 ppm Candy 0.9 ppm Baked goods 0.9 ppm Gelatins and puddings 0.9 ppm Chewing gum 0.9 ppm Milk, dairy products 0.9 ppm Cereals 0.9 ppm
Regulatory status	FDA 121.1164; FEMA No. 3097	FEMA No. 3443

REFERENCES

For References 1–5, see end of Part III.

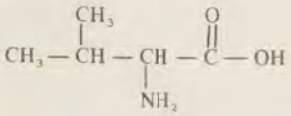
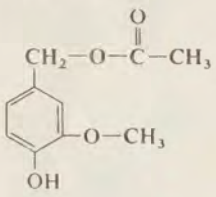
6. **Hunter et al.**, *J. Food Sci.*, 30, 1, 1965.
7. **Mac Leod**, *Tetrahedron Lett.*, p. 4779, 1965.
8. **Hunter et al.**, *J. Food Sci.*, 30, 383, 1965.
9. **Attaway**, *Phytochemistry*, 5, 1273, 1966.
10. **Maroni**, *Riv. Ital. EPPOS*, 55, 168, 1973.
11. **Van de Wal**, *Recl. Trav. Chim. Pays-Bas*, 87, 238, 1968; *J. Agric. Food Chem.*, 19, 276, 1971.
12. **Rohan**, *Food Process Mark.*, 38, 12, 1969.

	n-Valeraldehyde	Valeric acid
Other names	Amylaldehyde *n*-Pentanal Valeral *n*-Valeric aldehyde	Pentanoic acid Propylacetic acid
Empirical formula	$C_5H_{10}O$	$C_5H_{10}O_2$
Structure	$CH_3-CH_2-CH_2-CH_2-C(=O)-H$	$CH_3-(CH_2)_3-C(=O)-OH$
Physical/chemical characteristics		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	86.13	102.13
Melting point	−91.5°C	34°C
Boiling point	103.4°C	184–186°C (185.5–186.5 C)
Specific gravity	0.819 at 15°C	0.9459 at 20°C
Refractive index	1.3882 (1.3944) at 20°C	1.4100 at 20°C
Solubility	Very slightly soluble in water; soluble in alcohol, propylene glycol, and oils	Slightly soluble in water; soluble in alcohol and ether
Organoleptic characteristics	Powerful, acrid, pungent odor; at low levels taste is warm, slightly fruity, and nut-like	Unpleasant odor and flavor, similar to butyric acid
Synthesis	By distillation of calcium valerate and calcium formate;[6] by reduction of *n*-valeric acid	By oxidation of *n*-amyl alcohol or, together with other isomers, by distillation of valerian roots. Also by reacting butyl bromide and sodium cyanide with subsequent saponification of the formed butyl nitrile
Natural occurrence	Reported found among the constituents of several essential oils: Brazilian sassafras,[7] Bulgarian rose,[8] Bulgarian clary sage,[9] and others; also in the distillates from leaves of various *Eucalyptus* species: *E. cinerea*,[10] *E. globulus*,[11] *E. dives*,[12] *E. maideni*,[13] and *E. hemilampra*[14]	The acid is not too common in nature. Reported (as the corresponding ester) found in the essential oil of *Boronia anemonifolia*, in pineapple fruits, and in other plants; also identified as acid or the corresponding ester in the essential oil of lemon petitgrain[15]
Reported uses[3]	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 5.0 ppm Candy 4.2 ppm Baked goods 5.4 ppm	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 1.8 ppm Candy 2.5 ppm Baked goods 8.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3098	FDA 121.1164; FEMA No. 3101

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For References 1–5, see end of Part III.

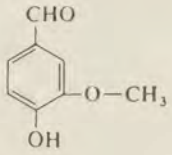
6. **Lieben and Rossi,** *Justus Liebigs Ann. Chem.*, 159, 70, 1871.
7. **Paul and Jachan,** *Perfum. Essent. Oil Rec.*, 42, 416, 1951.
8. **Panayotov and Ivanov,** *Perfum. Essent. Oil Rec.*, 49, 231, 1958.
9. **Panayotov,** *Perfum. Essent. Oil Rec.*, 49, 233, 1958.
10. **Baker and Smith,** *Res. Eucalyptus Essent. Oils* (Sidney), p. 119, 1920.
11. *Schimmel Ber.*, 4, 47, 1904.
12. *Schimmel Ber.*, p. 46, 1928; p. 41, 1930.
13. **Rutowski et al.,** *Riechstoffindustrie*, 1, 159, 1926.
14. **Baker and Smith,** *Res. Eucalyptus Essent. Oils* (Sidney), p. 57, 1910.
15. **Peyron,** *Riv. Ital. EPPOS*, 8, 413, 1965.

	d,l-Valine	Vanillin acetate
Other names	α-Aminoisovaleric acid 2-Amino-3-methylbutanoic acid 2-Amino-3-methylbutyric acid 2-Isopropyl glycine	Acetyl vanillin 3-Methoxy-4-acetoxy benzaldehyde Vanillyl acetate
Empirical formula	$C_5H_{11}NO_2$	$C_{10}H_{12}O_4$
Structure		
Physical/chemical characteristics		
Appearance		Crystalline solid
Molecular weight	117.15	194.19
Melting point	156–157.5°C (decomposes at 293°C)	78–79°C
Optical rotation	−6,1° at 25°C (water) −23,6° at 25°C (1*N* HCl) −29,4° at 25°C (6*N* HCl) −39,1° at 25°C (acetone)	
Solubility	184 parts in water at 24°C	Slightly soluble in water; soluble in alcohol and ether
Organoleptic characteristics		Mild balsamic, floral odor; non-vanillin flavor
Synthesis	By the action of ammonia on α-bromoisovaleric acid;[6-8] also through a hydantoin intermediate[9,10]	By acetylation of vanillin or by oxidation of isoeugenyl acetate with chromic acid in the presence of sulfanilic acid;[11] also by electrolytic reduction of vanillin, followed by acetylation of vanillyl alcohol
Natural occurrence	In many fruit, plant, and animal tissues; in milk and dairy products	
Reported uses[3]	Non-alcoholic beverages 15 ppm Ice cream, ices, etc. 40 ppm Candy 80 ppm Baked goods 60 ppm Gelatins and puddings 80 ppm Chewing gum 200 ppm Milk, dairy products 40 ppm	Non-alcoholic beverages, 11 ppm; ice cream, ices, etc., 11 ppm; candy, 28 ppm; baked goods, 28 ppm
Regulatory status	FEMA No. 3444	FDA 121.1164; FEMA No. 3108

REFERENCES

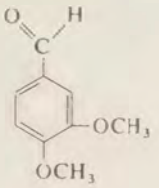
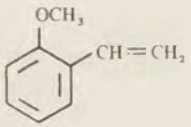
For References 1–5, see end of Part III.

6. **Clark et al.,** *Annalen,* 139, 202, 1866.
7. **Schmidt et al.,** *Annalen,* 193, 101, 1878.
8. **Marvel,** *Org. Synth.,* 20, 106, 1940.
9. **Goldsmith et al.,** U.S. Patent 2,480,644, assigned to Merck & Co.
10. **White,** U.S. Patents 2,557,920 and 2,700,054, assigned to Dow Chemical Co.
11. **Fritzsch & Co.,** German Patent 207,702, August 29, 1905 (March 10, 1909); *Chem. Zentralbl.,* 80, 1207, 1909.

	Vanillin
Other names	4-Hydroxy-3-methoxybenzaldehyde Methyl protocatechuic aldehyde Protocatechualdehyde-3-methylether
Empirical formula	$C_8H_8O_3$
Structure	
Physical/chemical characteristics[5]	
Appearance	White to yellowish crystalline powder
Molecular weight	152.14
Melting point	81 C (83 C); sublimes when heated
Boiling point	284–285 C (with decomposition)
Specific gravity	1.06 (liquid)
Relative humidity	0.5% max (weight loss %)
Solubility	1:3 in 70% alcohol; 1:2 in 95% alcohol; soluble in ether, chloroform, and hot ligroin; rather soluble in water and glycerol
Organoleptic characteristics	Characteristic strong vanilla-like odor; very sweet taste
Synthesis	From eugenol by direct oxidation or by previous transformation of eugenol in isoeugenol; the oxidation is carried out in alkaline solution after acetylation of the phenol group. From safrole obtained from camphor or sassafras oil by converting to isosafrole; by subsequent methylation and oxidation of isosafrole, a mixture of vanillin and isovanillin is obtained; the separation of the two isomers is a somewhat tedious operation. By introduction of the aldehyde group to the guaiacol molecule, a mixture of vanillin and isovanillin is also obtained.
Natural occurrence	Vanillin widely occurs in nature. It has been reported in the essential oil of Java citronella (*Cymbopogon nardus* Rendl.), in benzoin, Peru balsam, clove bud oil, and chiefly vanilla pods (*Vanilla planifolia, V. tahitensis, V. pompona*). More than 40 vanilla varieties are cultivated. Vanillin is also present in the plants as glucose and vanillin. Another source for vanilla is from the waste (liquor) of the wood-pulp industry. Vanillin is extracted with benzene after saturation of the sulfite waste liquor with CO_2.
Reported uses[3]	Non-alcholic beverages, 63 ppm; ice cream, ices, etc., 95 ppm; candy, 200 ppm; baked goods, 220 ppm; gelatins and puddings, 120 ppm; chewing gum, 270 ppm; syrups, 330–20,000 ppm; chocolate, 970 ppm; toppings, 150 ppm; margarine, 0.20 ppm
Regulatory status	FDA GRAS; FEMA No. 3107

REFERENCES

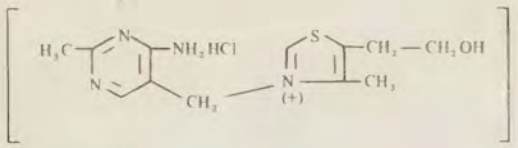
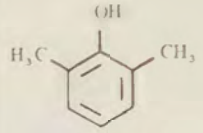
For References 1–5, see end of Part III.

	Veratraldehyde	o-Vinylanisole
Other names	3,4-Dimethoxybenzaldehyde 3,4-Dimethoxybenzenecarbonal Methyl vanillin Protocatechualdehyde dimethylether Vanillin methyl ether	1-Methoxy-2-vinylbenzene
Empirical formula	$C_9H_{10}O_3$	$C_9H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Needles (from ether); oxidizes in air to odorless veratric acid	
Molecular weight	166.17	134.17
Melting point	43–45°C	
Solubility	Almost insoluble in cold water; soluble in hot water, alcohol, and oils	
Organoleptic characteristics	Very sweet, woody, vanilla-like odor; warm, sweet, vanilla-like taste	
Synthesis	Prepared from vanillin[6] by methylation of vanillin with dimethylsulfate under mildly alkaline conditions	
Natural occurrence	Reported among the constituents of the essential oils of *Cymbopogon javanensis*,[7] and *Eryngium poterium*[8]	In *Origanum vulgare*[9,10]
Reported uses[3]	Non-alcoholic beverages 9.0 ppm Ice cream, ices, etc. 9.2 ppm Candy 32 ppm Baked goods 30 ppm Gelatins and puddings 15 ppm	Non-alcoholic beverages 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 3109	FEMA No. 3248

REFERENCES

For References 1–5, see end of Part III.

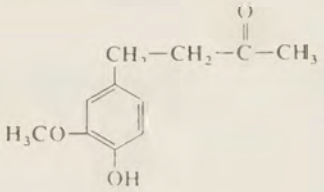
6. **Tiemann and Haarmann,** *Ber. Dtsch. Chem. Ges.*, 8, 1115, 1875.
7. **Hoffman,** *Chem. Zentralbl.*, 3, 886, 1919.
8. **Salgues,** *C. R. Séances Acad. Sci. Paris*, 241, 987, 1955.
9. **Maarse,** Ph.D. dissertation, University of Groningen, Germany, 1971.
10. **Maarse et al.,** *Flavour Ind.*, 4, 477, 1973.

	Vitamin B_1	2,6-Xylenol
Other names	3-(4′-Amino-2′-methyl-5′-pyrimidyl methyl)-5-(2-hydroxyethyl)-4-methyl thiazolium chloride Thiamine hydrochloride Thiamine chloride Aneurin and many other trade names	2,6-Dimethylphenol
Empirical formula	$C_{12}H_{17}ClN_4OS \cdot HCl$	$C_8H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Plates in rosette-like clusters; mildly hygroscopic	
Molecular weight	337.28	122.2
Melting point	248°C (decomposes)	49°C 212°C
Specific gravity		1.169 at 15°C
Solubility	Very soluble in water; slightly soluble in alcohol; insoluble in ether, benzene, hexane, and chloroform; soluble in propylene glycol	
Organoleptic characteristics	Odor slightly reminiscent of thiazole; bitter taste	
Synthesis	See References 6–9	From coal tar oil or coal hydrogenation[10]
Natural occurrence	Rice husks are reportedly the principal source of vitamin B_1; in variable amounts it is a constituent of yeast, milk, green leaves, roots, and tubers; it is also present in high concentration in seeds, and in lesser amounts in different animal organs and muscles	In whisky[11] and coffee[12,14]
Reported uses[3]	Non-alcoholic beverages 50.0 ppm Baked goods 50.0 ppm Condiments, pickles 50.0 ppm Meat, meat sauces, soups 50.0 ppm Milk, dairy products 50.0 ppm Cereals 50.0 ppm	Baked goods 1.0 ppm Condiments 1.0 ppm
Regulatory status	FEMA No. 3322	FEMA No. 3249

REFERENCES

For References 1–5, see end of Part III.

6. Williams, *J. Am. Chem. Soc.*, 57, 229, 1935; 58, 1063, 1936.
7. Williams and Cline, *J. Am. Chem. Soc.*, 58, 1504, 1936.
8. Williams, Ruehle and Finkelstein, *J. Am. Chem. Soc.*, 59, 526, 1937.
9. Gravin, *J. Appl. Chem. U.S.S.R.*, 16, 105, 1943.
10. Bocher, in *Ullmanns Encyklopädie der Technischen Chemie*, Vol. 13, Urban and Schwarzenberg, 1962, 440.
11. Nishimura et al., *J. Food Sci.*, 36, 819, 1971.
12. Goldmann et al., *Helv. Chim. Acta*, 50, 628, 1967.
13. Stoffelsma et al., *J. Agric. Food Chem.*, 16, 1000, 1968.
14. Walter et al., *Z. Ernährungswiss.*, 9, 123, 1969.

	Zingerone
Other names	4-Hydroxy-3-methoxy benzylacetone (4-Hydroxy-3-methoxyphenylethyl)methyl ketone 3-Methoxy-4-hydroxy benzylacetone 4-(3-Methoxy-4-hydroxyphenyl)-2-butanone Vanillyl acetone
Empirical formula	$C_{11}H_{14}O_3$
Structure	
Physical/chemical characteristics:	
Appearance	Crystals (from ether and petroleum ether). The commercial product is a yellowish liquid.
Assay	93% min
Molecular weight	194.23
Melting point	40°C (approx. 41°C)
Boiling point	185.5°C at 13 mm Hg Approximately 102°C
Specific gravity	1.138–1.139 at 25°C
Refractive index	1.5440–1.5450 at 20°C
Solubility	1:1 in 50% alcohol
Organoleptic characteristics	Strong, pungent odor reminiscent of ginger; sharp taste similar to ginger
Synthesis	By condensation of vanillin with acetone followed by hydrogenation
Natural occurrence	Reported found in the essential oil of *Zingiber officinale*[6] It was isolated by Lapwort and collaborators.[7]
Reported uses[3]	Non-alcoholic beverages 6.9 ppm Ice cream, ices, etc. 7.8 ppm Candy 11 ppm Baked goods 11 ppm Chewing gum 15 ppm
Regulatory status	FDA 121.1164; FEMA No. 3124

REFERENCES

For References 1–5, see end of Part III.

6. **Nomura,** *J. Chem. Soc.* (London), 111, 716, 769, 1917.
7. **Lapwort et al.,** *J. Chem. Soc.* (London), 111, 785, 1917.

REFERENCES FOR PART III

The following references have been used in Part III with respect to physical/chemical constants, methods, and use:

1. **Fenaroli, G.,** *Sostanze Aromatiche Naturali,* Vol. 1, Hoepli, Milan, Italy, 1963.
2. *EOA Specification and Standards,* Essential Oil Association of U.S.A., Inc., 60 East 42nd Street, New York, 10017.
3. FEMA (Flavor and Extract Manufacturers' Association) list of GRAS substances as published in various issues of *Food Technology,* starting with Vol. 19, 1965.
4. *Official Methods of Analysis of the Association of Official Agricultural Chemists,* Section 0.091, 10th edition, 1965.
5. **Fenaroli, G.,** *Sostanze Aromatiche Isolate e Sintetiche,* Vol. 2, Parts 1 and 2, Hoepli, Milan, Italy, 1968.

BIBLIOGRAPHY FOR PART III

Information on natural and synthetic flavoring ingredients is quite plentiful, but scattered throughout several texts, often in limited availability. Nonetheless, good central technical libraries should have these available as reference material. The following texts should be consulted for more detailed information:

Arctander, S., *Perfume and Flavor Chemicals,* Steffan Arctander, Montclair, N.J., 1969.
Arctander, S., *Perfume and Flavor Materials of Natural Origin,* Steffan Arctander, Elizabeth, N.J., 1960.
Bedoukian, P. Z., *Perfumery and Flavoring Synthetics,* 2nd ed., American Elsevier Publishing Co., 1967.
Chemicals Used in Food Processing, Publication 1274, National Academy of Sciences/National Research Council, 1965.
Clair, C., *Of Herbs and Spices,* Abelard-Schuman Ltd., 1961.
Gildemeister, E. and Hoffmann, F. R., *Die Aetherischen Oele,* Vols. 3a–3c, Akademie Verlag, 1960–1963.
Givaudan Index, 2nd ed., Givaudan-Delawanna, Inc., 1961.
Guenther, E., *The Essential Oils,* Vols. 1–6, D. Van Nostrand Co., 1948.
Merory, J. M., *Food Flavorings,* 2nd ed., Avi Publishing Co., 1968.

PART IV

The Use of Flavor Ingredients in Food



RELATIONSHIP OF CERTAIN FLAVOR INGREDIENTS TO TASTE AND FLAVOR

Before entering a discussion of complex flavor formulations representing specific food products, a classification of some important natural and synthetic flavor ingredients according to taste and corresponding flavor type may be helpful as a guideline. As indicated in Table 1, while each ingredient can be classified readily into a primary taste, the flavor type best represented by the ingredient can vary. In many instances the same ingredient can deliver several flavor impressions. For this reason and because food substrates are known to alter or modify flavor (*e.g.*, high-protein foods), the single ingredients presented in Table 1 are seldom, if ever, used in rendering a finished flavor.

TABLE 1

Classification of Flavor Ingredients by Primary Taste and Flavor Type

Flavor ingredient	Taste			Flavor type
	Sweet	Bittersweet	Bitter	
Acetophenone			x	—
Allyl anthranilate		x		Green leaves
Allyl benzoate		x		Cherry
Allyl butyrate		x		Apple, apricot
Allyl caproate		x		Pineapple
Allyl cyclohexylacetate		x		Pineapple
Allyl cyclohexylbutyrate		x		Pineapple
Allyl cyclohexylcaproate		x		Peach, apricot
Allyl cyclohexylpropionate		x		Pineapple
Allyl cyclohexylvalerate		x		Peach, apricot, apple
Allyl formate				Mustard
Allyl isovalerate		x		Apple, cherry
Allyl 2-nonylenate				Pineapple
Allyl pelargonate		x		Cognac, pineapple
Allyl phenoxyacetate		x		Pineapple, honey
Allyl phenylacetate			x	Honey
Allyl propionate		x		Apple, apricot
Allyl salicylate		x		Wintergreen, grape
Allyl undecylate		x		Coconut, peach
n-Amyl butyrate		x		Cherry, apple
Amyl phenylacetate	x			Apricot, peach
Anethol	x			Anise
Anisyl alcohol	x			Peach
Anisyl butyrate		x		Cherry, peach
Anisyl formate	x			Strawberry
Anisyl propionate		x		Cherry
Benzyl acetate			x	—
Benzyl butyrate	x			Pear
Benzyl cinnamate	x			Honey
Benzyl formate	x			Apricot, pineapple
Benzyl isobutyrate	x			Strawberry
Benzyl isovalerate	x			Apple
Benzyl propionate	x			Apricot, peach

TABLE 1 (Continued)

Classification of Flavor Ingredients by Primary Taste and Flavor Type

Flavor ingredient	Taste			Flavor type
	Sweet	Bittersweet	Bitter	
Benzyl salicylate	x			Raspberry
Bornyl acetate	x			Pineapple
n-Butyl acetate	x			Pineapple
Butyl formate				Plum
Butyl isobutyrate	x			Pineapple
Butyl isovalerate	x			Apple
Butyl propionate	x			Apricot
Butyl valerate				Apple
Carvacryl acetate		x		Honey
Cinnamaldehyde		x		Cinnamon, melon
Cinnamic acid	x			Apricot
Cinnamyl acetate	x			Pineapple
Cinnamyl alcohol			x	—
Cinnamyl anthranilate		x		Grape
Cinnamyl butyrate	x			Honey
Cinnamyl formate		x		Apple
Cinnamyl isobutyrate	x			Apple
Citral				Lemon
l-Citronellol	x			Peach
Citronellyl acetate	x			Apricot
Citronellyl butyrate	x			Plum
Citronellyl formate	x			Plum
Citronellyl isovalerate	x			Apple
Citronellyl propionate		x		Plum
Coumarin			x	—
p-Cresyl acetate				Honey
p-Cresyl ethyl ether	x			Honey
m-Cresyl phenylacetate	x			Honey
p-Cresyl phenylacetate	x			Honey
Cuminic alcohol		x		Strawberry
Cyclohexyl acetate		x		Apple, banana
Cyclohexyl butyrate		x		Banana, apple, currant
Cyclohexyl caproate		x		Peach, cognac
Cyclohexyl cinnamate				Peach, cherry
Cyclohexyl formate		x		Cherry
Cyclohexyl isovalerate		x		White apple
Cyclohexyl phenylacetate		x		Honey
Cyclohexyl propionate		x		Apple, banana
γ-Decalactone		x		Plum, apricot, peach
Decanal dimethyl acetal			x	Citrus
Decyl acetate	x			Pineapple
Decyl formate	x			Grape

TABLE 1 (Continued)

Classification of Flavor Ingredients by Primary Taste and Flavor Type

Flavor ingredient	Taste			Flavor type
	Sweet	Bittersweet	Bitter	
Diacetyl	x			Butter
Dimethylbenzylcarbinol			x	—
Dimethyl hydroquinone			x	—
Dimethyl phenethyl carbinyl acetate			x	—
Dimethyl phenethyl carbinyl propionate	x			Rose-like
Diphenyl ether	x			Black currant
γ-Dodecalactone		x		Apricot, peach
Ethyl acetate		x		Wine
2-Ethylbutyl acetate		x		Pear
Ethyl butyrate	x			Pineapple
Ethyl cinnamate	x			Apricot, peach
Ethyl formate			x	Rum
2-Ethyl-3-furylacrolein		x		Cola
Ethyl heptylate	x			Wine, pear
Ethyl hexadienoate		x		Pineapple, melon
Ethyl isovalerate	x			Apple
Ethyl methylphenylglycidate	x			Strawberry
Ethyl-2-octynoate	x			—
Ethyl phenoxyacetate		x		Pineapple, honey
Ethyl phenylacetate		x		Honey
Ethyl phenylglycidate	x			Strawberry
Ethyl undecylate		x		Coconut
Ethyl undecynoate			x	—
Ethyl valerate		x		Apple, banana
Ethyl vanillin		x		Vanilla
Eugenol			x	Clove buds
Geraniol			x	Rose-like
Geraniol "palmarosa"	x			Peach, apricot
Geranyl acetate			x	—
Geranyl anthranilate			x	—
Geranyl butyrate	x			Apricot
Geranyl formate			x	—
Geranyl isobutyrate	x			Apricot
Geranyl isovalerate	x			Apricot
Geranyl propionate			x	—
Guaiol acetate	x			Black currant, grape
Guaiol butyrate	x			Plum
Guaiol phenylacetate	x			Honey
Heptyl acetate	x			Apricot
Heptyl formate				Plum
Heptyl propionate		x		Apricot
Hexyl acetate		x		Pear
Hexyl butyrate	x			Pineapple