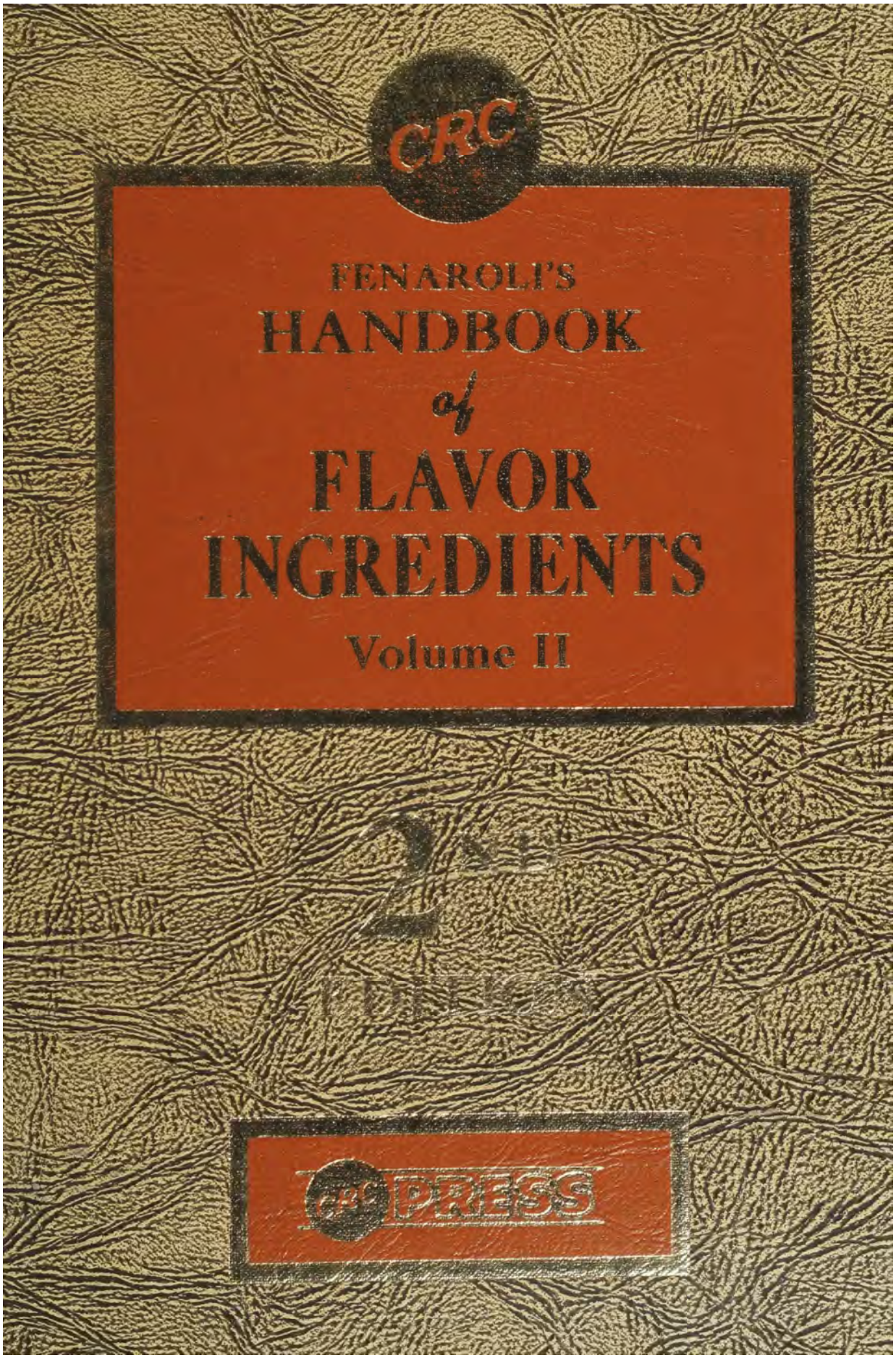
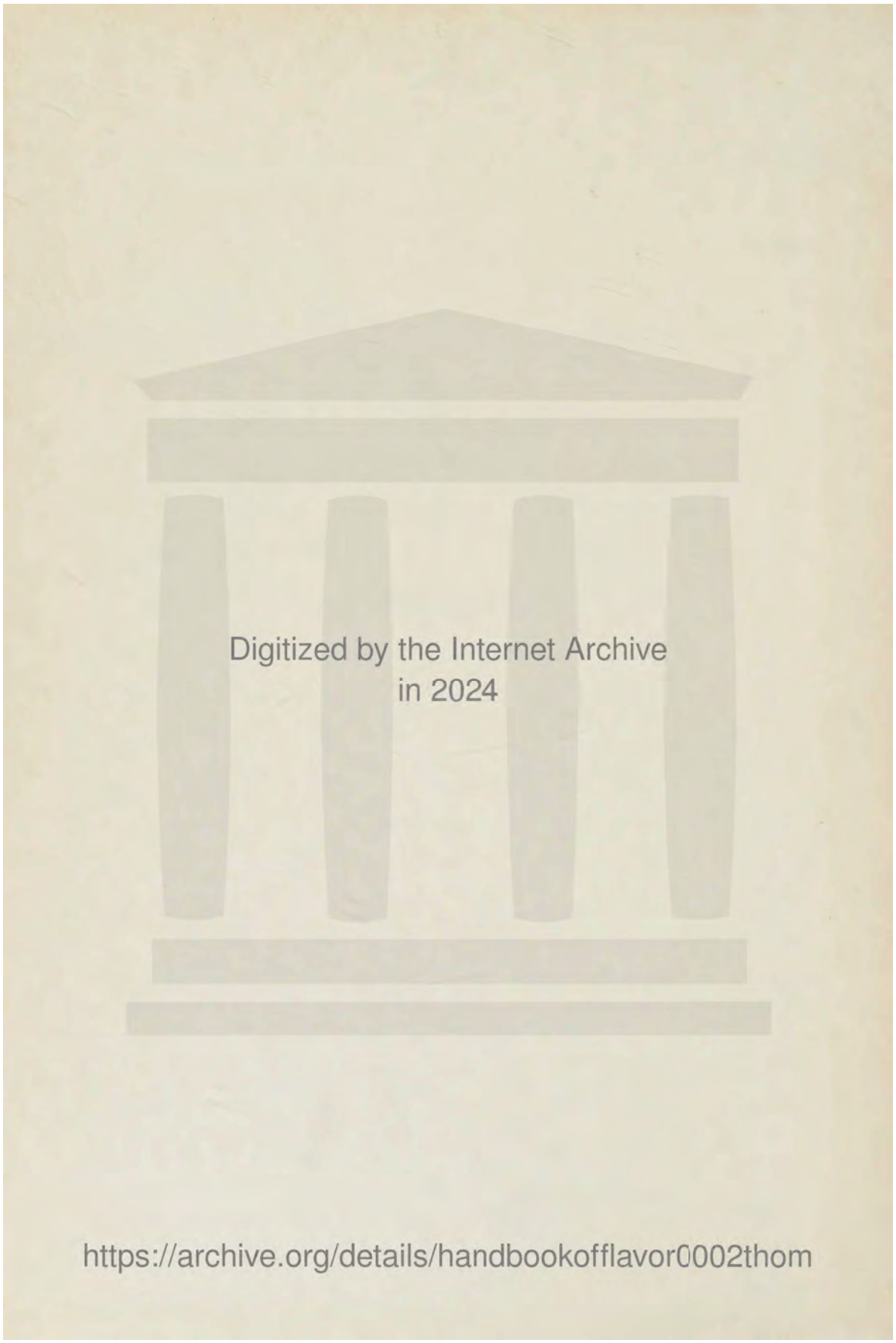


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FENAROLI'S HANDBOOK of FLAVOR INGREDIENTS

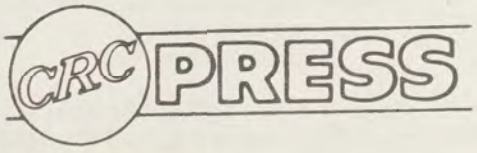
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Volume 2

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by
THOMAS E. FURIA and NICOLÓ BELLANCA
Dynapol
Palo Alto, California

Adapted from the Italian language works of
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Director, Center for Studies of Aromatic Substances
University of Milano, Milano, Italy

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EDITORIAL FOREWORD, FIRST EDITION

The subject of flavor and flavor ingredients, much like its close allies fragrance and perfumery, is still viewed by many through a veil of mystery. To contemporary practitioners of the "pure sciences," the subject of flavors is grossly misunderstood, suggestive of alchemy, and at times subject to condescending criticism. No such indictments are further from reality; few areas of research are more serious or embellished more by sound, scientific thought, and sophisticated techniques. The giants of chemistry have often resorted to problems in flavors and fragrances as a platform for hallmark contributions. It is true that the final assessment of flavor is subjective in character, but, prior to reaching that level of development, most, if not all, of the more objective measuring parameters are *fully* utilized. TLC, GLC, Mass Spec, NMR, UV, and IR, to mention a few, are *routinely* employed not only for resolving flavor components and elucidating structures but also as product control measures. The interdisciplinary nature of the flavor and fragrance industry is characterized by numerous scientific specialties, including analytical, organic, physical, and natural products, chemistry, agronomy, botany, genetics, and taxonomy; food technology; engineering; and finally the artistic efforts of the *flavorist*.

The chemical armament of the flavor industry contains the most numerous constituents of all food ingredients. In the United States it consists of no less than 1,200 ingredients of which approximately 200 are well characterized products of natural origin, while approximately 1,000 are precisely defined synthetics. The task of selecting and blending those ingredients capable of imparting a desired flavor characteristic to complex substrates (often having flavor backgrounds of their own) and at the same time being mindful of toxicological, regulatory, and economic considerations is indeed formidable.

While detailed treatises on various aspects of flavor technology have appeared from time to time, first-source reference texts on the subject as a whole are not readily available in the English language. Those seriously interested in flavor technology have had to wade through numerous journals to locate pertinent information, while the novice or cursory inquirer had only one or two general sources. The scope of this volume is therefore to present a current, authoritative, first-source description of natural and synthetic flavor ingredients, their detailed characteristics, and their application in food. It is primarily intended for those using flavors rather than for the accomplished *flavorist*. Furthermore, it is our intent to revise and up-date this handbook periodically in order to keep pace with advancing technology.

We especially wish to thank Prof. Dr. Giovanni Fenaroli, who arranged to be with us late in 1968 for editorial sessions, and Ulrico Hoepli and L. di G. Pirola, publishers of Prof. Dr. Fenaroli's Italian language books (*Sostanze Aromatiche*, Vols. I, II, and III, and *Aromatizzazione*), for their kind permission to translate and adapt the information for this work. We are grateful to those members of the flavor and fragrance industry who supplied valuable information; outstanding among these is Mr. Frank Fischetti, Jr., of Fritzsche Dodge & Olcott, Inc. We also wish to thank Naarden, Inc., for their permission to reproduce the fold-out schematic flow sheet (Figure 1) in Part I, Volume 1.

Ardsley, New York
November, 1970

T.E.F./N.B.

PREFACE, FIRST EDITION

Flavor is undoubtedly a basic characteristic stimulating the desirability of food; together with color, texture, and nutrition, it forms the cornerstone of contemporary food industries throughout the world. The economic importance of flavor ingredients (essential oils, synthetics, compounded formulations, etc.) is evident from current estimates placing their value at about two-thirds the total sales of all products offered by the flavor and fragrance industry. It is widespread opinion that within a few years an even greater shift in the value of flavors as opposed to fragrances will occur not only from normal increases in productivity but mainly as the result of demands for new food products by both affluent societies and those now in the process of increasing their living standards. Within the decade, however, sharpest increases in the demand for flavor ingredients will arise from new requirements for finished foods geared toward solving the critical starvation problem in most underdeveloped nations. It is therefore evident that while present achievements in flavor technology are indeed remarkable, considering the wide range of products currently offered by the food industry, the tempo will increase sharply. New techniques and more sophisticated flavor formulations designed to respond more precisely to the exacting specifications of future food manufacturers will be required. An example of the quickening pace and exacting specifications that we speak of is the problem of countering flavor modification and alteration in high-protein foods ("protein breakthrough").

With these basic thoughts in mind, it is my primary goal to summarize for the reader my personal experiences lived in this climate of continuing evolution and to rapidly update current efforts in flavor technology. I am convinced that the present state of the art furnishes a sufficiently broad and dynamic base to permit subsequent advances; it is therefore appropriate to describe and examine it in some detail. Certain flavor secrets employed by nature and their exact function are not as yet disclosed, but the investigational means are at our disposal; this makes us confident of the future success in identifying extremely complex systems. The more difficult problems concerning biological factors linked in the formation of naturally occurring flavors, as well as the assessment of the physiological reactions connected with their perception and assimilation by humans and animals, will also be resolved in due course. In the present work I wish to define flavor ingredients as to what they are, how they are manufactured, and how they are used.

In attempting to organize this handbook into a logical sequence capable of future expansion, my primary concern was to present as broad an information base as possible. This was accomplished by presenting the information in four interrelated parts. Part I treats definitions, nomenclature, assessment, and general methods of preparing flavor ingredients; in this section the viewpoint is generalized. (Those who argue that flavor manufacturing methods deserve detailed attention are probably correct, and we shall endeavor to do so in subsequent editions.) Parts II and III consist of detailed descriptions of the natural and synthetic flavor ingredients including the FDA regulatory status and FEMA proposals. Part IV deals exclusively with formulation technology and the uses of compounded flavors of natural and synthetic origin to achieve the most effective flavoring of foods and kindred products. From a technical viewpoint this section presents the greatest challenge, since I felt obliged to discuss not only the organoleptic effects of flavor ingredients and their combined effects in certain food substrates but also auxiliary flavor components, such as non-nutritive sweeteners and flavor potentiators. The flavor formulations presented in Part IV under various substrate categories are typical; while faithfully reproduced and tested, they are intended as guidelines only. In this sense I have attempted to explain the study and evolution of a formulation by stressing those general concepts that must be kept in focus (together with personal taste and experience) during the compounding of a flavor complex or flavoring a finished food product. While of paramount importance, the examples must be considered in light of current regulatory statutes, since it is nearly impossible to predict future restrictions aimed toward safeguarding public health. No doubt, future editions of the handbook will reflect significant changes of this section to keep pace with the application of flavors to food manufacturing problems.

The information presented in this text is partially derived from other works that I have written. Thanks to the Italian publishers Ulrico Hoepli (Milano) and L. di G. Pircla, I was able to summarize

and enlarge herein the more basic parts concerning flavor ingredients appearing in *Sostanze Aromatiche Isolate e Sintetiche*, Vol. II, Tomo II, U. Hoepli, Milano, 1968, and *Aromatizzazione*, L. di G. Pirola, Milano, 1969. A personal note of thanks to Dr. U. Hoepli and Messrs. L. A. Bosisio and D. Caremoli of Curt Georgi Imes for their kind cooperation and assistance.

Finally, if I am at all successful in fulfilling my goal, it will be through the invaluable cooperative efforts of T. Furia and N. Bellanca, who not only translated and edited the original manuscript but also interpreted it in its present fashion so as to stress those areas of importance, especially with regard to U.S. regulatory statutes.

Longmeadow, Massachusetts
December 15, 1968

GIOVANNI FENAROLI

PREFACE TO THE SECOND EDITION

The scientific and technological progress which has characterized numerous sectors of industry during the latter half of the 20th century has likewise been extremely apparent in the area of flavor ingredients. Since the publication of the first edition in 1971 (certainly since its inception in 1968), the flavor industry has traveled a rather precipitous road at what must often appear to peripheral observers as hurtling speeds. However, during this period several bench marks have been established:

1. The need for flavors has been recognized at all levels of food processing.
2. The concept that flavor ingredients should be considered food ingredients rather than isolated components of the flavor subunit has been accepted as rational from a technological viewpoint and punctuated by regulatory agencies concerned with safety.
3. Possibly most important, a more valid scientific notion of "flavoring" has been formulated with respect to the preparation of flavors and their uses.

In addition, the food industry is constantly presenting flavor manufacturers with new and increasingly difficult problems. To meet such needs, the number of new flavor ingredients has been expanded, and many await review by regulatory agencies.

Towards this end, the preparation of a revised and expanded second edition, rather than a second printing, was initiated.

As in the first edition, the same four-part format has been maintained, with corrections, additions, and the contributions of specific authors inserted in what was felt to be appropriate sections. The new material presented includes the following:

1. Data on new synthetic flavor ingredients appearing in FEMA lists 4 through 8 (1970–74).
2. Updating of the natural occurrence of flavor ingredients.
3. Addition of references, augmenting many of the topics already discussed while inserting new ones.
4. Through the cooperation of CRC Press, utilization of new, comprehensive reviews on significant flavor topics.

In expressing my thanks to all those who have contributed to the publication of this edition, I would like to highlight the efforts of Thomas E. Furia and Nicolo Bellanca of Dynapol (Palo Alto, California), who edited, translated, and revised the overall publication. Further, during the intervening years since publication of the first edition, they have maintained a close watch on developments in the flavor industry, reminding us, among other things of regulatory issues and gathering new material for review.

Milano
April 1, 1975

Giovanni Fenaroli

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INTRODUCTION AND REFERENCE NOTATIONS FOR PARTS II* AND III

Introduction

The naturally derived and synthetic flavor ingredients listed in Parts II and III represent only those currently employed and approved for use in the United States under provisions of the Federal Food, Drug and Cosmetic Act (November, 1966) as administered by the FDA. While recent developments and changes in the regulations governing the use of flavor ingredients in the United States have been updated and bear the appropriate *date notice*, the reader is cautioned not to use this listing as an "official" statement of current legal status, since it is impossible in a work of this type to post the latest changes. Accordingly, the reader is advised to consult the *Federal Register* for latest official notices applicable under U.S. law.

Regulatory Status Citations

The following general citations are used in Parts II and III with respect to regulatory status:

GRAS Indicates products *generally recognized as safe* when used:
I. in foods as the spice, herb, or botanical and/or
II. in foods when used as the essential oil, oleoresin (solvent-free), and natural extractives, including distillates. All GRAS substances receive this status when prepared and used in accordance with "good manufacturing practice." The reader is advised to consult with FDA for opinions regarding "good manufacturing practices."

§121.1163 Refers to that section of the Federal Food, Drug and Cosmetic Act stating that the indicated natural flavoring substances and natural adjuvants may be used safely in food in accordance with the following conditions:
1. used in minimum quantity required to produce their intended effect and in accordance with all principles of "good manufacturing practice", and
2. they consist of one or more appropriate forms (e.g., plant parts, fluid and solid extracts, concretes, absolute, oils, gums, balsams, resins, oleoresins, waxes, and distillates) used alone or in combination with flavoring substances and adjuvants generally recognized as safe in food, previously sanctioned for use in food, or regulated in any section. The reader is advised to consult the full text of §121.1163 for an official statement of the provision.

§121.1164 Refers to that section of the Federal Food, Drug and Cosmetic Act stating that the indicated synthetic flavoring substances and adjuvants may be safely used in food in accordance with the following conditions:
1. used in minimum quantity required to produce their intended effect and in accordance with all principles of "good manufacturing practice", and
2. they consist of one or more of the appropriate forms used alone or in combination with flavoring substances and adjuvants generally recognized as safe in food, previously sanctioned for use in food or regulated in any section. The reader is advised, as in the case of natural flavoring substances and adjuvants, to consult the full text of §121.1164 for an official statement of the provision.

*For Part II, see volume I.

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.

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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:

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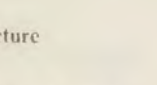
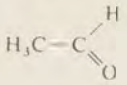
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PART III

Synthetic Flavors



	Acetal	Acetaldehyde
Other names	Acetaldehyde diethyl acetal; 1,1-diethoxyethane; diethyl acetal	Ethanal
Empirical formula	$C_6H_{14}O_2$	C_2H_4O
Structure		
Physical chemical characteristics		
Appearance	Colorless, mobile, flammable liquid; tends to polymerize on aging	Colorless, volatile, flammable liquid
Assay	97% min; free of dissolved metals, chlorides, sulfates, and water	
Molecular weight	118.18	44.05
Melting point		120 C (−123.3 C)
Boiling point	97–112 C (20 C at 20 mm Hg)	20.8 C
Flash point		30 C
Specific gravity	0.826–0.830 (0.8264) at 20 C	0.8009
Refractive index	1.3805 at 20 C	1.3392 at 18 C
Solubility	Slightly soluble in water (1:20); completely miscible with ethyl alcohol and ether; soluble in various aliphatic alcohols and other solvents	Water, ethyl alcohol, and ether; commercially available as a 50% aqueous solution or 99% pure in small steel cylinders
Organoleptic characteristics	Pleasant odor with a taste similar to nut	Characteristic pungent and penetrating odor
Synthesis	From ethyl alcohol and acetaldehyde in the presence of anhydrous calcium chloride[6] or small amounts of mineral acids (HCl)	a. By oxidation of ethyl alcohol with potassium dichromate or manganese dioxide in the presence of sulfuric acid b. By addition of water to acetylene c. Forming during the natural alcoholic fermentation process. Recovery is effected by suitable fractionation, subsequent preparation of the acetaldehyde ammonia, and final treatment of the addition compound with diluted sulfuric acid.
Natural occurrence	Present in some liquors (e.g., sake and whisky); also detected and quantitatively assessed in rum[8]	In oak and tobacco leaves; in the fruital aromas of: pear,[9] apple,[10] raspberry,[11] strawberry,[11] and pineapple;[11] in the distillation waters of *Monarda punctata*,[12] orris, cumin, chenopodium; in the essential oils of: *Litsea cubeba*,[13] *Magnolia grandiflora*,[14] *Artemisia brevifolia*, rosemary, balm, clary sage, *Mentha arvensis*, daffodil, bitter orange, camphor, angelica, fennel, mustard, etc.; in rum[8]
Reported uses[3]	Non-alcoholic beverages, 7.3 ppm; ice cream, ices, etc., 52 ppm; candy, 39 ppm; baked goods, 60–120 ppm	Non-alcoholic beverages, 3.9 ppm; ice cream, ices, etc., 25 ppm; candy, 22 ppm; baked goods, 12 ppm; gelatins and puddings, 6.8 ppm; chewing gum, 20–270 ppm
Regulatory status	FDA 121.1164; FEMA No. 2002	FDA GRAS

REFERENCES

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

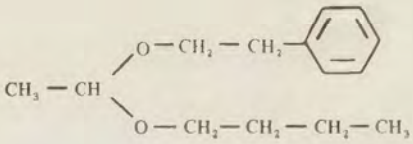
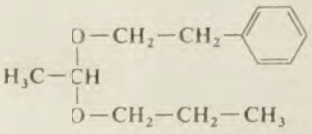
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Gildemeister and Hoffmann, *Die Aetherischen Oele*, Vol. 3c, Akademie Verlag, 1963, 8.

Guenther, *The Essential Oils*, Vol. 2, D. Van Nostrand Co., 1949.

	Acetaldehyde, butyl phenethyl acetal		Acetaldehyde phenethyl propyl acetal
Other names	2-Butoxy-2-phenylethoxy-ethane		Acetal R Pepital 1-Phenethoxy-1-propoxy-ethane Propyl phenethyl acetal
Empirical formula	$C_{14}H_{22}O_2$		$C_{13}H_{20}O_2$
Structure			
Physical/chemical characteristics[5]			
Appearance			Colorless, stable liquid
Molecular weight	222.32		208.30
Flash point			95 C
Specific gravity			0.944–0.950 at 25 /25 C
Refractive index			1.4770–1.4820 at 20 C
Solubility			1:7 in 70% ethanol; 1:2 in 80% ethanol
Organoleptic characteristics			Very strong odor of green leaves
Synthesis			From acetaldehyde with a mixture of propyl and β-phenyl ethyl alcohols
Natural occurrence			Not reported found in nature
Reported uses[3]	Non-alcoholic beverages	5.0 ppm	Candy 2.5 ppm
	Ice cream, ices, etc.	5.0 ppm	Baked goods 2.5 ppm
	Candy	5.0 ppm	
	Gelatins and puddings	5.0 ppm	
	Chewing gum	5.0 ppm	
Regulatory status	FEMA No. 3125		FDA 121.1164; FEMA No. 2004

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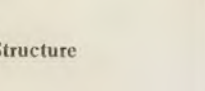
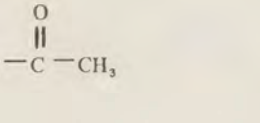
For References 1–5, see end of Part III.

	Acetanisole	Acetic acid
Other names	*p*-Acetyl anisole 4′-Methoxyacetophenone *p*-Methoxyacetophenone Navatone	Ethanoic acid
Empirical formula	$C_9H_{10}O_2$	$C_2H_4O_2$
Structure		$CH_3—COOH$
Physical/chemical characteristics[5]		
Appearance	Yellowish-white crystals at room temperature	Colorless liquid
Assay	98% min.[2] (as a ketone)	
Molecular weight	150.18	60.05
Melting point	38 C (36°C)	17 C (16.6–16.7°C)
Boiling point	158/256 C	118 C (118.2–118.5 C)
Freezing point	34.7 C (not less than 36°C)[2]	
Specific gravity	1.0959 at 25 C; 1.0818 at 41.1 C	1.049 at 20 C
Refractive index	1.55489 at 25 C; 1.547 at 41.1 C	1.3718 at 20 C
Halogens	Free[2]	
Optical rotation	±0°	
Solubility	Slightly soluble in water; from 1:4–1:5 in 50% ethanol; soluble in most organic solvents	Completely miscible with water, ethanol, ether, and carbon tetrachloride; insoluble in carbon disulfide
Organoleptic characteristics	Odor similar to that of *p*-methylacetophenone; suggestive of hawthorn and floral note of heliotrope; bitter, unpleasant taste	Strong, purgent, characteristic odor
Synthesis	From anisole and acetyl chloride in the presence of aluminum chloride and carbon disulfide; from anisole and acetic acid in the presence of boron trifluoride	From the destructive distillation of wood; from acetylene and water; via acetaldehyde by subsequent oxidation with air
Natural occurrence	In anise seed	Identified among the constituents of petitgrain lemon oil,[6] in bitter orange oil,[7] and in strawberry aroma[8]
Reported uses[3]	Non-alcoholic beverages 2.3 ppm Ice cream, ices, etc. 2.5 ppm Candy 4.6 ppm Baked goods 5.8 ppm Chewing gum 840 ppm	Non-alcoholic beverages 39 ppm Ice cream, ices, etc. 32 ppm Candy 52 ppm Baked goods 38 ppm Gelatins and puddings 15 ppm Chewing gum 60 ppm Condiments 5,900 ppm
Regulatory status	FDA 121.1164; FEMA No. 2005	FDA GRAS; FEMA No. 2006

REFERENCES

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

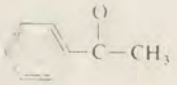
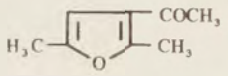
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8. **Willhalm et al.,** *Helv. Chim. Acta*, 49, 66, 1966.

	Acetone	Acetoin
Other names	2-Propanone Dimethyl ketone β-Ketopropane Pyroacetic ether	Acetyl methyl carbinol 2,3-Butanolone Dimethylketol 3-Hydroxy-2-butanone γ-Hydroxy-β-oxobutane
Empirical formula	C_3H_6O	$C_4H_8O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, mobile, highly flammable liquid	Yellowish liquid; forms dimer on standing that reconverts to monomer by melting
Molecular weight	58.08	88.10
Melting point	−95.35°C	15 C
Boiling point	57°C	148 C (140/142 C)
Flash point	−20°C	
Specific gravity	0.788 at 25°C 0.8186 at 0°C	0.9972 at 17 C
Refractive index	1.3588 at 20°C	1.4190 at 17.3 C
Optical rotation		−39.4 (pure) and −105 (aqueous solution) at 20 C; *also see* Synthesis (following)
Solubility	Soluble in water in all proportions; soluble in alcohol, ether, benzene, and chloroform	Miscible with water; soluble in ethanol; slightly soluble in ether
Organoleptic characteristics	Characteristic aromatic odor; pungent, somewhat sweet taste	Pleasant, butter-like odor and flavor
Synthesis	By fermentation, or by chemical synthesis from isopropanol, cumene, or propane[9]	From diacetyl by partial reduction with zinc and acid,[6] also a product of fermentation Acetoin is an optically active compound. The *d* (−) acetyl methyl carbinol is obtained from fermentation and, in mixture with other products, from the catalytic oxidation of 2,3-butanediol.[7] The *l* (−) acetyl methyl carbinol is obtained from fermentation. The optically pure form has not been isolated; the optically inactive form is prepared synthetically.
Natural occurrence	In apple, pear, grape, pineapple, strawberry, raspberry, tomato, black currant, citrus, onion, and potato; also reported found in cocoa leaves, in Mexican goosefoot, and in the oils of coriander and lavender; in trace amounts it has been reportedly identified in the oil of bitter orange, in distilled wine, and in coffee aroma[10]	Present in corn, wine, vinegar (from grape or other sources), honey, cocoa, butter, and roasted coffee; identified also in currant and strawberry aromas[8]
Reported uses	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	Non-alcoholic beverages 7.4 ppm Ice cream, ices, etc. 3.3 ppm Candy 18 ppm Baked goods 32 ppm Gelatins and puddings 0.60–21 ppm Shortening 8.0 ppm Margarine 0.80–50 ppm Cheese (cottage) 7.0 ppm
Regulatory status	FEMA No. 3326	FDA GRAS; FEMA No. 2008

REFERENCES

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

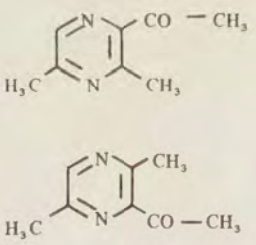
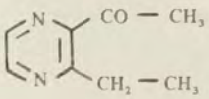
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7. Blom, *J. Am. Chem. Soc.*, 67, 484, 1945.
8. Coppens and Hoejenbons, *Chem. Zentralbl.*, 2, 2339, 1939.
9. Weiss, *Chem. Eng. News*, 36, 79, 1958.
10. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.

	Acetophenone	3-Acetyl-2,5-dimethyl furan
Other names	Acetyl benzene Hypnone Methyl phenyl ketone	2,5-Dimethyl-3-acetyl furan
Empirical formula	C_8H_8O	$C_8H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Almost colorless liquid at room temperature	
Assay	98% min.	
Molecular weight	120.14	138
Melting point	19.5–20.5°C	
Boiling point	202°C	
Freezing point	19.5°C	
Flash point	76°C	
Specific gravity	1.0329 at 15°C (1.025–1.028 at 25°/25°C)[2]	
Refractive index	1.53631 at 15°C (1.533–1.5350 at 20°C)[2]	
Solubility	1:5 in 50% ethanol; soluble in essential oils and most organic solvents; insoluble in water	
Organoleptic characteristics	Characteristic sweet, pungent odor (acacia) and bitter, aromatic flavor	
Synthesis	From benzene and acetylchloride in the presence of aluminum chloride or by catalytic oxidation of ethyl benzene; also prepared by fractional distillation and crystallization from the essential oil of *Stirlingia latifolia*	
Natural occurrence	In the oils of labdanum, *Stirlingia latifolia*, *Urtica dioica*,[6] *Elsholtzia argyi* var. *nipponica*,[7] *Elsholtzia ciliata*,[8] in various species of *Orthodon*[9] (*O. citraliferum*, *O. linalooliferum* var. *lacrolinalooliferum*, *O. linaloiferum*, *O. sabinoliferum* var. *taiwanense*), and in castoreum absolute[10]	
Reported uses[3]	Non-alcoholic beverages 0.98 ppm Ice cream, ices, etc. 2.8 ppm Candy 3.6 ppm Baked goods 5.6 ppm Gelatins and puddings 7.0 ppm Chewing gum 0.60–20 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 0.6 ppm Candy 1.5 ppm Baked goods 2.0 ppm Gelatins and puddings 1.5 ppm Meat, meat sauces, soups 1.0 ppm Milk, dairy products 0.6 ppm
Regulatory status	FDA 121.1164; FEMA No. 2009	FEMA No. 3391

REFERENCES

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

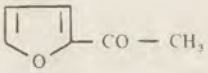
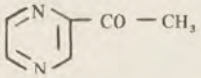
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7. Fujita and Ueda, *J. Chem. Soc. Jap. Pure Chem. Sect.*, 79, 1067, 1958.
8. Fujita and Ueda, *J. Chem. Soc. Jap. Pure Chem. Sect.*, 80, 1495, 1959.
9. Fujita and Ueda, *Miltizer Ber.*, 91, 1959; *J. Chem. Soc. Jap. Pure Chem. Sect.*, 1957, 1958, 1959.
10. Lederer, *Schimmel Ber.*, 25, 1950.

	2-Acetyl-3,5 (and 6)-dimethylpyrazine	2-Acetyl-3-ethylpyrazine
Other names	(1) 2-Acetyl-3,5-dimethylpyrazine (2) 3-Acetyl-2,5-dimethylpyrazine	2-Acetyl-3-ethyl-1,4-diazine 3-Ethyl-2-pyrazinyl methyl ketone
Empirical formula	$C_8H_{10}N_2O$	$C_8H_{10}N_2O$
Structure		
Physical/chemical characteristics		
Assay	C: 63.98%; H: 6.71%; N: 18.65%; O: 10.65%	C: 63.98%; H: 6.71%; N: 18.65%; O: 10.65%
Molecular weight	150.18 (calculated = 150.079312)	150.18 (calculated = 150.079312)
Boiling point		55°C at 1.1 mm Hg
Mass spectra[6]		150, 43, 107, 52, 79, 27
IR spectra[6]		3.3, 3.39, 3.41, 5.5, 5.9, 6.05, 6.45, 6.55, 6.85, 7.09, 7.14, 7.4, 7.6, 7.85, 8.02, 8.45, 8.6, 8.7, 9.2, 9.3, 9.45, 9.72, 10.3, 10.5, 11.65μ
NMR spectra[6]		($CDCl_3$) δ 1.28 (t, 3, $-CH_2-CH_3$), 2.69 (s, 3, $-C(=O)-CH_3$), 3.15 (q, 2, $-CH_2-CH_3$) 8.44 (d-1, ring –H), 8.61 (d,1, ring –H)
Synthesis	From the corresponding dimethylethylpyrazine by bromination, followed by oxidation to the ketone[6]	From 2-ethyl-3-methylpyrazine by bromination, followed by oxidation to the ketone[7]
Reported uses[3]	Ice cream, ices, etc. 1.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 1.0 ppm Meat, meat sauces 5.0 ppm Soups 5.0 ppm Cereals 5.0 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 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
Regulatory status	FEMA No. 3327	FEMA No. 3250

REFERENCES

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

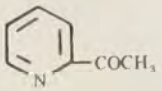
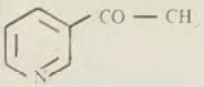
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7. Mookherjee and Klaiber, *J. Org. Chem.*, 37, 511, 1972.

	2-Acetylfuran	Acetylpyrazine
Other names	2-Furyl methyl ketone 2-Acetofuran	Methylpyrazinyl ketone 2-Acetylpyrazine
Empirical formula	$C_6H_6O_2$	$C_6H_6ON_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless crystals	
Assay		C: 59.01%, H: 4.95%; O: 13.10%; N: 22.94%
Molecular weight	110.11	122.13
Melting point	33°C	79–80°C
Boiling point	173°C 67°C at 10 mm Hg 60°C at 12 mm Hg	
Mass spectra[13]		43 (100), 52 (44), 53 (34), 79 (27), 80 (45), 122 (37)
IR spectra[14]		1683, 1570, 1282, 1163, 1102, 1043, 1020, 950, 858 cm^{-1}
UV spectra[14]		λ_{max}^{ETOH} 269 nm
NMR spectra[14]		T = 0.82 (1, db, ring – H), 1.28 (1, db, ring – H), 1.37 (1, qd, ring – H), 7.28 (3, S, $-CH_3$)
Specific gravity	1.098 at 20°C	
Refractive index	1.5017 at 20°C	
Solubility	Insoluble in water; soluble in alcohol, ether, and propylene glycol	
Organoleptic characteristics	Powerful, balsamic-sweet odor	Flavor reminiscent of popcorn
Synthesis	From furan and acetyl chloride by a Friedel-Kraft condensation[6]	By the ester condensation of EtO_2 C-pyrazine;[10] by dehydrating pyrazynamide with $POCl_3$ and then reacting the resulting 2-cyanopyrazine with methyl magnesium bromide[11]
Natural occurrence	Reported found as a constituent in coffee aroma;[7] also isolated from beech and oak wood tar oils; an aroma component of yellow passion fruit (*Passiflora edulis* f. flavicarpa);[8] also a volatile flavor component of potato chips[9]	Reported present in peanuts, filberts, popcorn, and sesame oil[12]
Reported uses[3]	Baked goods 20.0 ppm Condiments 20.0 ppm Meats, meat sauces 20.0 ppm Soups 20.0 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 5.0 ppm Baked goods 5.0 ppm
Regulatory status	FEMA No. 3163	FEMA No. 3126

REFERENCES

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

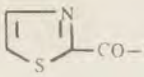
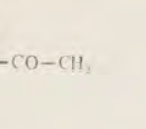
6. Reichstein, *Helv. Chim. Acta*, 13, 356, 1930.
7. Gianturco, Gianmarino and Friedel, *Nature*, 210, 1358, 1966.
8. Winter and Klöti, *Helv. Chim. Acta*, 55(6), 1916, 1972.
9. Deck, Pokorny, and Chang, *J. Food Sci.*, 38(2), 345, 1973.
10. Shindo, *Chem. Pharm. Bull.* (Tokyo), 8, 33, 1960.
11. British Patent 1,164,050, assigned to R. J. Reynolds Tobacco Co.
12. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
13. Walradt et al., *J. Agric. Food Chem.*, 18, 926, 1970.
14. Roberts, U.S. Patent 3,402,051, 1968.

	2-Acetylpyridine	3-Acetylpyridine
Other names	Methyl-2-pyridyl ketone 2-Acetopyridine	3-Acetylpyridine Methyl-3-pyridyl ketone
Empirical formula	C_7H_7ON	C_7H_7ON
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid; tends to yellow on exposure to air	Colorless liquid; turns yellow in air
Molecular weight	121.14	121.13
Boiling point	192°C 78°C at 12 mm Hg	220°C 106°C at 12 mm Hg
Refractive index	1.5203 at 20°C	
Solubility	Soluble in alcohol, ether, and acids	Soluble in water, ethanol, ether, and acids
Organoleptic characteristics	Tobacco-like aroma	
Synthesis	From ethyl picolinate[6]	Dry distillation of calcium nicotinate with calcium acetate[7]
Natural occurrence		In roasted filberts[8]
Reported uses[3]	Candy 3.0 ppm Baked goods 5.0 ppm Meats, meat sauces 3.0 ppm Soups 3.0 ppm Milk, dairy products 3.0 ppm Cereals 3.0 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm Gelatins and puddings 2.0 ppm
Regulatory status	FEMA No. 3251	FEMA No. 3424

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

6. Kolloff and Hunter, *J. Am. Chem. Soc.*, 63, 490, 1941.
7. Engler et al., *Chem. Ber.*, 22, 597, 1889.
8. Kinlin et al., *J. Agric. Food Chem.*, 20, 1021, 1972.

	2-Acetyl thiazole	Aconitic acid
Other names	Methyl-2-thiazolyl ketone 5-Acetyl thiazole Methyl-5-thiazolyl ketone	Achilleic acid Citridic acid Equisetic acid 1-Propene-1,2,3-tricarboxylic acid
Empirical formula	C_5H_5NOS	$C_6H_6O_6$
Structure		
Physical/chemical characteristics		
Appearance	Oily liquid	White or yellowish crystalline solid
Molecular weight	127.16	174.11
Melting point	64.5–65.5°C	194–195°C (with decomposition)
Boiling point	95–105°C at 15 mm Hg 74°C at 11 mm Hg	
Refractive index	n_D^{20} 1.5480	
Solubility		Soluble in water and alcohol; slightly soluble in ether
Synthesis	By oxidation of the corresponding carbinol using dichromate[6]	By dehydration of citric acid with concentrated H_2SO_4.[7] Aconitic acid prepared by this or other methods has the *trans* configuration. The *cis*-isomer is little known.
Natural occurrence	In beef broth	In beet root, sugar cane, the leaves of *Aconitum napellus*, and other natural products (*Pelargonium* species)
Reported uses[3]	Non-alcoholic beverages 0.2 ppm Ice cream, ices, etc. 0.9 ppm Candy 1.4 ppm Chewing gum 0.6 ppm Protein foods 0.7 ppm	Non-alcoholic beverages 0.20–2.0 ppm Alcoholic beverages 20 ppm Ice cream, ices, etc. 0.60 ppm Candy 0.60–30 ppm Baked goods 0.60–15 ppm Chewing gum 28 ppm
Regulatory status	FEMA No. 3328	FDA GRAS; FEMA No. 2010

REFERENCES

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

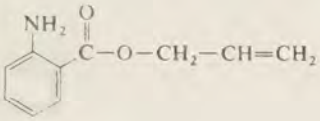
6. Berand and Metzger, *Bull. Soc. Chim. Fr.*, p. 2072, 1962.
7. Bruce, *Org. Synth.*, 2, 12, 1943.

	Adipic acid	β-Alanine
Other names	1,4-Butanedicarboxylic acid Hexanedioic acid	β-Aminopropionic acid 3-Aminopropanoic acid 3-Aminopropionic acid
Empirical formula	$C_6H_{10}O_4$	$C_3H_7O_2N$
Structure	$HOOC-(CH_2)_4-COOH$	$H_2N-CH_2-CH_2-COOH$
Physical/chemical characteristics[5]		
Appearance	White, crystalline solid	Needles (from water)
Molecular weight	146.14	89.10
Melting point	153°C	207°C (decomposes)
Boiling point	216°C at 15 mm Hg	
Specific gravity	1.360 at 25°C	1.437 at 19°C
Solubility	Slightly soluble in cold water; soluble in hot water; soluble in alcohol; insoluble in benzene	Soluble in water; slightly soluble in alcohol; insoluble in ether and acetone
Organoleptic characteristics		Slightly sweet taste
Synthesis	By oxidation of cyclohexanol with concentrated nitric acid; by catalytic oxidation of cyclohexanone with air[6,7]	By heating acrylic acid with concentrated aqueous ammonia under pressure;[8] by addition of acrylonitrile to phthalimide or to ammonia;[9] from β-aminopropionitrile;[10] from succinimide by the Hofmann degradation;[11] patented process[12]
Natural occurrence	In beet juice	Reported to occur as a component in amino acids: carnosine, auserine, pantothenic acid
Reported uses[3]	Non-alcoholic beverages 40 ppm Gelatins and puddings 5,000 ppm It can usually replace tartaric acid in baking powders because of its lower hygroscopicity	Non-alcoholic beverages 10.0 ppm Baked goods 10.0 ppm Condiments, pickles 10.0 ppm Meat, meat sauce 10.0 ppm Soups 10.0 ppm Milk, dairy products 10.0 ppm Cereals 10.0 ppm
Regulatory status	FDA 121 1164; FEMA No. 2011	FEMA No. 3252

REFERENCES

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

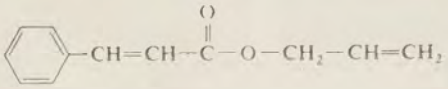
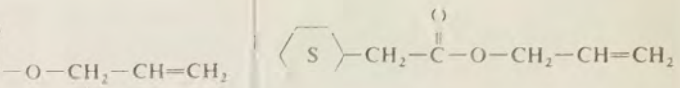
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8. **Baker and Ollis,** *J. Chem. Soc.*, p. 345, 1949.
9. **Horning,** *Organic Syntheses*, Coll. Vol. 3, Wiley & Sons, New York, 1955, 34.
10. **Blatt,** *Organic Syntheses*, Coll. Vol. 2, Wiley & Sons, New York, 1943, 19.
11. **Clarke and Behr,** *Org. Synth.*, 16, 1, 1936.
12. U.S. Patents 2,734,081 and 2,956,080.

	Allyl anthranilate	Allyl butyrate
Other names	Allyl 2-aminobenzoate Allyl *o*-aminobenzoate	
Empirical formula	$C_{10}H_{11}NO_2$	$C_7H_{12}O_2$
Structure		$CH_3-(CH_2)_2-\overset{\overset{O}{\|}}{C}-O-CH_2-CH=CH_2$
Physical/chemical characteristics[5]		
Appearance		Liquid
Molecular weight	177.21	128.17
Boiling point		44–45°C at 15 mm Hg
Flash point		
Specific gravity		0.9017 at 20°C
Refractive index		1.4158 at 20°C
Synthesis		From allyl alcohol and butyric acid in the presence of concentrated H_2SO_4 or *p*-toluenesulfonic acid in benzene[6–8]
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 0.67 ppm Candy 2.0 ppm Baked goods 0.02–1.0 ppm Gelatins and puddings 2.0 ppm	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 0.50–1.0 ppm Candy 1.3 ppm Baked goods 0.50–3.0 ppm Gelatins and puddings 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2020	FDA 121.1164; FEMA No. 2021

REFERENCES

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

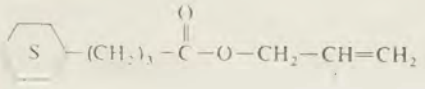
6. Golendejew, *Zh. Obshch, Khim.*, 6, 1844, 1936.
7. Jeffery and Vogel, *J. Chem. Soc.*, p. 663, 1948.
8. Salmi and Leimu, *Suom. Kemistil. B*, 20, 47, 1947.

	Allyl cinnamate	Allyl cyclohexaneacetate
Other names		
Empirical formula	$C_{12}H_{12}O_2$	$C_{11}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Almost colorless liquid	Liquid
Molecular weight	188.22	182.26
Boiling point	150–152°C	66°C at 1 mm Hg
Specific gravity	1.048 at 23°C	
Refractive index	1.5661 (1.530) at 23°C	1.4574 at 20°C
Solubility	Allyl 3-phenylpropenoate; allyl β-phenylacrylate	
Organoleptic characteristics	Peach or apricot-like aroma	Intense fruital (pineapple, peach, apricot) aroma
Synthesis	By esterification of cinnamic acid with allyl alcohol in the presence of concentrated H_2SO_4[6]	By esterification of cyclohexane acetic acid and allyl alcohol in the presence of benzene
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.4 ppm Candy 1.8 ppm Baked goods 2.6 ppm	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 1.6 ppm Candy 3.5 ppm Baked goods 4.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2022	FDA 121.1164; FEMA No. 2023

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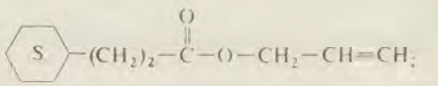
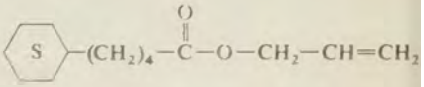
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6. Seeligmann, Dissertation, Technical University of Karlsruhe, Germany, 1906, 17.

	Allyl cyclohexane butyrate	Allyl cyclohexanehexanoate
Other names		Allyl cyclohexylcaproate Allyl cyclohexylcapronate
Empirical formula	$C_{13}H_{22}O_2$	$C_{15}H_{26}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Liquid	
Molecular weight	210.31	238.37
Boiling point	104°C at 1 mm Hg	
Refractive index	1.4608 at 20.5°C	
Organoleptic characteristics	Pineapple aroma	
Synthesis	By direct esterification in the presence of benzene	By direct esterification of the acid with allyl alcohol
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.4 ppm Candy 3.3 ppm Baked goods 3.8 ppm	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 3.3 ppm Candy 8.0 ppm Baked goods 8.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2024	FDA 121.1164; FEMA No. 2025

REFERENCES

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

	Allyl cyclohexane propionate	Allyl cyclohexanevalerate
Other names	Allyl-3-cyclohexylpropionate Allyl-β-cyclohexylpropionate	Allyl cyclohexylpentanoate
Empirical formula	$C_{12}H_{20}O_2$	$C_{14}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid
Molecular weight	98% min.[2] (ester content)	224.34
Melting point	196.29	
Boiling point	91°C at 1 mm Hg	119 C at 1 mm Hg
Specific gravity	0.945-0.950[2] at 25°/25°C	
Refractive index	1.4595 (1.4570–1.4620)[2] at 22°C	1.4605 at 22°C
Acid value	Not more than 5.0	
Solubility	1:4 in 80% ethanol[2]	
Organoleptic characteristics	Pineapple aroma	Characteristic fruital (peach, apricot, apple) aroma
Synthesis	By direct esterification of cyclohexylpropionic acid with allyl alcohol in the presence of benzene	By direct esterification in the presence of benzene
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.7 ppm Ice cream, ices, etc. 3.1 ppm Candy 13 ppm Baked goods 7.1 ppm Gelatins and puddings 7.7 ppm Chewing gum 30 ppm Icings 0.20 ppm	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 2.3 ppm Candy 4.4 ppm Baked goods 4.8 ppm
Regulatory status	FDA 121.1164; FEMA No. 2026	FDA 121.1164; FEMA No. 2027

REFERENCES

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

	Allyl disulfide	Allyl 2-ethylbutyrate
Other names	Diallyl disulfide	
Empirical formula	$C_6H_{10}S_2$	$C_9H_{16}O_2$
Structure	$CH_2=CH-CH_2-S-S-CH_2-CH=CH_2$	$CH_3-CH_2-CH(-CH_2-CH_3)-C(=O)-O-CH_2-CH=CH_2$
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	146.26	156.23
Boiling point	138/139°C (79°C at 16 mm Hg)	165–167°C; 58–60°C at 6 mm Hg
Specific gravity	1.010 at 15°C	
Refractive index	1.541 at 20°C	1.4240 at 15°C
Solubility	Insoluble in water; soluble in most common organic solvents	
Organoleptic characteristics	Characteristic garlic odor	Ethereal aroma with a slightly fruit-like note
Synthesis	By oxidation of allyl mercaptan with iodine in the presence of pyridine and ethanol;[6] from sodium allyl thiosulfate with potassium hydroxide[7]	By prolonged heating of 2-ethylbutyric acid (sodium salt) with allyl bromide in xylene;[9] by direct esterification of the acid with allyl alcohol[1,0]
Natural occurrence	Main constituent of *Allium sativum* essential oil[8]	Not reported found in nature
Reported uses[3]	Condiments 6.5 ppm Meats 7.0 ppm	Non-alcoholic beverages 0.50–1.0 ppm Candy 2.0 ppm Gelatins and puddings 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2028	FDA 121.1164; FEMA No. 2029

REFERENCES

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

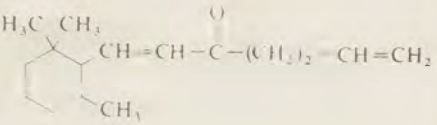
6. Smoll, Bailey and Cavallito, *J. Am. Chem. Soc.*, 69, 1711, 1947.
7. Challenger and Greenwood, *Biochem. J.*, 44, 90, 1949.
8. Semmler, *Arch. Pharm.* (Wernheim), 230, 438, 1892.
9. Arnold and Liggett, *J. Am. Chem. Soc.*, 64, 2877, 1942.
10. Seldner, *Am. Perfum.*, 54(3), 296, 1949.

	Allyl heptylate	Allyl hexanoate
Other names	Allyl heptanoate Allyl heptoate Allyl oenanthate	Allyl caproate Allyl capronate 2-Propenyl hexanoate
Empirical formula	$C_{10}H_{18}O_2$	$C_9H_{16}O_2$
Structure	$H_3C-(CH_2)_5-\overset{\overset{O}{\|}}{C}-O-CH_2-CH=CH_2$	$H_3C-(CH_2)_4-\overset{\overset{O}{\|}}{C}-O-CH_2-CH=CH_2$
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless to light-yellow, mobile liquid; stable
Assay		98% min
Molecular weight	170.25	156.23
Boiling point	210°C	75/76 C at 15 mm Hg
Flash point		68 C
Specific gravity	0.890 at 15.5°C	0.8869 at 20 C; 0.885–0.890 at 25 C
Refractive index	1.4290 at 20°C	1.4243 (1.422–1.426) at 20 C
Acid value		1 max
Solubility		Insoluble in water; soluble in most organic solvents; 1:2 in 80% ethanol
Organoleptic characteristics	Characteristic wine odor with a slight banana note and banana-like flavor	Fruit-like aroma (pineapple)
Synthesis		By esterification of *n*-capronic acid with allyl alcohol in the presence of concentrated H_2SO_4[6] or of naphthalene-β-sulfonic acid in benzene under a nitrogen blanket[7]
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. 2.7 ppm Candy 6.4 ppm Baked goods 6.4 ppm Gelatins and puddings 2.9 ppm Chewing gum 86 ppm	Non-alcoholic beverages 7.0 ppm Ice cream, ices, etc. 11 ppm Candy 32 ppm Baked goods 25 ppm Gelatins and puddings 22 ppm Chewing gum 210 ppm
Regulatory status	FDA GRAS; FEMA No. 2031	FDA 121.1164; FEMA No. 2032

REFERENCES

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

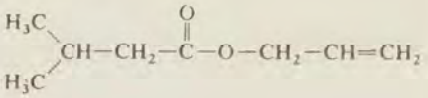
6. Golendejew, *Zh. Obshch. Khim.*, 10, 1411, 1940; *Chem. Abstr.*, p. 3067, 1941.
7. Swern and Jordan, *J. Am. Chem. Soc.*, 70, 2336, 1948.

	Allyl α-ionone	Allyl isothiocyanate
Other names	Butenyl α-cyclocitrylidenemethyl ketone Cetone V α-Cyclocitrylidenemethyl butenyl ketone 1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-1,6-heptadiene-3-one	Mustard oil (mustard oil volatile, synthetic)
Empirical formula	$C_{18}H_{24}O$	C_4H_5NS
Structure		$CH_2=CH-CH_2-N=C=S$
Physical/chemical characteristics[5]		
Appearance	Yellow liquid	Colorless liquid; tends to darken on aging
Assay	88% min	
Molecular weight	232.35	99.19
Melting point		−102.5°C
Boiling point	102/104°C at 0.15 mm Hg	152°C
Flash point	100°C	
Specific gravity	0.9289 at 20°C; 0.928–0.935 at 25/25°C	1.02356 at 15°C
Refractive index	1.50402 (1.5030–1.5070) at 20°C	1.52481 at 15°C
Solubility	1:8 in 70% ethanol	1:8 in 80% ethanol; slightly soluble in water; completely miscible with ether, chloroform, and benzene
Organoleptic characteristics	Strong fruital aroma reminiscent of pineapple	Strong, pungent odor; lachrymatory
Synthesis	By condensation of citral and allyl acetone in the presence of sodium methoxide and subsequent ring closure in the presence of boron trifluoride	By distillation of sodium thiocyanate and allyl chloride
Natural occurrence	Not reported found in nature	In the essential oil from seeds of *Brassica nigra* Koch.,[6] *Brassica juncea* Hook. and Thoms.,[7] and *Thlaspi arvense*;[8] in the essential oil from roots of *Cochlearia armoracia*;[9] in the seeds and roots of *Alliaria officinalis*;[10,11] in onion juice;[12] and in the seeds of various *Cruciferae*[13–16]
Reported uses[3]	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 1.4 ppm Candy 2.6 ppm Baked goods 3.1 ppm Gelatins and puddings 1.0 ppm Jellies 2.0 ppm	Non-alcoholic beverages 0.02–0.50 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50 ppm Baked goods 5.2 ppm Condiments 52 ppm Meats 87 ppm Syrups 10–88 ppm
Regulatory status	FDA 121.1164; FEMA No. 2033	FDA 121.1164; FEMA No. 2034

REFERENCES

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

6. **Will,** *Ann. Chem.*, 52, 1, 1840–44.
7. **Gildemeister and Hoffmann,** *Die Aetherischen Oele*, 3rd ed., Vol. 1, Akademie Verlag, 1963, 686.
8. **Pless,** *Ann. Chem.*, 58, 38, 1845.
9. **Hubatka,** *Ann. Chem.*, 47, 153, 1840.
10. **Pless,** *Ann. Chem.*, 58, 38, 1845.
11. **Wertheim,** *Ann. Chem.*, 52, 52, 1840.
12. **Kooper,** *Chem. Zentralbl.*, 2, 331, 1910.
13. **Raquet,** *Chem. Zentralbl.*, 2, 457, 1912.
14. **Grimme,** *Chem. Zentralbl.*, 2, 613, 1912.
15. **Carles,** *Chem. Zentralbl.*, 2, 297, 1913.
16. **Imbert and Juillet,** *Chem. Zentralbl.*, 2, 1170, 1913.

	Allyl isovalerate	Allyl mercaptan
Other names		Allyl sulfhydrate Allylthiol 2-Propene-l-thiol
Empirical formula	$C_8H_{14}O_2$	C_3H_6S
Structure		$CH_2=CH-CH_2-SH$
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless liquid; tends to darken on aging
Molecular weight	142.19	74.14
Boiling point	89–90°C	67–68°C
Refractive index	1.4162 at 21°C	0.925 at 23°C
Solubility		Insoluble in water; completely miscible with alcohol and ether
Organoleptic characteristics	Fruit-like (apple, cherry) aroma	Strong, garlic odor
Synthesis	By direct esterification in the presence of benzene	
Natural occurrence	Not reported found in nature	In onion and garlic
Reported uses[3]	Non-alcoholic beverages 8.6 ppm Ice cream, ices, etc. 18 ppm Candy 22 ppm Baked goods 15–48 ppm Gelatins and puddings 1.0 ppm	Non-alcoholic beverages 0.25 ppm Ice cream, ices, etc. 0.50–2.0 ppm Candy 0.50 ppm Baked goods 0.50–2.0 ppm Chewing gum 2.0–3.0 ppm Condiments 0.50 ppm
Regulatory status	FDA 121.1164; FEMA No. 2045	FDA 121.1164; FEMA No. 2035

REFERENCES

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

	Allyl methyl disulfide	Allyl methyl trisulfide
Other names		Methyl allyl trisulfide
Empirical formula	$C_4H_8S_2$	$C_4H_8S_3$
Structure	$CH_2=CH-CH_2-S-S-CH_3$	$CH_2=CH-CH_2-S-S-S-CH_3$
Physical/chemical characteristics		
Molecular weight	120.23	152.30
Boiling point	30–33°C at 20 mm Hg	47°C at 0.8 mm Hg
Refractive index	n_D^{25} 1.5453	n_D^{21} 1.5930
Synthesis	By treating a mixture of corresponding aliphatic thiosulfates with an alkali metal sulfide[6]	
Natural occurrence	It occurs in *Allium sativum* (garlic), *Allium chinense*, and *Allium ampeloprasum*,[7] it is the main component of *Allium victorialis*[8]	It is a main volatile component of flavor of caucas (*Allium rictorialis*)
Reported uses[3]	Baked goods 1.0 ppm Condiments, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm	Baked goods 2.0 ppm Condiments, pickles 2.0 ppm Meat, meat sauces, soups 2.0 ppm
Regulatory status	FEMA No. 3127	FEMA No. 3253

REFERENCES

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

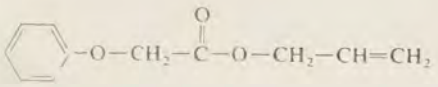
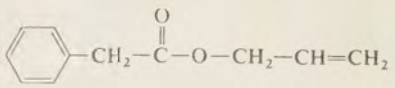
6. German Patent 2,020,051; *Chem. Abstr.*, 74, 86571z, 1971.
7. **Jacobsen, Bernhard and Mann.**, *Arch. Biochem. Biophys.*, 104(3), 473, 1964.
8. **Nishimura et al.**, *J. Agric. Food Chem.*, 19, 992, 1971.

	Allyl nonanoate	Allyl octanoate
Other names	Allyl pelargonate	Allyl caprylate Allyl octylate
Empirical formula	$C_{12}H_{22}O_2$	$C_{11}H_{20}O_2$
Structure	$CH_3-(CH_2)_7-\overset{\overset{O}{\|}}{C}-O-CH_2-CH=CH_2$	$CH_3-(CH_2)_6-\overset{\overset{O}{\|}}{C}-O-CH_2-CH=CH_2$
Physical/chemical characteristics[5]		
Appearance	Mobile liquid	Light, mobile liquid
Molecular weight	198.31	184.28
Boiling point	151°C at 50 mm Hg	87–88°C at 5.5 mm Hg
Specific gravity	0.8702 at 30°C	0.8729 at 30°C
Refractive index	1.4302 at 30°C	1.4271 at 30°C
Solubility		
Organoleptic characteristics	Characteristic fruital aroma (cognac, pineapple)	Fruit-like aroma
Synthesis	By esterification of nonanoic acid with allyl alcohol in benzene solution in the presence of naphthalene-β-sulfonic acid[6]	By esterification of caprylic acid with allyl alcohol in benzene in the presence of naphthalene-β-sulfonic acid[7]
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 0.70 ppm Ice cream, ices, etc. 0.50–3.0 ppm Candy 5.0 ppm Baked goods 3.0–5.0 ppm Meats 1.0 ppm	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 3.3 ppm Candy 5.1 ppm Baked goods 4.0 ppm Gelatins and puddings 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2036	FDA 121.1164; FEMA No. 2037

REFERENCES

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

6. Swern and Jordan, *J. Am. Chem. Soc.*, 70, 2337, 1948.
7. Swern and Jordan, *J. Am. Chem. Soc.*, 70, 2336, 1948.

	Allyl phenoxyacetate	Allyl phenylacetate
Other names	Acetate PA	Allyl α-toluate
Empirical formula	$C_{11}H_{12}O_3$	$C_{11}H_{12}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	192.22	176.22
Boiling point	100–102°C at 1 mm Hg	89–93°C at 3 mm Hg
Specific gravity		
Refractive index	1.5131 at 25.5°C	1.5122 at 13.5°C
Solubility		
Organoleptic characteristics	Honey and pineapple-like aroma	Honey-like aroma
Synthesis	By direct esterification in benzene solution	By direct esterification in benzene solution
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.82 ppm Ice cream, ices, etc. 0.004–40 ppm Candy 2.3 ppm Baked goods 0.02–1.0 ppm Gelatins and puddings 3.0 ppm	Non-alcoholic beverages 0.06–3.0 ppm Ice cream, ices, etc. 8.0 ppm Candy 14 ppm Baked goods 40 ppm
Regulatory status	FDA 121.1164; FEMA No. 2038	FDA 121.1154; FEMA No. 2039

REFERENCES

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

	Allyl propionate	Allyl sorbate
Other names		Allyl-2,4-hexadienoate
Empirical formula	$C_6H_{10}O_2$	$C_9H_{12}O_2$
Structure	$CH_3-CH_2-\overset{\overset{O}{\|}}{C}-O-CH_2-CH=CH_2$	$CH_3-CH=CH-CH=CH-\overset{\overset{O}{\|}}{C}-O-CH_2-CH=CH_2$
Physical/chemical characteristics[5]		
Appearance	Liquid	
Molecular weight	114.15	152.19
Boiling point	122–123°C (121°C)	
Specific gravity	0.9140 at 20°C	
Refractive index	1.4105 at 20°C; 1.4142 at 14°C	
Solubility		
Organoleptic characteristics	Fruital (apricot, apple) aroma	
Synthesis	By direct esterification of the acid with allyl alcohol in benzene solution in the presence of concentrated H_2SO_4[6] or of *p*-toluene sulfonic acid[7]	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.06–3.0 ppm Ice cream, ices, etc. 16 ppm Candy 6.5 ppm Baked goods 10 ppm	Non-alcoholic beverages 0.86 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50–5.0 ppm Baked goods 1.0 ppm Gelatins and puddings 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2040	FDA 121.1164; FEMA No. 2041

REFERENCES

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

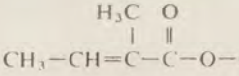
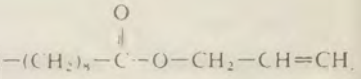
6. Jeffery and Vogel, *J. Chem. Soc.*, p. 663, 1948.
7. Salmi and Leimu, *Chem. Abstr.*, 42, 4031, 1948.

	Allyl sulfide	Allyl thiopropionate
Other names	Diallyl sulfide Thioallyl ether	Propionic acid, thioacrylic ester Thiopropionic acid, allyl ester
Empirical formula	$C_6H_{10}S$	$C_6H_{10}OS$
Structure	$CH_2=CH-CH_2-S-CH_2-CH=CH_2$	$CH_3-CH_2-\overset{\overset{S}{\|}}{C}-O-CH_2-CH=CH_2$
Physical/chemical characteristics		
Appearance	Colorless liquid	
Molecular weight	114.20	130.21
Boiling point	139°C	
Specific gravity	0.888 at 27°C	
Refractive index	1.4877 at 27°C	
Solubility	Insoluble in water; miscible with alcohol, ether, and other organic solvents	
Organoleptic characteristics	Characteristic garlic odor	
Synthesis	See *Beilstein* BI[2], 478, and also reference 6	
Natural occurrences	Identified in garlic and garlic extracts;[6] also identified in the leaves of *Diplotazis tenuifolia* and the roots of *Armoracia lapathifolia*. Allyl disulfide appears to be a secondary rather than primary natural product.	
Reported uses[3]	Non-alcoholic beverages 0.04 ppm Ice cream, ices, etc. 0.06 ppm Candy 0.07 ppm Baked goods 0.05 ppm Condiments 13 ppm Meats 3.7 ppm	Baked goods 0.25 ppm Condiments, pickles 0.25 ppm Meat, meat sauces, soups 0.25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2042	FEMA No. 3329

REFERENCES

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

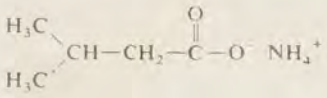
6. **Wertheim,** *Annalen,* 51, 289, 1844; 55, 297, 1845.

	Allyl tiglate	Allyl 10-undecenoate
Other names	Allyl-*trans*-2,3-dimethylacrylate Allyl-*trans*-2-methyl-2-butenoate	Allyl hendecenoate Allyl undecylenate Allyl undecylenoate
Empirical formula	$C_8H_{12}O_2$	$C_{14}H_{24}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Liquid
Molecular weight	140.18	224.34
Boiling point		180 C at 30 mm Hg; 114–118 C at 1 mm Hg
Specific gravity		0.8802 at 30 C; 0.935 at 15.5 C
Refractive index		1.4448 at 30 C; 1.4479 at 23 C
Solubility		Insoluble in water; miscible with most organic solvents
Organoleptic characteristics		Fruital aroma suggestive of pineapple
Synthesis		By azeotropic distillation of a benzene solution of the corresponding acid and allyl alcohol in the presence of naphthalene-β-sulfonic acid[6]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.28 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50–3.0 ppm Baked goods 0.50–3.0 ppm	Non-alcoholic beverages 0.25–1.0 ppm Ice cream, ices, etc. 0.50 ppm Candy 0.50 ppm Baked goods 0.50 ppm
Regulatory status	FDA 121.1164; FEMA No. 2043	FDA 121.1164; FEMA No. 2044

REFERENCES

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

6. Jordan and Swern, *J. Am. Chem. Soc.*, 71, 2378, 1949.

	Ammonium isovalerate	Ammonium sulfide
Other names	Isovaleric acid, ammonium salt	Ammonium monosulfide
Empirical formula	$C_5H_{13}O_2N$	H_8N_2S
Structure		$H_4N-S-NH_4$
Physical/chemical characteristics[5]		
Appearance	Deliquescent crystals	Liquid at room temperature (>−18°C, yellow crystals); tends to decompose at higher temperatures
Molecular weight	109	68.15
Solubility	Soluble in alcohol and in water	Very soluble in ammonia and in cold water; decomposes in hot water; soluble in alcohol
Organoleptic characteristics	Odor reminiscent of valeric acid; sharp, sweet taste; used in butter, nut, and cheese flavors	
Synthesis		
Natural occurrence		
Reported uses[3]	Baked goods 58 ppm Syrups 0.20 ppm	Baked goods 5.0 ppm Condiments 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2054	FDA 121.1164; FEMA No. 2053

REFERENCES

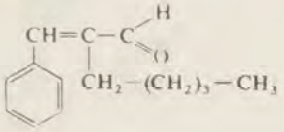
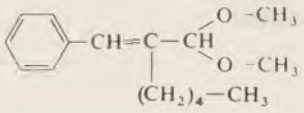
For References 1–5, see end of Part III.

	Amyl alcohol	Amyl butyrate
Other names	1-Pentanol Pentyl alcohol	Pentyl butyrate
Empirical formula	$C_5H_{12}O$	$C_9H_{18}O_2$
Structure	$CH_3-CH_2-CH_2-CH_2-CH_2OH$	$CH_3-(CH_2)_2-\overset{\overset{O}{\|\|}}{C}-O-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	88.15	158.24
Melting point	−73.85°C (−78.5°C)	
Boiling point	138.06°C (137.8–138°C)	185–186°C
Flash point	39°C	
Specific gravity	0.8144 at 20°C	0.8659 at 20°C
Refractive index	1.4113 at 20°C	1.4123 at 20°C
Solubility	1:5 in water at 30°C; miscible with most organic solvents	
Organoleptic characteristics	Characteristic fusel-like odor and burning taste; somewhat more toxic than ethyl alcohol	Strong, penetrating odor; sweet taste
Synthesis	By hydrogenation of valeric aldehyde with sodium amalgam; from amyl chloride	From *n*-amyl alcohol and butyric acid in the presence of H_2SO_4[7]
Natural occurrence	In the essential oils of Brazilian and American peppermint, Spanish "origanum", *Thymus marshallianus*, *Artemisia herba-alba*, *Eucalyptus cornuta*, *Eucalyptus aggregata*, oreganum, and cottonseed oil. It has been identified also among the constituents of bitter orange oil[6]	Found in several natural products
Reported uses[3]	Non-alcoholic beverages 18 ppm Ice cream, ices, etc. 15 ppm Candy 35 ppm Baked goods 24 ppm Gelatins and puddings 7.7–50 ppm Chewing gum 150–340 ppm	Non-alcoholic beverages 19 ppm Ice cream, ices, etc. 32 ppm Candy 76 ppm Baked goods 43 ppm Gelatins and puddings 0.50–1.4 ppm Chewing gum 760 ppm Syrups 58 ppm
Regulatory status	FDA 121.1164; FEMA No. 2056	FDA 121.1164; FEMA No. 2059

REFERENCES

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

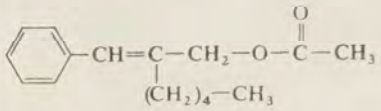
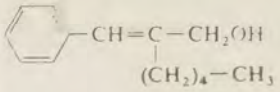
6. Mehlitz and Minas, *Ind. Obst. Gemueseverwert.*, 50, 861, 1965.
7. Vogel, *J. Chem. Soc.*, p. 629, 1948.

	α-Amylcinnamaldehyde	α-Amylcinnamaldehyde dimethyl acetal
Other names	Amyl cinnamic aldehyde α-Amyl-β-phenylacrolein 2-Benzylidene heptanal α-Pentylcinnamaldehyde	α-*n*-Amyl-β-phenylacroleindimethylacetal 1,1-Dimethoxy-2-amyl-3-phenyl-2-propene 1,1-Dimethoxy-2-benzylidene-heptane
Empirical formula	$C_{14}H_{18}O$	$C_{16}H_{24}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Yellowish, clear liquid	Yellowish liquid; stable
Assay	97% min	
Molecular weight	202.29	248.37
Melting point		
Boiling point	153–154°C at 10 mm Hg	
Flash point		92°C
Specific gravity	0.9715 at 15°C; 0.963–0.968 at 25°C	0.953–0.958 at 25°/25°C; 0.935 at 15.5°C
Refractive index	1.5552 (1.5540–1.5590) at 20°C	1.5050–1.5080 at 20°C; 1.5245 at 20°C
Acid value		1 max.
Solubility	1:6 in 80% ethanol; miscible with most organic solvents	1:9 in 80% alcohol; 1:2 in 90% alcohol
Organoleptic characteristics	Distinct floral (jasmine, lily) note	Floral note reminiscent of jasmine
Synthesis	By condensation of *n*-amyl aldehyde with cinnamic aldehyde. This method of condensation of aromatic aldehydes with aliphatic aldehydes has the maximum yield in α-amylcinnamic aldehyde with little formation of the inferior homologs. The methyl, ethyl, and propyl amylcinnamic aldehyde analogs exhibit a characteristic scent[6]	
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. 1.5 ppm Candy 4.0 ppm Baked goods 4.5 ppm Gelatins and puddings 0.03–0.05 ppm Chewing gum 15 ppm	Non-alcoholic beverages 0.80 ppm Ice cream, ices, etc. 1.5–2.0 ppm Candy 2.0 ppm Baked goods 2.6 ppm
Regulatory status	FDA 121.1164; FEMA No. 2061	FDA 121.1164; FEMA No. 2062

REFERENCES

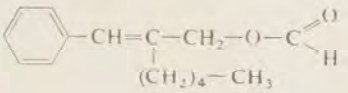
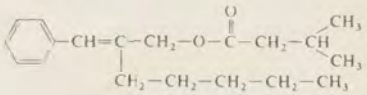
For References 1–5, see end of Part III.

6. **Bedoukian,** *Perfumery Synthetics and Isolates,* D. Van Nostrand, 1951, 43.

	α-Amylcinnamyl acetate	α-Amylcinnamyl alcohol
Other names	α-*n*-Amyl-β-phenylacryl acetate Floxin acetate α-Pentylcinnamyl acetate	*n*-Amyl cinnamic alcohol 2-Amyl-3-phenyl-2-propen-1-ol 2-Benzylidene-heptanol α-Pentylcinnamyl alcohol
Empirical formula	$C_{16}H_{22}O_2$	$C_{14}H_{20}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Yellowish liquid
Assay		95% min. (97%)
Molecular weight	246.36	204.31
Flash point		>100°C
Specific gravity	>1.0	0.954–0.962 at 25°C; 0.9675–0.9705 at 15°C
Refractive index		1.5330–1.5400 (1.5365–1.5385) at 20°C
Solubility	Soluble in alcohol	1:3 in 70% ethanol; miscible with water and ether
Organoleptic characteristics	Mild, fruity, green odor with a balsamic and slightly floral undernote; somewhat fruity flavor	Light, floral note
Synthesis	From amylcinnamic alcohol and acetic acid	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.92 ppm Ice cream, ices, etc. 3.5 ppm Candy 3.5 ppm Baked goods 3.0 ppm Chewing gum 3.0 ppm	Non-alcoholic beverages 0.47 ppm Ice cream, ices, etc. 1.5 ppm Candy 1.6 ppm Baked goods 1.5 ppm Chewing gum 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2064	FDA 121.1164; FEMA No. 2065

REFERENCES

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

	α-Amylcinnamyl formate	α-Amylcinnamyl isovalerate
Other names	α-*n*-Amyl-β-phenylacryl formate α-Pentylcinnamyl formate	α-*n*-Amyl-β-phenylacryl isovalerate Floxin isovalerate α-Pentylcinnamyl isovalerate
Empirical formula	$C_{15}H_{20}O_2$	$C_{19}H_{28}O_2$
Structure		
Physical, chemical characteristics[3]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	232.33	288.43
Solubility	Soluble in alcohol	Soluble in alcohol
Organoleptic characteristics	Sweet, oily, herbaceous, and somewhat green odor	Mild, fruity, somewhat tobacco-like odor; oily, fruity, hay-like, somewhat spicy flavor
Synthesis	By formylation of the alcohol	From amylcinnamic alcohol and isovaleric acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.17 ppm Ice cream, ices, etc. 0.93 ppm Candy 1.5 ppm Baked goods 1.5 ppm Chewing gum 1.0 ppm	Non-alcoholic beverages 0.36 ppm Ice cream, ices, etc. 1.2 ppm Candy 1.3 ppm Baked goods 1.7 ppm Chewing gum 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2066	FDA 121.1164; FEMA No. 2067

REFERENCES

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

	Amyl formate	Amyl heptanoate
Other names	Pentyl formate	Amyl heptoate Amyl heptylate Pentyl heptanoate
Empirical formula	$C_6H_{12}O_2$	$C_{12}H_{24}O_2$
Structure	$CH_3-(CH_2)_4-O-\overset{\overset{O}{\|}}{C}-H$	$CH_3-(CH_2)_5-\overset{\overset{O}{\|}}{C}-O-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	116.16	200.32
Melting point	−73.5 C	−49.5 C (from pentane)
Boiling point	130.4 C	245.4 C (240 C)
Specific gravity	0.8846 at 20 C, 1.8926 at 15 C	0.85427 at 20 C; 0.882 at 15.5 C
Refractive index	1.3997 at 20 C; 1.3951 at 11.5 C	1.42627 (1.4240) at 20 C
Solubility	Very slightly soluble in water; miscible with alcohol, ether, and other organic solvents	Soluble in most organic solvents
Organoleptic characteristics	Fruit-like aroma	Characteristic, strong, ethereal, fruital (unripe banana) odor and corresponding taste
Synthesis	From *n*-amyl alcohol and formic acid in the presence of H_2SO_4[6]	From the corresponding heptanoic acid and *n*-amyl alcohol in the presence of mineral acids[7] or in benzene solution in the presence of *p*-toluene sulfonic acid[8]
Natural occurrence	Identified as a constituent of *Pyrus malus*	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 13 ppm Ice cream, ices, etc. 11 ppm Candy 31 ppm Baked goods 8.0 ppm Chewing gum 170 ppm	Non-alcoholic beverages 7.0 ppm Ice cream, ices, etc. 3.8 ppm Candy 7.5 ppm Baked goods 3.0 ppm Gelatins and puddings 3.5 ppm Chewing gum 53 ppm
Regulatory status	FDA 121.1164; FEMA No. 2068	FDA 121.1164; FEMA No. 2073

REFERENCES

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

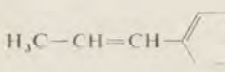
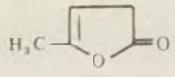
6. **Kohlraush and Pongratz,** *Z. Phys. Chem. Abt. B.*, 22, 379, 1933.
7. **Gartenmeister,** *Justus Liebigs Ann. Chem.*, 233, 284, 1886; Bilterys and Gisseleire, *Bull. Soc. Chem. Belg.*, 44, 569, 572, 1935.
8. **Hoback, Parsons and Bartlett,** *J. Am. Chem. Soc.*, 65, 1606, 1943.

	Amyl hexanoate	Amyl octanoate
Other names	Amyl caproate Amyl hexylate Pentyl hexanoate	Amyl caprylate Amyl octylate Pentyl octanoate
Empirical formula	$C_{11}H_{22}O_2$	$C_{13}H_{26}O_2$
Structure	$CH_3-(CH_2)_4-\overset{\overset{O}{\|}}{C}-O-(CH_2)_4-CH_3$	$CH_3-(CH_2)_6-\overset{\overset{O}{\|}}{C}-O-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid
Molecular weight	186.30	214.35
Melting point	−47°C	−34 to −35°C
Boiling point	226°C (116°C at 20 mm Hg)	260°C (124–216°C at 12 mm Hg)
Specific gravity	0.8612 at 25°C	0.8562 at 25°C
Refractive index	1.4202 at 25°C	1.4262 at 25°C
Solubility		
Organoleptic characteristics	Characteristic fruit-like (banana, pineapple) aroma	Odor suggestive of orris
Synthesis	By esterification of hexanoic acid with *n*-amyl alcohol in benzene solution in the presence of *p*-toluenesulfonic acid[6]	By esterification of octanoic acid with *n*-amyl alcohol in benzene solution in the presence of *p*-toluenesulfonic acid[6]
Natural occurrence	Occurs in several natural products	In strawberry and apple
Reported uses[3]	Non-alcoholic beverages 5.3 ppm Ice cream, ices, etc. 16 ppm Candy 22 ppm Baked goods 8.3 ppm Gelatins and puddings 0.30–3.7 ppm Chewing gum 110 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 3.5 ppm Candy 6.0 ppm Baked goods 3.5 ppm Gelatins and puddings 2.1 ppm
Regulatory status	FDA 121.1164; FEMA No. 2074	FDA 121.1164; FEMA No. 2079

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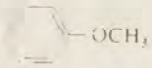
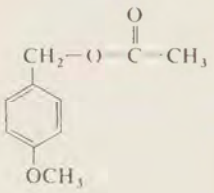
For References 1–5, see end of Part III.

6. Hoback, Parsons and Bartlett, *J. Am. Chem. Soc.*, 65,1606, 1943.

	Anethole	α-Angelica lactone
Other names	Isoestragole 1-Methoxy-4-propenyl benzene *p*-Methoxypropenyl benzene *p*-Propenyl anisole *p*-Propenylphenyl methyl ether	4-Hydroxy-3-pentenoic acid lactone β, γ-Angelica lactone γ-Angelica lactone 5-Methyl-2 (3H)-furanone γ-Methyl-β-butenolide
Empirical formula	$C_{10}H_{12}O$	$C_5H_6O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White, crystalline solid; melts at room temperature	Needle-like crystals; readily isomerizes to the beta form
Molecular weight	148.20	98.10
Melting point	20–23°C	18°C
Boiling point	234–237°C	167–170°C 56°C at 12 mm Hg
Specific gravity	0.983–0.987 at 25°C	1.084 at 20°C
Refractive index	1.558–1.561 at 25°C	1.4476 at 20°C
Solubility	1:8 in 80% alcohol; 1:1 in 90% ethanol; almost water insoluble; miscible with chloroform and ether	Slightly soluble in water; soluble in alcohol, ether, and carbon disulfide
Organoleptic characteristics	Characteristic anise odor and corresponding sweet taste	Sweet, herbaceous odor reminiscent of tobacco
Synthesis	By esterification of *p*-cresol with methyl alcohol and subsequent condensation with acetaldehyde (Perkins). The most common method of preparation is from pine oil. By fractional distillation of the essential oils of anise, star anise, and fennel. The anise essences contain an average of 85% anethole; fennel, from 60 to 70%.	By dry distillation of levulinic acid[6]
Natural occurrence	In addition to the mentioned oils, it is also present in the oil of *Illicium anisatum* L., in the oil from leaves of *Piper peltatum* Sur., in the roots of *Osmorrhiza longistylis* Eberh., in the oils of common fennel and basil, and in the oils from leaves of *Clausena anisata* Hook., *Backhousia anisata*, and *Magnolia salicifolia*.	
Reported uses[3]	Non-alcoholic beverages 11 ppm Alcoholic beverages 1,400 ppm Ice cream, ices, etc. 26 ppm Candy 340 ppm Baked goods 150 ppm Chewing gum 1,500 ppm	Ice cream, ices, etc. 0.2 ppm Candy 2.0 ppm Baked goods 4.0 ppm Gelatins and puddings 2.0 ppm Meats 2.0 ppm Milk, dairy products 0.2 ppm Cereals 2.0 ppm
Regulatory status	FDA GRAS; FEMA No. 2086	FEMA No. 3293

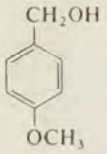
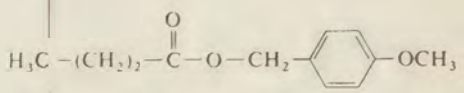
REFERENCES

For References 1–5, see end of Part III.
6. Wolff, *Annalen*, 229, 250, 1885.

	Anisole	Anisyl acetate
Other names	Methoxybenzene Methyl phenyl ether	*p*-Methoxybenzyl acetate
Empirical formula	C_7H_8O	$C_{10}H_{12}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to slightly yellow liquid
Assay		97% min.[2]
Molecular weight	108.13	180.21
Melting point	37–38°C	270°C
Boiling point	155°C	
Flash point	42°C	
Specific gravity	0.999 (0.9980–1.0010) at 15°C	1.104 1.107[2] at 25°/25°C; 1.014 at 20°C
Refractive index	1.5179 (1.5165–1.5175) at 20°C	1.5110–1.5160[2] at 20°C; 1.515 at 15°C
Acid value		Not more than 1.0[2]
Solubility	Insoluble in water; soluble in alcohol and ether	1:6 in 60% alcohol; insoluble in water
Organoleptic characteristics	Characteristic, pleasant aromatic odor	Floral fruit-like odor; a slight pungent, sweet taste
Synthesis	By reacting phenol and dimethyl sulfate in the presence of aqueous NaOH; by passing methyl chloride into a suspension of sodium phenolate in liquid ammonia	May be prepared by the reaction of anisic alcohol with acetic anhydride
Natural occurrence	Identified in the oil of *Artemisia dracunculus* var. *turkestanica*	In currants
Reported uses[3]	Non-alcoholic beverages 9.0 ppm Ice cream, ices, etc. 16 ppm Candy 51 ppm Baked goods 34 ppm	Non-alcoholic beverages 6.3 ppm Ice cream, ices, etc. 8.0 ppm Candy 15 ppm Baked goods 12 ppm Gelatins and puddings 11 ppm Chewing gum 30 ppm
Regulatory status	FDA 121.1164; FEMA No. 2097	FDA 121.1164; FEMA No. 2098

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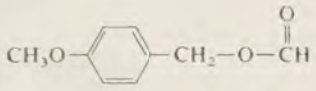
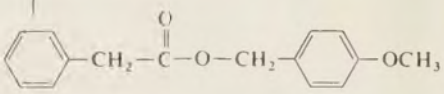
For References 1–5, see end of Part III.

	Anisyl alcohol	Anisyl butyrate
Other names	Anisic alcohol *p*-Methoxybenzyl alcohol	*p*-Methoxybenzyl butyrate
Empirical formula	$C_8H_{10}O_2$	$C_{12}H_{16}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow liquid	Colorless liquid
Assay	97% min.[2]	
Molecular weight	138.16	208.26
Melting point	23.8°C (25–27°C)	Approx. 270°C
Boiling point	259°C (145°C at 18 mm Hg)	
Freezing point	>23.5°C	
Specific gravity	1.110–1.115[2] (1.110–1.125) at 25°/25°C	
Refractive index	1.5430–1.5450[2] (1.5412–1.5430) at 25°C	
Acid value	Not more than 1.0[2]	
Aldehyde content	Not more than 1.0%[2]	
Solubility	1:1 in 50% alcohol; 1:13 in 30% alcohol; soluble in most organic solvents	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Floral odor; sweet, fruity (peach) taste	Weak, floral, intensely sweet, plum-like odor
Synthesis	By reduction from anisic aldehyde	From anisyl alcohol and *n*-butyric acid
Natural occurrence	Reported found in vanilla pods (Tahitian production) and anise seed oil[6]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 7.4 ppm Ice cream, ices, etc. 8.0 ppm Candy 11 ppm Baked goods 12 ppm Gelatins and puddings 1.9 ppm	Non-alcoholic beverages 3.1 ppm Ice cream, ices, etc. 5.7 ppm Candy 10 ppm Baked goods 13 ppm
Regulatory status	FDA 121.1164; FEMA No. 2099	FDA 121.1164; FEMA No. 2100

REFERENCES

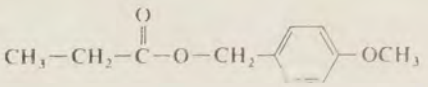
For References 1–5, see end of Part III.

6. Monod et al., *Chem. Abstr.*, 45, 3124, 1951.

	Anisyl formate	Anisyl phenylacetate
Other names	*p*-Methoxybenzyl formate	Anisyl α-toluate
Empirical formula	$C_9H_{10}O_3$	$C_{16}H_{16}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Assay	90% min	
Molecular weight	166.18	256.30
Boiling point	100°C	370°C
Specific gravity	0.138–0.142 at 25°C	
Refractive index	1.5220–1.5240 at 20°C	
Acid Value	3 max	
Solubility	Insoluble in water; soluble in most organic solvents; 1:3 in 70% alcohol	Soluble in alcohol
Organoleptic characteristics	Sweet, floral odor; fruity (strawberry) taste. The floral note varies, depending on whether synthetic or natural anisic alcohol has been used (probably because of the purity of the starting alcohol).	Anise and honey-like odor
Synthesis	By direct esterification of anisic alcohol with formic acid	From anisyl alcohol and phenylacetic acid by direct esterification
Natural occurrence	Reported in *Vanilla fragrans* and *Ribes* species	
Reported uses[3]	Non-alcoholic beverages 3.2 ppm Ice cream, ices, etc. 3.9 ppm Candy 7.9 ppm Baked goods 14 ppm Gelatins and puddings 0.20 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2101	FDA 121.1164

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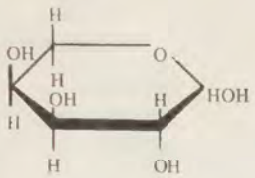
For References 1–5, see end of Part III.

	Anisyl propionate	Arabinogalactan
Other names	*p*-Methoxybenzyl propionate	Larch gum
Empirical formula	$C_{11}H_{14}O_3$	$[(C_5H_8O_4)(C_6H_{10}O_5)_6]_n$
Structure		$\left[(C_5H_8O_4)(C_6H_{10}O_5)_6\right]_n$
Physical/chemical characteristics[5]		
Appearance		Complex polysaccharide containing *d*-galactose and *l*-arabinose in the approximate ratio of 6:1
Molecular weight	194.23	
Boiling point	277°C (100–103°C at 0.5 mm Hg)	
Specific gravity	1.078 at 15.5°C	
Refractive index	1.5490 at 20°C; 1.5112 at 15°C	
Solubility		Soluble in water
Organoleptic characteristics	Herbaceous odor; fruity (cherry, peach) taste	
Synthesis	By esterification of anisic alcohol with propionic anhydride	From larch wood, white pine, Monterrey pine, and Jack pine[6]
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 5.6 ppm Ice cream, ices, etc. 6.1 ppm Candy 16 ppm Baked goods 20 ppm Gelatins and puddings 0.25 ppm	Candy, 85%
Regulatory status	FDA 121.1164; FEMA No. 2102	FEMA No. 3254

REFERENCES

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

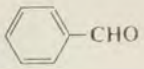
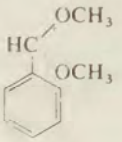
6. **Whistler,** in *Methods in Carbohydrate Chemistry,* Vol. 5, Whistler, R. L. and Wolfrom, M. L., Eds., Academic Press, New York, 1965, 75.

	L-Arabinose	Beechwood creosote
Other names	Pectin sugar	Wood creosote
Empirical formula	$C_5H_{10}O_5$	
Structure		A mixture of phenols (chiefly guaiacol, creosol, and *p*-cresol)
Physical/chemical characteristics[5]		
Appearance	Rhombic prisms	Colorless or yellowish oily liquid
Molecular weight	150.13	
Melting point	159.5°C	
Boiling point		200–220°C
Congealing point		Approx. −20°C
Specific gravity	α-, 1.585 at 20°C β-, 1.625 at 20°C	1.076–1.09 at 25°C
Optical rotation	+105° at 20°C (c = 3 in water)	
Solubility	Very soluble in water; slightly soluble in alcohol; insoluble in ether.	Insoluble in water; soluble in glycerol, glacial acetic acid, and alkali hydroxide solutions; miscible with alcohol, chloroform, and ether
Organoleptic characteristics		Characteristic smoky odor; caustic, burning taste
Synthesis	By partial hydrolysis of mesquite gum[6]	Starting materials are the heavy oils from wood tar. The material first is treated with NaOH to precipitate all saponifiable oils and subsequently with H_2SO_4. The raw creosote finally is purified by repeated fractional distillation.[7]
Reported uses[3]	Non-alcoholic beverages 450.0 ppm Candy 450.0 ppm Baked goods 450.0 ppm Condiments, pickles 450.0 ppm Preserves and spreads 450.0 ppm	
Regulatory status	FEMA No. 3255	FDA 121.1164

REFERENCES

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

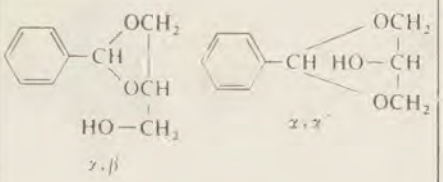
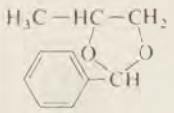
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	Benzaldehyde	Benzaldehyde dimethyl acetal
Other names	Benzenecarbonal Benzenemethylal Benzoic aldehyde	Dimethoxy-(phenyl)-methane α,α-Dimethoxy toluene
Empirical formula	C_7H_6O	$C_9H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid
Assay	98% min	
Molecular weight	106.12	152.19
Melting point	−26°C	
Boiling point	179°C	198°C (207°C)
Flash point	62°C	
Specific gravity	1.0500 at 15°C; 1.041–1.046 at 25°C	1.025 at 15.5°C
Refractive index	1.5450 (1.5440–1.5465) at 20°C	1.4950 at 20°C
Optical rotation	±0°	
Solubility	Miscible with alcohol and ether; 1:1–1:1.5 in 70% alcohol; 1:2.5 in 60% alcohol; 1:8 in 50% alcohol; 1:300 in water	
Organoleptic characteristics	Characteristic odor and aromatic taste similar to bitter almond	Floral note; also reminiscent of almond
Synthesis	By extraction and subsequent fractional distillation from botanical sources; synthetically, from benzyl chloride and lime or by oxidation of toluene	From benzaldehyde and methanol in the presence of calcium chloride and HCl;[7] from benzaldehyde and tetramethylorthosilicate in the presence of anhydrous HCl in methanol[8]
Natural occurrence	Present as cyanuric glucoside (amygdalin) in bitter almond, peach, apricot kernel, and other *Prunus* species. Amygdalin is also present in various parts of the following plants: *Sambucus nigra, Chrysophyllum arten, Anacyclus officinarum, Anacyclus pedunculatus, Davallia brasiliensis, Lacuma deliciosa, Lacuma multiflora*, and others. Free benzaldehyde has been reported found in several essential oils: hyacinth, citronella, orris, cinnamon, sassafras, labdanum, and patchouli.[6]	In potato
Reported uses[3]	Non-alcoholic beverages 36 ppm Alcoholic beverages 50–60 ppm Ice cream, ices, etc. 42 ppm Candy 120 ppm Baked goods 110 ppm Gelatins and puddings 160 ppm Chewing gum 840 ppm	Non-alcoholic beverages 26 ppm Alcoholic beverages 60 ppm Ice cream, ices, etc. 22 ppm Candy 56 ppm Baked goods 45 ppm Gelatins and puddings 50 ppm
Regulatory status	FDA GRAS; FEMA No. 2127	FDA 121.1164; FEMA No. 2128

REFERENCES

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

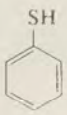
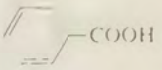
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7. Adams and Adkins, *J. Am. Chem. Soc.*, 47, 1365, 1925.
8. Helferich and Hansen, *Ber. Dtsch. Chem. Ges.*, 57, 797, 1924.

	Benzaldehyde glyceryl acetal	Benzaldehyde propylene glycol acetal
Other names	Phenyl-*m*-dioxan-5-ol (α,α') 2-Phenyl-1,3-dioxan-5-ol (α,α')	4-Methyl-2-phenyl-*m*-dioxolane
Empirical formula	$C_{10}H_{12}O_3$	$C_{10}H_{12}O_2$
Structure	 γ,β α,α'	
Physical/chemical characteristics[5]		
Appearance	α,α', solid α,β, oily liquid	
Molecular weight	180.21	164.21
Melting point	α,α'(*cis*), 63.5–64.5°C α,α' (*trans*), 83–84°C	
Boiling point	α,α', 185°C at 20 mm Hg α,β, 143–144°C at 2 mm Hg	
Specific gravity	α,β, 1.1916 at 17°C	
Refractive index	α,β, 1.5389 at 17°C	
Solubility	α,α', slightly soluble in a ligroin-benzene mixture at room temperature; α,β, soluble in a ligroin-benzene mixture at room temperature	
Organoleptic characteristics		
Synthesis	The α,α'- and α,β-isomers are obtained in mixture by heating glycerol and benzaldehyde to 145–170°C under a stream of CO_2.[6,7] The isomers are subsequently isolated, exploiting the solubility differences. The α,α'-isomer is readily converted to the α,β-form by heating in the presence of HCl.	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 21 ppm Ice cream, ices, etc. 24 ppm Candy 110 ppm Baked goods 73 ppm Gelatins and puddings 100 ppm Chewing gum 840 ppm	Non-alcoholic beverages 34 ppm Ice cream, ices, etc. 27 ppm Candy 110 ppm Baked goods 96 ppm Gelatins and puddings 50 ppm
Regulatory status	FDA 121.1164; FEMA No. 2129	FDA 121.1164; FEMA No. 2130

REFERENCES

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

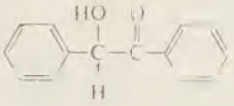
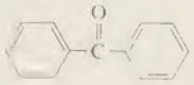
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7. **Verkade and Van Roon,** *Recl. Trav. Chim. Pays-Bas*, 61, 834, 1942.

	Benzenethiol	Benzoic acid
Other names	Phenyl mercaptan Thiophenol	Benzenecarboxylic acid Dracylic acid Phenylformic acid
Empirical formula	C_6H_6S	$C_7H_6O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Prism-like crystals from ligroin	Flexible, shiny plates or monoclinic needles
Molecular weight	110.04	122.12
Melting point	70°C	121–123 C (U.S.P.)
Boiling point	169.5 C	249 C 249–250 C
Specific gravity	1.0728 at 25°C	1.265 at 15.5 C
Refractive index	1.5931 at 14°C	
Solubility	Insoluble in water; slightly soluble in alcohol, ether, and benzene	1:380 in cold water; 1:15 in hot water; 1:2.5 in 90% alcohol; 1:10 in glycerol
Organoleptic characteristics	Repulsive, penetrating, garlic-like odor	Almost odorless or exhibiting a faint balsamic odor and a sweet-sour to acrid taste
Synthesis	By reduction of benzenesulfonyl chloride with zinc dust in sulfuric acid[6]	By oxidation of toluene with nitric acid or sodium bichromate or from benzonitrile
Natural occurrence	Not reported found in nature	Reported as being a constituent of various oils, resins, and flower absolutes: hyacinth, tuberose, neroli bigarade, Chinese cinnamon, cinnamon leaves, anise, vetiver, ylang-ylang, Tolu balsam, and clove. It is contained in fairly sizable amounts in gum benzoin, from which benzoic acid is extracted by sublimation.
Reported uses[3]		Non-alcoholic beverages 7.5 ppm Ice cream, ices, etc. 4.8 ppm Candy 8.9 ppm Baked goods 40 ppm Chewing gum 20–32 ppm Icings 250 ppm Used chiefly as a preservative at 0.1%; as a flavor ingredient it is used at ppm levels
Regulatory status	FDA 121.1164	FDA GRAS (0.1% preservative); FEMA No. 2131

REFERENCES

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

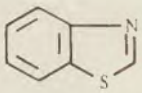
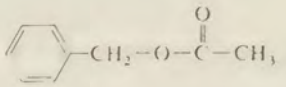
6. Adams and Marvel, *Org. Synth.*, 1, 71, 1921.

	Benzoin	Benzophenone
Other names	Benzoyl phenylcarbinol 2-Hydroxy-2-phenylacetophenone	Benzoyl benzene Diphenyl ketone
Empirical formula	$C_{14}H_{12}O_2$	$C_{13}H_{10}O$
Structure		
Physical/chemical characteristics[4]		
Appearance	Monoclinic prisms or needles	White, crystalline material
Molecular weight	212.22	182.21
Melting point	132–137 C	48.5 C
Boiling point		170 C at 15 mm Hg
Congealing point		47.0 C[2]
Specific gravity		1.0496 at 95 C
Refractive index		1.5893 at 45.2 C
Solubility	Soluble in acetone and boiling alcohol	1:10 in 80% alcohol;[2] insoluble in water; soluble in alcohol, ether, and acetic acid
Organoleptic characteristics		Delicate, persistent, rose-like odor
Synthesis	By treating an alcoholic solution of benzaldehyde with an alkali cyanide[6,7]	By Friedel-Craft condensation of benzene with benzoyl chloride in the presence of aluminum chloride[8]
Natural occurrence	Not reported found in nature	In grapes
Reported uses[3]	Non-alcoholic beverages 4.5 ppm Ice cream, ices, etc. 0.54 ppm Candy 2.0 ppm Baked goods 1.4 ppm Gelatins and puddings 0.10 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 0.61 ppm Candy 1.7 ppm Baked goods 2.4 ppm
Regulatory status	FDA 121.1164; FEMA No. 2132	FDA 121.1164; FEMA No. 2134

REFERENCES

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

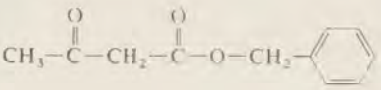
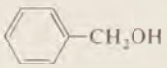
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7. Arnold and Fuson, *J. Am. Chem. Soc.*, 58, 1295, 1936.
8. Marvel and Sperry, *Org. Synth.*, 8, 26, 1928.

	Benzothiazole	Benzyl acetate
Empirical formula	C_7H_5NS	$C_9H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless liquid
Assay		98% min[2] (as benzyl acetate)
Molecular weight	135.19	150.18
Melting point	2°C	
Boiling point	223–225°C (234°C) 131°C at 34 mm Hg	215.5–216.0 C (71 C at 3 mm Hg)
Flash point		93 C
Specific gravity	1.2460 at 20°C	1.052–1.056 at 25 /25 C[2]
Refractive index	1.6379 at 20°C	1.5010–1.5030 at 20 C[2]
Optical rotation		±0
Acid value		Not more than 1.0
Solubility	Soluble in alcohol, acetone, and carbon disulfide; very slightly soluble in water	1:5 in 60% alcohol; 1:200 in 30% alcohol; slightly soluble in water; soluble in most organic solvents
Organoleptic characteristics	Odor similar to that of quinoline	Characteristic flowery (jasmine) odor; bitter, pungent taste
Synthesis	By refluxing a mixture of zinc *o*-aminophenylsulfide and formic acid, followed by steam distillation of the alkalized reaction mixture;[6] by heating formanilid or dimethylaniline with sulfur;[7] by oxidation of 2-mercaptobenzothiazole or of the corresponding disulfide[8]	By interaction of benzyl chloride and sodium acetate;[9] by acetylation of benzyl alcohol; or from benzaldehyde and acetic acid with zinc dust[10]
Natural occurrence		Present as a main constituent in several oils and flower absolutes: ylang-ylang, cananga, neroli, jasmine, hyacinth, gardenia, tuberose. It has been isolated in the essential oil from flowers of *Loiseleuria procumbens* Desv. (azalea).[11] Benzyl acetate can be isolated from natural sources (in which it may occur at levels up to 65%), but the commercial product is of synthetic origin.
Reported uses[3]	Non-alcoholic beverages 0.5 ppm Candy 0.5 ppm Baked goods 0.5 ppm Meat, meat sauces, soups 0.5 ppm Milk, dairy products 0.5 ppm	Non-alcoholic beverages 7.8 ppm Ice cream, ices, etc. 14 ppm Candy 34 ppm Baked goods 22 ppm Gelatins and puddings 23 ppm Chewing gum 760 ppm
Regulatory status	FEMA No. 3256	FDA 121.1164; FEMA No. 2135

REFERENCES

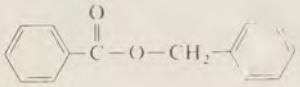
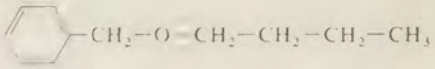
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9. Seelig, *J. Prakt. Chem.*, 39, 162, 1899.
10. Tiemann, *Berl. Ber.*, 19, 355, 1866.
11. Salgues, *C. R. Séances Acad. Sci.* (Paris), 240, 1136, 1955.

	Benzyl acetoacetate	Benzyl alcohol
Other names	Benzyl acetyl acetate Benzyl β-ketobutyrate Benzyl 3-oxobutanoate	α-Hydroxy toluene Phenyl carbinol Phenyl methanol
Empirical formula	$C_{11}H_{12}O_3$	C_7H_8O
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	Colorless liquid
Molecular weight	192.22	108.13
Melting point	Approx. 270 C (162–164 C at 16 mm Hg)	−15.3°C
Boiling point		205.45°C (202.5–206.5°C)
Specific gravity		1.04927 at 15 C; 1.041–1.046 at 25°C
Refractive index		1.54259 at 15 C; 1.5385–1.5405 at 20°C
Solubility	Soluble in alkali solutions at room temperature	Soluble 1:25 in water and most organic solvents; 1:8–9 in 30% alcohol; 1:1.5 in 50% alcohol
Organoleptic characteristics	Odor similar to that of ethyl acetate	Characteristic pleasant, fruity odor; slightly pungent, sweet taste. The note tends to become similar to that of benzyl aldehyde on aging.
Synthesis	By heating ethyl acetoacetate and benzyl alcohol to 160 C	By saponification of the ester present in Tolu and Peru balsams. Synthetically, it is obtained from benzyl chloride by the action of sodium or potassium carbonate.
Natural occurrence		The free alcohol is often present in several essential oils and extracts of: jasmine, tobacco, tea, neroli, copaiba, *Acacia farnesiana* Willd., *Acacia cavenia* Hook. and Arn., *Robinia pseudacacia*, ylang-ylang, *Pandanus odoratissimus*, *Michelia champaca*, *Prunus laurocerasus*, tuberose, orris, castoreum, violet leaves, clove buds, and others.
Reported uses[3]	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 6.0 ppm Candy 13 ppm Baked goods 13 ppm Gelatins and puddings 0.50–10 ppm Chewing gum 50 ppm	Non-alcoholic beverages 15 ppm Ice cream, ices, etc. 160 ppm Candy 47 ppm Baked goods 220 ppm Gelatins and puddings 21–45 ppm Chewing gum 1,200 ppm
Regulatory status	FDA 121.1164; FEMA No. 2136	FDA 121.1164; FEMA No. 2137

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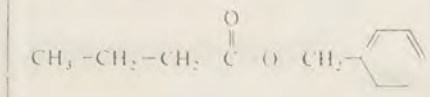
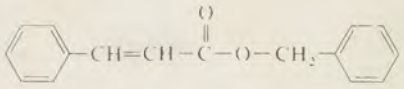
For References 1–5, see end of Part III.

	Benzyl benzoate	Benzyl butyl ether
Other names	Benzyl benzene carboxylate Benzyl phenylformate	Butyl benzyl ether
Empirical formula	$C_{14}H_{12}O_2$	$C_{11}H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Leaflets or oily liquid	Colorless liquid
Assay	98% min	
Molecular weight	212.24	164.25
Melting point	18–19°C	
Boiling point	324°C (170–171°C at 11 mm Hg)	220–221°C at 744 mm Hg
Congealing point	18°C	
Flash point	148°C	
Specific gravity	1.116–1.120 (1.1121) at 25/25°C	0.931 at 10°C
Refractive index	1.568–1.570 at 20°C; 1.5685 at 21.5°C	
Solubility	Insoluble in water or glycerol; soluble in alcohol, chloroform, and ether; 1:2 in 90% alcohol	Insoluble in water; miscible with alcohol and ether
Organoleptic characteristics	Light, balsamic odor reminiscent of almond; sharp, pungent taste	
Synthesis	By the dry esterification of sodium benzoate and benzoyl chloride in the presence of triethylamine[6] or by reaction of sodium benzylate on benzaldehyde[7]	Obtained in mixture by heating benzyl alcohol and butyl alcohol in the presence of sulfuric acid or sodium bisulfate[15,16]
Natural occurrence	Contained in Peru balsam[8] and in the concrete and absolute of tuberose flowers,[9] hyacinth,[10] *Narcissus jonquilla* L.,[11] and *Dianthus caryophillus* L.;[12] also in the oil of ylang-ylang and in Tolu balsam[13,14]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 4.5 ppm Ice cream, ices, etc. 12 ppm Candy 39 ppm Baked goods 33 ppm Chewing gum 280 ppm	Non-alcoholic beverages 0.50–2.0 ppm Ice cream, ices, etc. 3.5 ppm Candy 8.0 ppm Baked goods 2.0–8.0 ppm Gelatins and puddings 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2138	FDA 121.1164; FEMA No. 2139

REFERENCES

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

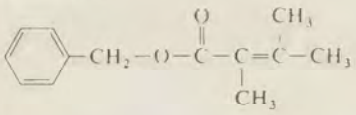
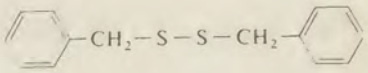
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10. Euklaar, *Chem. Weekbl.*, 7, 11, 1910.
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12. Treff and Wittrish, *J. Prakt. Chem.*, 122, 139, 1929.
13. Van Itallie and Harsma, *Pharm. Weekbl.*, 62, 898, 1926.
14. Van Itallie and Harsma, *Chem. Zentralbl.*, 1, 167, 1926.
15. Senderens, *Compt. Rend.*, 178, 1415, 1924.
16. Senderens, *Compt. Rend.*, 188, 1075, 1929.

	Benzyl butyrate	Benzyl cinnamate
Other names	Benzyl butanoate	Benzyl β-phenylacrylate Benzyl-3-phenylpropenoate Cinnamein
Empirical formula	$C_{11}H_{14}O_2$	$C_{16}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	White to pale-yellow, fused, crystalline solid, melting at room temperature to a yellowish liquid
Assay	98% min	99% min[2]
Molecular weight	178.23	238.29
Melting point		*trans*, 35–36 C;[8] *cis*, 30 C[9]
Boiling point	235–242 C (130–132 C at 15 mm Hg)	228–230 C at 22 mm Hg
Congealing point		33.0–34.5 C[2]
Flash point	>100 C	>100 C
Specific gravity	1.006–1.009 at 25/25 C;[2] 1.014 at 19 C	1.109 at 15 C
Refractive index	1.4920–1.4960 at 20 C[2]	
Acid value	Not more than 1.0[2]	Not more than 1.0[2]
Solubility	Insoluble in water; miscible with alcohol and ether	1:8 in 90% alcohol
Organoleptic characteristics	Characteristic fruity (apricot) odor; sweet, pear-like taste	Sweet, balsamic odor; honey-like taste
Synthesis	By heating benzyl chloride and sodium butyrate in water[6] or butyric acid and benzyl chloride under pressure[7]	Usually prepared by esterification of benzyl alcohol and cinnamic acid[2] By heating benzyl chloride and excess sodium cinnamate in water to 110–115 C;[10] by heating sodium cinnamate with an excess of benzyl chloride in the presence of diethylamine[11]
Natural occurrence	In passion fruit	Reported found in Peru[12] and Tolu[13] balsam, in Sumatra and Penang benzoin,[14] and as the main constituent of copaiba balsam[15]
Reported uses[3]	Non-alcoholic beverages 4.5 ppm Ice cream, ices, etc. 6.9 ppm Candy 7.7 ppm Baked goods 9.9 ppm Gelatins and puddings 3.0 ppm Chewing gum 310 ppm	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 2.5 ppm Candy 6.7 ppm Baked goods 6.6 ppm Gelatins and puddings 3.0–5.0 ppm Chewing gum 5.3–120 ppm
Regulatory status	FDA 121.1164; FEMA No. 2140	FDA 121.1164; FEMA No. 2142

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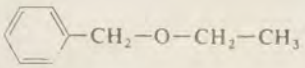
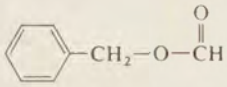
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10. Gomberg and Buchler, *J. Am. Chem. Soc.*, 42, 2065, 1920.
11. Volwiler and Vliet, *J. Am. Chem. Soc.*, 43, 1674, 1921.
12. Tschirch and Trog, *Arch. Pharm.*, 232, 91, 1894.
13. Tschirch and Oberländer, *Arch. Pharm.*, 232, 559, 1894.
14. Tschirch and Ludy, *Arch. Pharm.*, 231, 43, 1893.
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	Benzyl 2,3-dimethylcrotonate	Benzyl disulfide
Other names	Benzyl 2,3-dimethyl-2-butenoate Benzyl methyl tiglate	Dibenzyl disulfide
Empirical formula	$C_{13}H_{16}O_2$	$C_{14}H_{14}S_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Pale-yellow leaflets (from alcohol)
Molecular weight	204.27	246.40
Melting point		71–72°C (74°C)
Boiling point		>270°C (with decomposition)
Solubility		Almost insoluble in water; soluble in hot alcohol and ether
Organoleptic characteristics		Powerful, burnt-caramel odor; irritating when concentrated
Synthesis		From benzyl chloride and Na_2S_2; also from benzyl mercaptan via oxidation
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. 2.8 ppm Candy 1.8 ppm Baked goods 1.5 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2143	FDA 121.1164

REFERENCES

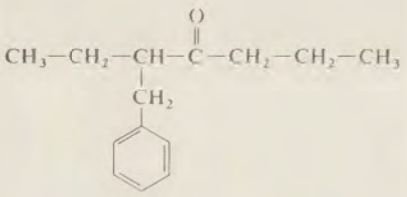
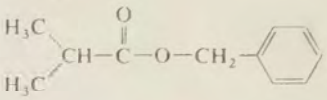
For References 1–5, see end of Part III.

	Benzyl ethyl ether	Benzyl formate
Other names	Ethyl benzyl ether	Formic acid benzyl ester
Empirical formula	$C_9H_{12}O$	$C_8H_8O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	Colorless liquid
Assay		95% min
Molecular weight	136.19	136.15
Boiling point	186 C	202–203°C
Flash point		83°C
Specific gravity	0.9490 at 20°C	1.0930–1.0965 at 15°C
Refractive index	1.4955 (1.4970) at 20°C	1.5100–1.5120 at 20°C
Acid value		0.2 max
Solubility	Insoluble in water; miscible with alcohol and ether	1:3–4 in 70% alcohol
Organoleptic characteristics	Pleasant, fruity (pineapple) odor	Intense, pleasant, floral-fruity odor; sweet taste reminiscent of apricot and pineapple
Synthesis	From benzyl chloride and sodium ethylate in alcoholic solution[6]	By heating a mixture of formic/acetic anhydride and benzyl alcohol to 50°C;[7] by passing a mixture of formic acid and excess benzyl alcohol over a catalyst (ThO_2 or TiO_2) at high temperature[8]
Natural occurrence	In cocoa	It has been isolated from the oil of *Rosa rugosa*.[9]
Reported uses[3]	Non-alcoholic beverages 0.50–1.0 ppm Ice cream, ices, etc. 2.5 ppm Candy 7.5 ppm Baked goods 7.5 ppm	Non-alcoholic beverages 2.4 ppm Ice cream, ices, etc. 8.0 ppm Candy 12 ppm Baked goods 8.6 ppm Chewing gum 3.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2144	FDA 121.1164; FEMA No. 2145

REFERENCES

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

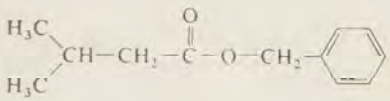
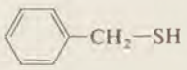
6. **Franzen,** *J. Prakt. Chem.*, 97, 82, 1918.
7. **Béhal,** *Ann. Chim. Paris*, 20, 421, 1900.
8. **Sabatier and Maihle,** *Compt. Rend.*, 152, 1045, 1911.
9. **Tsumotu et al.,** *Nippon Kagaku Zasshi*, 83, 745, 1962.

	3-Benzyl-4-heptanone	Benzyl isobutyrate
Other names	Benzyl dipropyl ketone Morellone	Benzyl 2-methyl propanoate
Empirical formula	$C_{14}H_{20}O$	$C_{11}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Assay		97% min[2]
Molecular weight	204.31	178.23
Boiling point		105–108 C at 4 mm Hg
Flash point		100 C
Specific gravity		1.001–1.005 at 25°/25°C[2]
Refractive index		1.4890–1.4920 at 20°C[2]
Acid value		Not more than 1.0
Solubility		1:6 in 70% alcohol
Organoleptic characteristics		Fruity, somewhat jasmine-like odor; sweet, strawberry-like taste
Synthesis		May be prepared from benzyl alcohol and isobutyric acid;[2] by the action of aluminum ethylate on a mixture of benzyl and butyric aldehydes[6]
Natural occurrence	Not reported found in nature	In mint
Reported uses[3]	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 4.6 ppm Candy 11 ppm Baked goods 11 ppm	Non-alcoholic beverages 5.2 ppm Ice cream, ices, etc. 12 ppm Candy 12 ppm Baked goods 25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2146	FDA 121.1164; FEMA No. 2141

REFERENCES

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

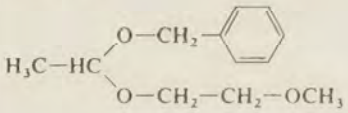
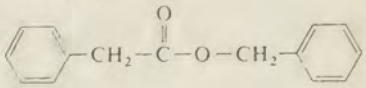
6. Orlow, *Bull. Soc. Chim. Fr.*, 35, 362, 1924.

	Benzyl isovalerate	Benzyl mercaptan
Other names	Benzyl 3-methyl butyrate	Benzyl hydrosulfide Thiobenzyl alcohol α-Toluenethiol
Empirical formula	$C_{12}H_{16}O_2$	C_7H_8S
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay	98% min[2]	
Molecular weight	192.26	124.19
Boiling point	245 C	194–195°C
Flash point	>100 C	
Specific gravity	0.985–0.991 at 25°/25°C;[2] 0.9932–0.9983 at 15°C	1.058 at 20°C
Refractive index	1.4860–1.4900 at 20°C[2]	
Acid value	Not more than 1.0[2]	
Solubility	1:2 in 80% ethanol; 1:1 in 90% ethanol	
Organoleptic characteristics	Fruity odor reminiscent of apple or pineapple	Repulsive, garlic-like odor; oxidizes in air to dibenzyl disulfide
Synthesis	May be prepared by esterification of isovaleric acid with benzyl alcohol[6]	From benzyl chloride and potassium hydrosulfide[7,8]
Natural occurrence	Not reported found in nature	In coffee
Reported uses[3]	Non-alcoholic beverages 2.2 ppm Ice cream, ices, etc. 3.4 ppm Candy 16 ppm Baked goods 9.4 ppm Gelatins and puddings 56 ppm Chewing gum 200 ppm	Non-alcoholic beverages 0.15–0.25 ppm Ice cream, ices, etc. 0.15–0.50 ppm Candy 0.50–0.75 ppm Baked goods 0.50–0.75 ppm
Regulatory status	FDA 121.1164; FEMA No. 2152	FDA 121.1164; FEMA No. 2147

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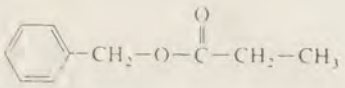
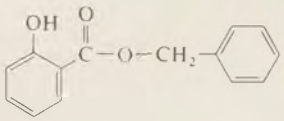
For References 1–5, see end of Part III.

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7. Scheibler and Voss, *Ber. Dtsch. Chem. Ges.*, 53, 382, 1920.
8. Hoffman and Reid, *J. Am. Chem. Soc.*, 45, 1883, 1923.

	Benzyl methoxyethyl acetal	Benzyl phenylacetate
Other names	Acetaldehyde benzyl β-methoxyethyl acetal 1-Benzoxy-1-(2-methoxyethoxy)-ethane 1-Benzyloxy-1-(β-methoxy)-ethoxyethane	Benzyl α-toluate
Empirical formula	$C_{12}H_{18}O_3$	$C_{15}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay		98% min
Molecular weight	210.27	226.28
Boiling point		320°C
Flash point		>100°C
Specific gravity		1.095–1.099 at 25°C
Refractive index		1.5530–1.5580 at 20°C
Acid value		Not more than 1.0
Solubility		1:3 in 90% ethanol
Organoleptic characteristics	Mild, sweet, green, fruital odor	Sweet, floral (jasmine-rose) odor; a slight honey-like taste
Synthesis		By direct esterification of benzyl alcohol with phenylacetic acid
Natural occurrence	Not reported found in nature	Not reported found in nature. Phenylacetic acid, on the other hand, has been reported in several essential oils.
Reported uses[3]	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 2.6 ppm Candy 6.6 ppm Baked goods 4.3 ppm Toppings 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2148	FDA 121.1164; FEMA No. 2149

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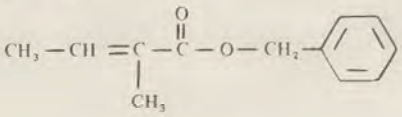
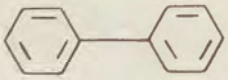
For References 1–5, see end of Part III.

	Benzyl propionate	Benzyl salicylate
Other names	Benzyl propanoate	Benzyl *o*-hydroxybenzoate
Empirical formula	$C_{10}H_{12}O_2$	$C_{14}H_{12}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Assay	98% min[2]	98% min[2]
Molecular weight	164.21	228.25
Boiling point	219–220°C (227°C)	208°C at 26 mm Hg; 170–175°C at 7 mm Hg
Congealing point		-23.5°C[2]
Flash point	100°C	>100°C
Specific gravity	1.028–1.032 at 25°/25°C;[2] 1.040 at 15.5°C	1.176–1.180 at 25°/25°C;[2] 1.1799 at 20°C
Refractive index	1.496–1.500[2] (1.5100) at 20°C	1.5790–1.5820[2] (1.5805) at 20°C
Acid value	1.0 max[2]	Not more than 1.0[2]
Solubility	1:3 in 70% alcohol	1:9 in 90% ethanol
Organoleptic characteristics	Sweet, fruity odor; peach-, apricot-like taste	Faint, sweet odor; a sweet, currant-like taste
Synthesis	By esterification of benzyl alcohol with propionic acid[2]	By esterification of salicylic acid with benzyl alcohol[2]
Natural occurrence	In strawberry	It has been reported in small amounts in carnation oil (*Dianthus caryophyllus* L.)[6] and in larger amounts in the oil of *Primula auricula*.[7]
Reported uses[3]	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 5.8 ppm Candy 19 ppm Baked goods 17 ppm Chewing gum 19–150 ppm Icings 40 ppm	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 0.89 ppm Candy 1.8 ppm Baked goods 0.01–2.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2150	FDA 121.1164; FEMA No. 2151

REFERENCES

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

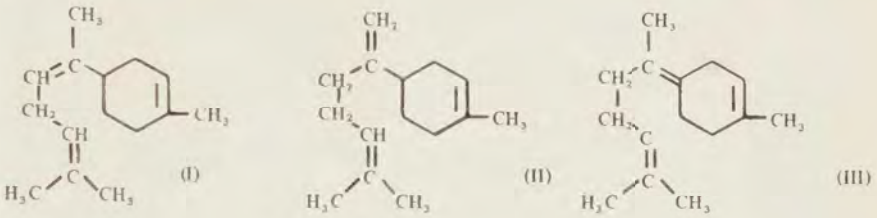
6. **Treff and Wittrisch,** *J. Prakt. Chem.*, 122, 339, 1939.
7. *Ullmanns Enzyklopädie der Technischen Chemie,* Vol. 5, Urban and Schwarzenberg, 1953, 313.

	Benzyl tiglate	Biphenyl
Other names	Benzyl *trans*-2-methyl 2-butenoate Benzyl *trans*-2,3-dimethyl acrylate Benzyl *trans*-2-methyl crotonate	Phenylbenzene Diphenyl
Empirical formula	$C_{12}H_{14}O_2$	$C_{12}H_{10}$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	White to slightly yellow crystals
Molecular weight	190.24	154.21
Melting point		71°C
Boiling point		254–255°C 227°C at 400 mm Hg 217°C at 300 mm Hg 145°C at 22 mm Hg 70–78°C at 0.2 mm Hg
Specific gravity		0.8660 at 20°C
Refractive index		1.475 at 20°C
Solubility	Insoluble in water; soluble in alcohol and oils	Insoluble in water; soluble in alcohol and ether; very soluble in benzene, methanol, carbon tetrachloride, and carbon disulfide
Organoleptic characteristics	Odor reminiscent of mushroom, with a rosy undertone	Pungent odor, reminiscent of rose on dilution
Synthesis	By direct esterification of tiglic acid with benzyl alcohol under azeotropic conditions	By thermal dehydrogenation of benzene[6]
Natural occurrence		Reported found in coal tar
Reported uses[3]	Baked goods 8.0 ppm Condiments 8.0 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
Regulatory status	FEMA No. 3330	FEMA No. 3129

REFERENCES

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

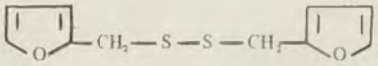
6. **Kirk and Othmer,** *Encyclopedia of Chemical Technology*, 2nd Ed., Vol. 7, Wiley & Sons, 1965, 191.

	Bisabolene
Other names	Limene (I) α-Bisabolene; 1-methyl-4-(1,5-dimethyl-1,4-hexadienyl)-1-cyclohexene (II) β-Bisabolene; 1-methyl-4-(5-methyl-1-methylene-4-hexenyl)-1-cyclohexene (III) γ-Bisabolene; 1-methyl-4-(1,5-dimethyl-4-hexenylidene)-1-cyclohexene
Empirical formula	$C_{15}H_{24}$
Structure	 (I) (II) (III)
Physical/chemical characteristics[5]	
Appearance	Colorless oil
Molecular weight	204
Boiling point	148°C at 18 mm Hg (β-bisabolene)
Refractive index	1.4893 at 15°C (β-bisabolene)
Optical rotation	−67° at 15°C (β-bisabolene); for the γ-form widely different values characterize products obtained from different natural sources
Solubility	Soluble in alcohol; insoluble in water
Organoleptic characteristics	Pleasant balsamic odor
Synthesis	Reported isolated from bisabol myrrh;[6] also from nerolidol by dehydration (γ-form)[7]
Natural occurrence	Reported found in bisabol myrrh,[6] in bergamot oil,[8] and in several essential oils: *Orthodon asaroniferum, O. methyliso-eugenoliferum, O. tenuicaule*;[9] *Citrus medica* var. *acida* (*C. aurantifolia*);[10] *Cinnomomum kanahirai*;[11] *Citrus limonia* from California;[12] *Illicium verum*;[13] French lavender (*Lavendula vera*).[14] For additional listings of natural occurrence, please consult Reference 15
Reported uses[3]	Non-alcoholic beverages 3.0 ppm 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 Preserves and spreads 3.0 ppm
Regulatory status	FEMA No. 3331

REFERENCES

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

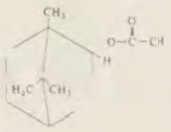
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7. Rodd, *Chemistry of Carbon Compounds*, 2nd ed., Vol. 2, Part C, American Elsevier, 1959, 259.
8. Burgess and Page, *J. Chem. Soc.*, 85, 1327, 1904.
9. Huzita and Fujita, *J. Chem. Soc. Jap.*, 61, 782, 1940; 64, 356, 599, 1943; 65, 79, 1944.
10. Guenther and Langenau, *J. Am. Chem. Soc.*, 65, 959, 1943.
11. Naito, *J. Chem. Soc. Jap.*, 64, 1024, 1943.
12. Poore, *Perfum. Essent. Oil Rec.*, 23, 166, 1932.
13. Jackson and Short, *J. Soc. Chem. Ind.*, 55, 8T, 1936.
14. Seidel, Müller and Schinz, *Helv. Chim. Acta*, 27, 738, 1944.
15. Ruzička and Capato, *Helv. Chim. Acta*, 8, 263, 1925.

	Bis (2-furfuryl) disulfide	Borneol
Other names	Difurfuryl disulfide Furfuryl disulfide	2-Bornanol; borneo camphor; bornyl alcohol; 2-camphanol
Empirical formula	$C_{10}H_{10}O_2S_2$	$C_{10}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Pale-yellow oily liquid	Colorless plates
Molecular weight	226.32	154.24
Melting point	10°C	208°C (*dl*-borneol)
Boiling point	112–113°C at 0.5 mm Hg	212 C
Flash point		150 C
Specific gravity		1.011 at 20°C
Optical rotation		+37°44′ at 20°C
Solubility	Slightly soluble in water; very soluble in alcohol and organic solvents	Insoluble in water; soluble in alcohol, chloroform, and ether
Organoleptic characteristics	Powerful, repulsive sulfide odor	Pungent, camphor-like odor and burning taste somewhat reminiscent of mint
Synthesis	From furfural and sodium hydrogen sulfide[6]	Racemic borneol is prepared synthetically by reduction of camphor or from pinene.
Natural occurrence		Unlike isoborneol free or esterified borneol has been identified in more than 250 distillates from plants, herbs, leaves, or bark: *Compositae*, *Ericaceae*, *Lauraceae*, *Labiatae*, *Rutaceae*. Natural borneol can be *d* or *l* rotatory but very seldom also racemic. Most frequently encountered is the *l*-borneol characteristic of *Compositae*, *Graminaceae*, and almost all *Pinaceae*. *d*-Borneol is characteristic of *Cupressaceae*, *Zingiberaceae*, lavender, lavandin, and spike oils.
Reported uses[3]	Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm Gelatins and puddings 3.0 ppm Chewing gum 3.0 ppm Condiments, pickles 3.0 ppm Meat, meat sauces, soups 3.0 ppm Milk, dairy products 3.0 ppm	Non-alcoholic beverages, 0.25–1.4 ppm; ice cream, ices, etc., 1.4 ppm; candy, 3.7 ppm; baked goods, 5.1 ppm; chewing gum, 0.30 ppm; syrups, 0.30 ppm
Regulatory status	FEMA No. 3257	FDA 121.1164; FEMA No. 2157

REFERENCES

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

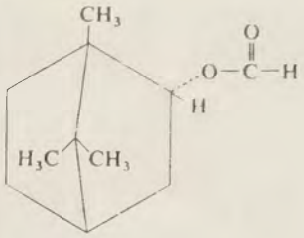
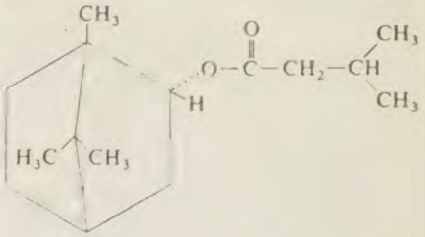
6. Gilman and Hewlett, *J. Am. Chem. Soc.*, 52, 2141, 1930.

	Bornyl acetate
Other names	Bornyl acetic ether Bornyl ethanoate
Empirical formula	$C_{12}H_{20}O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid at room temperature solidifies in a crystalline mass below 26–27° C
Assay	98% min[2]
Molecular weight	196.29
Melting point	*l*, 27.4°C; *d*, 27.7°C
Boiling point	*l*, 225–226°C; *d*, 225–226°C
Freezing point	25°C[2]
Flash point	89°C
Specific gravity	*l*, 0.981–0.985 at 25°/25°C;[2] *d*, 0.9910 at 15°C
Refractive index	*l*, 1.4620–1.4655 at 20°C;[2] *d*, 1.4639
Optical rotation	*l*, −39.5° to −45.0°;[2] *d*, +44°23′ *l*, 1:3 in 70% alcohol; *d*, —
Organoleptic characteristics	Fresh, strong, piney odor; fresh, burning taste
Synthesis	*l*-Bornyl acetate occurs naturally in many oils distilled from the leaves of plants of the family Pinaceae; *d*-bornyl acetate is found in the oils distilled from plants of the family Cupressaceae. Bornyl acetate therefore may be isolated by distillation and crystallization from these oils; however, it is commonly prepared by direct acetylation of borneol. The first synthesis dates to 1889.[6]
Natural occurrence	*l*-Bornyl acetate has been reported in the oils of *Abies canadensis, Abies concolor, Picea canadensis, Picea rubens, Picea orientalis, Pinus densiflora, Larix americana, Callitris drummondi, Abies alba, Pinus punulio, Abies sibirica* L., etc., and also in coriander, thyme, and valerian oil. It has been identified also in the essence from flowers of *Chrysanthemum sincuse* Sabin,[7] in the distillate of *Teucrium chamaedris* L.,[8] and in the fresh rhizomes of *Valeriana officinalis* L.[9] *d*-Bornyl acetate is found in the essential oils of *Callitris glauca, C. robusta, C. gracilis, C. verrucosa,* and *C. calcarata.* The presence of bornyl acetate has been excluded from the essence of lavender and lavandin.[10]
Reported uses[3]	Non-alcoholic beverages, 1.1 ppm; ice cream, ices, etc., 1.8 ppm; candy, 1.9 ppm; baked goods, 1.4 ppm; gelatins and puddings, 70 ppm; chewing gum, 0.30 ppm; syrups, 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2159

REFERENCES

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

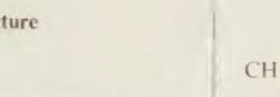
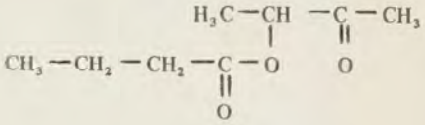
6. Haller, *C. R. Séances Acad. Sci.* (Paris), 109, 29, 1889.
7. Kotake and Nonaka, *Miltizer Ber.*, p. 26, 1958.
8. Rovesti, *Riv. Ital. EPPOS*, 40, 163, 1958.
9. Stoll et al., *Helv. Chim. Acta*, 40, 1205, 1957.
10. Naves, *Helv. Chim. Acta*, 42, 2744, 1959.

	Bornyl formate	Bornyl isovalerate
Other names	Bornyl methanoate	Bornyl-3-methylbutanoate Bornyval
Empirical formula	$C_{11}H_{18}O_2$	$C_{15}H_{26}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless oil
Assay	95% min	
Molecular weight	182.66	238.37
Boiling point	106–108°C at 21 mm Hg	*d*, 151–152°C at 26 mm Hg; *l*, 255–260°C at 760 mm Hg
Specific gravity	1.010 at 20°C	*d*, 0.9486 at 18°C
Refractive index	1.4689 at 20°C	*d*, 1.4605 at 18°C
Optical rotation	At 20°C: *l*, −48.6°; *d*, +48.45°	*d*, +36.7°
Solubility		*d*, 1:4 in 80% alcohol
Organoleptic characteristics	Odor similar to that of bornyl acetate	Aromatic odor similar to valerian and borneol
Synthesis	The corresponding ester is prepared by heating to 50°C a mixture of formic/acetic anhydride with *d*-bornyl alcohol[6]	*d*-Bornyl isovalerate can be prepared by heating to 140°C *d*-borneol and isovaleric acid.[9]
Natural occurrence	It has been reported in the essential oil from roots of valerian.[7,8]	*l*-Bornyl isovalerate has been reported in valerian root oil.[7,8] *d*-Bornyl isovalerate is not reported found in nature.
Reported uses[3]	Non-alcoholic beverages 3.7 ppm Ice cream, ices, etc. 0.30–3.0 ppm Candy 0.80–2.0 ppm Baked goods 0.80–2.0 ppm Syrups 0.04 ppm	Non-alcoholic beverages 0.06–1.0 ppm Ice cream, ices, etc. 0.40–1.0 ppm Candy 0.90–2.0 ppm Baked goods 0.90–2.0 ppm Syrups 1.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2161	FDA 121.1164; FEMA No. 2165

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

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7. Bruylants, *Ber. Dtsch. Chem. Ges.*, 11, 455, 1878.
8. Haller, *Ann. Chim. Paris*, 27, 396, 1892.
9. Vavon and Peignier, *Bull. Soc. Chim. Fr.*, 39, 936, 1926.

	2-Butanone	Butan-3-one-2-yl butanoate
Other names	Ethyl methyl ketone Methyl ethyl ketone	Acetoyl butyrate
Empirical formula	C_4H_8O	$C_8H_{14}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, flammable liquid	
Molecular weight	72.10	158.19
Melting point	−85.9°C (−86.4 C)	
Boiling point	78.6–79.57°C	
Specific gravity	0.8255 at 4°C; 0.8054 at 20°C	
Refractive index	1.3785 (1.3790) at 20°C	
Solubility	Soluble in water, alcohol, and ether; miscible with oils	
Organoleptic characteristics	Acetone-like odor	
Synthesis	By catalytic dehydrogenation of secondary butyl alcohol; by dehydration of butane-2,3-diol by refluxing with 25% aqueous H_2SO_4[6,7] Industrially, it is also prepared by controlled oxidation of butane, by dry distillation of calcium acetate and calcium propionate, or by refluxing methyl acetoacetate and diluted H_2SO_4.	Reported not found in nature
Natural occurrence	It has been reported found as an impurity among the products from the dry distillation of wood and in the oil (extracted with ether) of black tea.[8] It is also present in coffee, cheese, bread, some citrus oils, and some other natural products (grape, raspberry).	
Reported uses[3]	Non-alcoholic beverages 70 ppm Ice cream, ices, etc. 270 ppm Candy 100 ppm Baked goods 100 ppm	Non-alcoholic beverages 5.0 ppm Alcoholic beverages 25.0 ppm Ice cream, ices, etc. 25.0 ppm Candy 50.0 ppm Baked goods 75.0 ppm Gelatins and puddings 30.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2170	FEMA No. 3332

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

6. Akabori, *J. Chem. Soc. Jap.*, 59, 1132, 1938.
7. Neish et al., *Can. J. Res.*, 23, 281, 1945.
8. Takei et al., *Bull. Inst. Phys. Chem. Res. Abstr. Tokyo*, 10, 45, 1937.

	Butter acids	Butter esters
Description	Naturally occurring fatty acids in butter	Ethyl ester of the mixed acids in butter
Physical/chemical characteristics[5]		
Appearance	Waxy solid	Waxy solid
Assay	Oleic/palmitic acids, 50–70%; stearic/myristic acids, about 20%; butyric acid, 3–4%; linoleic, lauric, palmitic, caproic, capric, and caprylic acids, < 1.0% each	See Butter acids
Melting point	Low melting, variable	Low melting, variable
Solubility	Poorly soluble in alcohol; soluble in oils	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Typical odor and flavor of fatty acids	Fatty, oily, waxy odor and flavor
Synthesis	Isolated from butter; mixtures of the acids from other sources	By esterification of the mixed butter acids with ethanol
Natural occurrence	In butter	
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 2,800 ppm Baked goods 8.3 ppm	Ice cream, ices, etc. 24 ppm Candy 78 ppm Baked goods 86 ppm Toppings 2.0 ppm Popcorn oil 1,200 ppm
Regulatory status	FDA 121.1164; FEMA No. 2171	FDA 121.1164; FEMA No. 2172

REFERENCES

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

	Butter starter distillate	Butyl acetate
Other names	Flavor compounds distilled from cultured reconstituted skim milk	
Empirical formula		$C_6H_{12}O_2$
Structure		$CH_3-CH_2-CH_2-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_3$
Physical chemical characteristics[5]		
Appearance	Slightly viscous, clear liquid	Colorless liquid
Assay	Main component diacetyl; variable from 1–15 mg diacetyl/ml	95% min
Molecular weight		116.16
Melting point		−76.8°C
Boiling point		126.5°C
Flash point		38°C (22°C)
Specific gravity		0.882 at 20°C; 0.8830–0.8870 at 15°C
Refractive index		1.3942 (1.3930–1.3970) at 20°C
Acid value		0.2 max
Solubility	Soluble in water; partially soluble in oil	Very slightly soluble in water; soluble in most common organic solvents
Organoleptic characteristics		Strong, fruity odor; burning and then sweet taste reminiscent of pineapple
Synthesis	By steam-water distillation at 100°C of specially cultured skim milk	By esterification of *n*-butyl alcohol with acetic acid
Natural occurrence		Reported present in rum ether[6] and other natural products
Reported uses[3]	Ice cream, ices, etc. 20–40 ppm Candy 420 ppm Baked goods 720 ppm Shortenings 750–12,000 ppm	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 16 ppm Candy 32 ppm Baked goods 32 ppm Gelatins and puddings 13 ppm Chewing gum 220 ppm
Regulatory status	FDA 121.1164; FEMA No. 2173	FDA 121.1164; FEMA No. 2174

REFERENCES

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

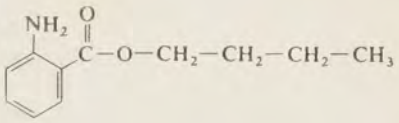
6. Fenaroli et al., *Riv. Ital. EPPOS*, 9, 484, 1965; 2, 75, 1966.

	Butyl acetoacetate	Butyl alcohol
Other names	Butyl-β-ketobutyrate Butyl 3-oxobutanoate	1-Butanol *n*-Butyl alcohol
Empirical formula	$C_8H_{14}O_3$	$C_4H_{10}O$
Structure	$CH_3-C(=O)-CH_2-C(=O)-O-(CH_2)_3-CH_3$	$CH_3-CH_2-CH_2-CH_2OH$
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless liquid
Molecular weight	158.20	74.12
Boiling point	100–103°C at 16 mm Hg	117–118°C
Freezing point		−90°C
Flash point		35–36°C
Specific gravity	0.9761 at 25°C	0.8096–0.8099 at 20°C
Refractive index	1.4245 at 25°C	1.39949 at 20°C
Solubility		1:11–1:12 in water; soluble in alcohol and ether
Organoleptic characteristics		Odor similar to amyl alcohol; dry, burning taste
Synthesis	By heating butyl acetate and sodium or potassium butylate; from ethyl acetoacetate and *n*-butyl alcohol; by reacting diketene and butyl alcohol in the presence of acetic acid and pyridine	*n*-Butyl alcohol is obtained by fermentation of glycerol, mannite, starches, and sugars in general, using *Bacillus butylicus* sometimes synergized by the presence of *Clostridium acetobutyricum*; synthetically, from acetylene
Natural occurrence		Reported present in peppermint oil from Brazil,[6] *Achillea ageratum*, tea, and in the apple aroma
Reported uses[3]	Non-alcoholic beverages 4.2 ppm Ice cream, ices, etc. 7.3 ppm Candy 26 ppm Baked goods 26 ppm	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
Regulatory status	FDA 121.1164; FEMA No. 2176	FDA 121.1164; FEMA No. 2178

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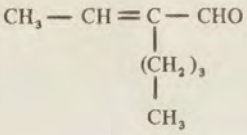
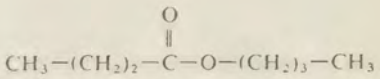
For References 1–5, see end of Part III.

6. Garnero, Bénezet and Igolen, *Ind. Parfum.*, 3, 353, 1958.

	Butylamine	Butyl anthranilate
Other names	1-Aminobutane *m*-Butylamine	Butyl-2-aminobenzoate Butyl *o*-aminobenzoate
Empirical formula	$C_4H_{11}N$	$C_{11}H_{15}NO_2$
Structure	$CH_3—CH_2—CH_2—CH_2—NH_2$	
Physical/chemical characteristics		
Appearance	Colorless liquid	Liquid at room temperature
Assay		
Molecular weight	73.14	193.25
Melting point	-50°C	Approx 0°C
Boiling point	78°C	303°C
Flash point	45°C	
Specific gravity	0.7327 at 25/4°C	1.060 at 15.5°C
Refractive index		1.5420 at 20°C
Solubility	Miscible with water, alcohol, and ether	
Organoleptic characteristics	Ammoniacal odor	Sweet, faint, fruity (plum, petitgrain) note
Synthesis	Catalytic alkylation of ammonia with butyl alcohol	Prepared by transesterification of methyl anthranilate (methyl 2-aminobenzoate) with *n*-butyl alcohol in the presence of HCl
Natural occurrence	In mulberry leaves	Not reported found in nature
Reported uses[3]	Alcoholic beverages 0.1 ppm Ice cream, ices, etc. 0.1 ppm Candy 0.1 ppm Baked goods 0.1 ppm Gelatins and puddings 0.1 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 2.6 ppm Candy 9.0 ppm Baked goods 6.7 ppm
Regulatory status	FEMA No. 3130	FDA 121.1164; FEMA No. 2181

REFERENCES

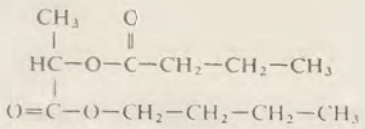
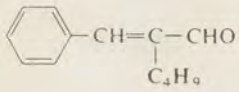
For References 1–5, see end of Part III.

	2-Butyl-2-butenal	Butyl butyrate
Other names	2-Ethylidene hexanal	
Empirical formula	$C_8H_{14}O$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Liquid
Molecular weight	126.19	144.21
Boiling point		165°C (162°C)
Specific gravity	1.4540 at 20°C	0.8692 at 20°C
Refractive index		1.4064 at 20°C
Solubility		Insoluble in water; miscible with alcohol and ether
Organoleptic characteristics		Fruity (pear-pineapple-like) odor
Synthesis	By isomerization of 2-butyl-3-butene-1,2-diol in acid media[6]	By passing vapors of *n*-butyl alcohol over MnO_2 or ZnO at 400°C;[6] also by passing vapors of *n*-butyl alcohol over CuO-VO at 180–200°C[7,8]
Natural occurrence		Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 0.5 ppm Ice cream, ices, etc. 0.6 ppm Candy 1.5 ppm Baked goods 2.0 ppm Gelatins and puddings 1.5 ppm Milk, dairy products 0.6 ppm	Non-alcoholic beverages 8.6 ppm Ice cream, ices, etc. 22 ppm Candy 24 ppm Baked goods 22 ppm Gelatins and puddings 14 ppm Chewing gum 150–1,500 ppm
Regulatory status	FEMA No. 3392	FDA 121.1164; FEMA No. 2186

REFERENCES

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

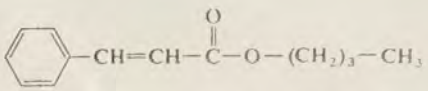
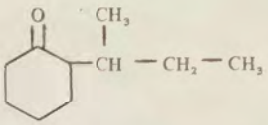
6. Gelin et al., *Bull Soc. Chim. Fr.*, p. 720, 1972.
7. E. I. du Pont de Nemours & Co., U.S. Patent 1,857,921, 1928.
8. Iwannikow and Gawrilowa, *Zh. Prikl. Khim.*, 9, 491, 1936.
9. Iwannikow and Gawrilowa, *Zh. Obshch. Khim.*, 17, 1103, 1947.

	Butyl butyryllactate	α-Butylcinnamaldehyde
Other names	Lactic acid, butyl ester, butyrate	2-Benzylidene hexanal Butyl cinnamic aldehyde α-Butyl-β-phenylacrolein
Empirical formula	$C_{11}H_{20}O_4$	$C_{13}H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	216.28	188.27
Boiling point	90°C at 2 mm Hg	265°C
Specific gravity	0.9731 at 20°C	0.825 at 15.5°C
Refractive index	1.4215 at 20°C	
Solubility		
Organoleptic characteristics		Characteristic floral, jasmine, lily-like odor
Synthesis	By direct acetylation of the butyl ester of lactic acid with butyric anhydride in the presence of H_2SO_4[6,7]	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 13 ppm Ice cream, ices, etc. 9.0 ppm Candy 44 ppm Baked goods 58 ppm	Non-alcoholic beverages 0.50–1.0 ppm Ice cream, ices, etc. 1.0–2.8 ppm Candy 2.0–8.0 ppm Baked goods 2.0–8.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2190	FDA 121.1164; FEMA No. 2191

REFERENCES

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

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7. Fein and Fisher, *Ind. Eng. Chem.*, 36, 235, 1944.

	Butyl cinnamate	2-*sec*-Butylcyclohexanone
Other names	Butyl β-phenyl acrylate Butyl 3-phenyl propenoate	2-(1-Methylpropyl)-cyclohexanone
Empirical formula	$C_{13}H_{16}O_2$	$C_{10}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Mobile liquid	Colorless viscous liquid; solidifies to an opaque mass
Molecular weight	204.27	154.25
Boiling point	145°C at 13 mm Hg (295°C at 760 mm Hg)	76–78°C at 8 mm Hg
Specific gravity	1.012 at 18°C; 1.015 at 15.5°C	0.9152 at 20°C
Refractive index	1.5470 at 20°C	1.4586 at 20°C
Solubility	Soluble in 95% alcohol, chloroform, benzene, and ether; almost insoluble in water	Insoluble in water; soluble in alcohol; miscible with most oils
Organoleptic characteristics	Pleasant, balsamic, slightly cocoa-like odor	Woody, camphoraceous, somewhat dry and musty odor
Synthesis		By hydrogenation of *o-sec*-butyl phenol in the presence of palladium catalyst;[6] by hydrogenation of 2-*sec*-butylidene cyclohexanone[7]
Natural occurrence	Not reported found in nature	Reported found in yellow passion fruit[8]
Reported uses[3]	Non-alcoholic beverages 0.83 ppm Alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.6 ppm Candy 1.0–15 ppm Baked goods 1.0–15 ppm	Non-alcoholic beverages 25.0 ppm Ice cream, ices, etc. 25.0 ppm Candy 150.0 ppm Baked goods 100.0 ppm Chewing gum 1,000.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2192	FEMA No. 3261

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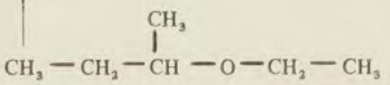
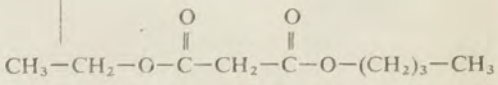
For References 1–5, see end of Part III.

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7. Barkhash, Smironova, Prudchenko and Machinskaya, *Zh. Obshch. Khim.*, 33(7), 2202, 1963.
8. Winter and Kloti, *Helv. Chim. Acta*, 55(6), 1916, 1972.

	Butyl 2-decenoate	1,3-Butylene glycol
Other names	*n*-Butyl decylenate	1,3-Butanediol β-Butyleneglycol 1,3-Dihydroxy butane
Empirical formula	$C_{14}H_{26}O_2$	$C_4H_{10}O_2$
Structure	$CH_3-(CH_2)_6-CH=CH-\overset{\overset{O}{\|\|}}{C}-O-(CH_2)_3-CH_3$	$CH_2(OH)-CH_2-CH(OH)-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Viscous liquid
Molecular weight	226.36	90.12
Boiling point		207°C
Specific gravity		1.00
Solubility	Insoluble in water; soluble in alcohol	Soluble in water and alcohol; insoluble in ether
Organoleptic characteristics	Rich, oily, fruity odor of peach and apricot; fruity, green taste	Sweet flavor with bitter aftertaste; odorless when pure
Synthesis	By esterification of *n*-butanol with 2-decenoic acid	From formaldehyde and propylene via pressure and a catalyst
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 8.0 ppm Candy 1.5–22 ppm Baked goods 30 ppm Chewing gum 2000 ppm	The compound is used as a solvent for flavors.
Regulatory status	FDA 121.1164; FEMA No. 2194	FDA 121.1176

REFERENCES

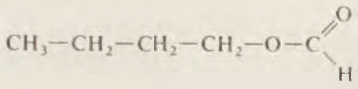
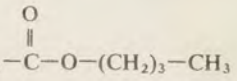
For References 1–5, see end of Part III.

	sec-Butyl ethyl ether	Butyl ethyl malonate
Other names		Ethyl butyl malonate
Empirical formula	$C_6H_{14}O$	$C_9H_{16}O_4$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	
Molecular weight	102.18	188.122
Boiling point	81°C	222°C
Specific gravity	0.7503 at 20°C	1.0257 at 17°C
Refractive index	1.3802 at 20°C	
Solubility	Insoluble in water; very soluble in alcohol and ether	
Synthesis	From *sec*-butyl alcohol and ethyl bromide or ethyl sulfate in the presence of sodium metal[6,7]	It can be prepared by passing vapors of ethyl butyl oxalacetate over coke or pumice at 350°C.[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	Non-alcoholic beverages 3.0 ppm Candy 0.13 ppm
Regulatory status	FEMA No. 3131	FDA 121.1164; FEMA No. 2195

REFERENCES

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

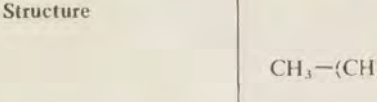
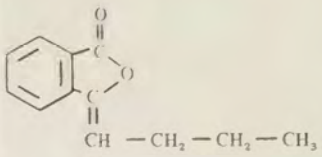
6. Norris and Rigby, *J. Am. Chem. Soc.*, 54, 2097, 1932.
7. Marks, Lipkin and Bestman, *J. Am. Chem. Soc.*, 59, 947, 1937.
8. D.R.P., German Patent, 427,856.

	Butyl formate	Butyl heptanoate
Other names		Butyl heptoate Butyl heptylate
Empirical formula	$C_5H_{10}O_2$	$C_{11}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	102.13	186.30
Melting point	−90°C	−68.4°C (from pentane)
Boiling point	106.8°C	226.2°C
Flash point	64°C	
Specific gravity	0.8917 at 20°C; 0.9108 at 0°C	0.85553 at 20°C
Refractive index	1.3890–1.3891 at 20°C	1.42280 at 20°C
Solubility	Slightly soluble in water; miscible with alcohol, ether, and other organic solvents	Soluble in most organic solvents
Organoleptic characteristics	Fruity, plum-like odor and corresponding taste	Characteristic herbaceous, slightly fruity odor and corresponding taste
Synthesis	By azeotropic distillation of formic acid and *n*-butyl alcohol with isopropyl formate,[6] by boiling *n*-butyl alcohol and formamide in the presence of ZnCl, $ZnSO_4$, or $HgCl_2$[7,8]	By direct esterification of the acid with *n*-butyl alcohol in the presence of mineral acids[6,7] or in benzene solution in the presence of *p*-toluene sulfonic acid.[11] It has been prepared together with other products from heptyl aldehyde and aluminum butylate in butyl alcohol at 25–30°C.[12]
Natural occurrence	Reported found in several natural products	Not reported found in nature. The acid has been reported present in various plants.
Reported uses[3]	Non-alcoholic beverages 2.9 ppm Ice cream, ices, etc. 3.2 ppm Candy 11 ppm Baked goods 9.1 ppm Gelatins and puddings 5.0 ppm	Non-alcoholic beverages 0.50–1.0 ppm Ice cream, ices, etc. 2.0–10 ppm Candy 2.0–25 ppm Baked goods 2.0–25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2196	FDA 121.1164; FEMA No. 2199

REFERENCES

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

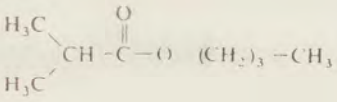
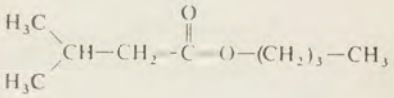
6. Consort. Elektrochem. Ind., German Patent 721,300, 1939.
7. Imp. Chem. Ind., U.S. Patent 1,877,847, 1928.
8. Imp. Chem. Ind., German Patent 523,189, 1928.
9. **Gartenmeister,** *Justus Liebigs Ann. Chem.*, 233, 284, 1886.
10. **Bilterys and Gisseleire,** *Bull. Soc. Chim. Belg.*, 44, 569, 1935.
11. **Hoback, Parsons and Bartlett,** *J. Am. Chem. Soc.*, 65, 1606, 1943.
12. **Kay-Fries,** U.S. Patent 2,412,469, 1943.

	Butyl hexanoate	3-Butylidenephthalide
Other names	Butyl caproate Butyl capronate Butyl hexylate	Ligusticum lactone
Empirical formula	$C_{10}H_{20}O_2$	$C_{12}H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Yellowish oily liquid
Assay		
Molecular weight	172.27	182.22
Melting point	−63°C to −64°C	82–83°C
Boiling point	208°C (99°C at 20 mm Hg)	134°C at 1.5 mm Hg (natural source) 141°C at 2.4 mm Hg (synthetic)
Specific gravity	0.8623 at 25°C; 0.865 at 15.5°C	1.0966 at 20°C (natural source) 1.1028 at 20°C (synthetic)
Refractive index	1.4153 at 25°C; 1.4170 at 20°C	1.5759 at 20°C (natural source) 1.5780 at 20°C (synthetic)
Solubility		Very slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics	Characteristic pineapple-like odor	Herbaceous odor reminiscent of lovage and celery
Synthesis	By esterification of hexanoic acid with *n*-butyl alcohol in benzene solution in the presence of *p*-toluene sulfonic acid.[6] It is also formed in the fermentation of carbohydrates yielding *n*-butyl alcohol and acetone.[7]	From sodium valerate, valeric anhydride, and phthalic anhydride[8]
Natural occurrence		Reported as occurring naturally in the fruits and roots of *Ligusticum acutilobum*
Reported uses[3]	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 3.9 ppm Candy 7.6 ppm Baked goods 10 ppm	Baked goods 8 ppm Condiments 5 ppm Meats 5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2201	FEMA NO. 3334

REFERENCES

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

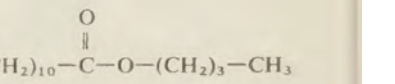
6. Hoback, Parsons and Bartlett, *J. Am. Chem. Soc.*, 65, 1606, 1943.
7. Fujita, *J. Chem. Soc. Jap.*, 64, 1008, 1943.
8. Berlingozzi and Lupo, *Gazz. Chim. Ital.*, 57, 259, 1927.

	Butyl isobutyrate	Butyl isovalerate
Other names	*n*-Butyl 2-methyl propanoate	
Empirical formula	$C_8H_{16}O_2$	$C_9H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid
Assay	97% min[2]	
Molecular weight	144.21	158.24
Boiling point	155–156°C	175–176°C
Specific gravity	0.859–0.864[2] at 25/25°C; 0.8618 at 20°C	0.8608 at 20°C
Refractive index	1.4010–1.4040[2] at 20°C; 1.4025 at 20°C	1.4087 at 20°C
Acid value	Not more than 1.0[2]	
Solubility	Insoluble in water; 1:7 in 60% alcohol[2]	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Strong, fruity odor and sweet, pineapple-like taste	Odor reminiscent of the isobutyl ester with a sweet, apple-like taste
Synthesis	Prepared from the corresponding acid and *n*-butyl alcohol by esterification in the presence of concentrated H_2SO_4 with or without solvent (boiling benzene)	By prolonged boiling of the acid with *n*-butyl alcohol in benzene in the presence of concentrated H_2SO_4[7]
Natural occurrence	Reported present in Roman camomile essential oil.	Reported found in the oil from leaves of *Eriostemon coxii* and *Phebalium dentatum*
Reported uses[3]	Non-alcoholic beverages 8.7 ppm Ice cream, ices, etc. 4.0–5.0 ppm Candy 19 ppm Baked goods 39 ppm Chewing gum 2,000 ppm	Non-alcoholic beverages 4.6 ppm Ice cream, ices, etc. 12 ppm Candy 13 ppm Baked goods 15 ppm Gelatins and puddings 50 ppm
Regulatory status	FDA 121.1164; FEMA No. 2188	FDA 121.1164; FEMA No. 2218

REFERENCES

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

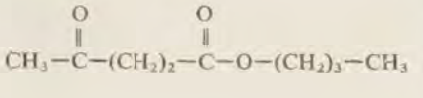
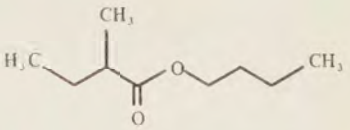
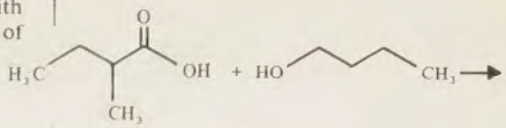
6. Salmi and Leimu, *Suom. Kemistil.*, 208, 47, 1947.
7. Vogel, *J. Chem. Soc.*, p. 630, 1948.

	Butyl lactate	Butyl laurate
Other names	Butyl 2-hydroxypropanoate Butyl α-hydroxypropionate	Butyl dodecanoate Butyl dodecylate
Empirical formula	$C_7H_{14}O_3$	$C_{16}H_{32}O_2$
Structure		
Physical/chemical characteristics[5]	*d-form* / *l-form* / *dl-form*	
Appearance	Liquid / Liquid / Liquid	Liquid
Molecular weight	146.16 / 146.16 / 146.16	256.44
Melting point		−7 °C
Boiling point	77 °C at 10 mm Hg / 70–73 °C at 10–11 mm Hg / 185 °C	154 °C at 4.5 mm Hg
Specific gravity	0.9744 at 27.6 °C / — / 0.973 at 20 °C	0.8603 at 20 °C
Refractive index	— / — / 1.4210 at 20 °C	1.4362 at 20 °C
Optical rotation	+13.63° at 27.3 °C / — / —	
Solubility	Slightly soluble in water	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Faintly sweet, pleasant odor	Characteristic fruity, peanut-like odor
Synthesis	Two optically active forms and one racemic form are known. The *d*-form is prepared by reacting zinc ammonium *l*-lactate with *n*-butyl alcohol in the presence of concentrated H_2SO_4.[6] The *l*-form is prepared by reacting zinc ammonium *d*-lactate with *n*-butyl alcohol in the presence of HCl.[7] The racemic form is prepared by several methods, one being from calcium or sodium lactate and *n*-butyl alcohol in benzene in the presence of H_2SO_4, with subsequent azeotropic distillation of the mixture.[8]	By esterification of lauric acid with *n*-butyl alcohol in the presence of H_2SO_4[9] or by conducting the esterification using gaseous HCl as a catalyst
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.66 ppm Ice cream, ices, etc. 2.8 ppm Candy 6.5 ppm Baked goods 7.7 ppm	Non-alcoholic beverages 0.40–3.0 ppm Ice cream, ices, etc. 0.60 ppm Candy 17 ppm Baked goods 1.0–40 ppm
Regulatory status	FDA 121.1164; FEMA No. 2205	FDA 121.1164; FEMA No. 2206

REFERENCES

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

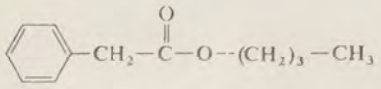
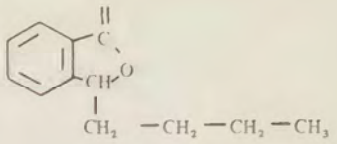
6. Wood, Such and Scarf, *J. Chem. Soc.*, 123, 610, 1923
7. Wassmer and Guye, *Chem. Zentralbl.*, 2, 1419, 1903.
8. Smith and Claborn, *Ind. Eng. Chem.*, 32, 693, 1940.
9. Rheinboldt, Konig and Otten, *Ann. Chem.*, 473, 258, 1929.

	Butyl levulinate	*n*-Butyl-2-methylbutyrate
Other names	Butyl γ-butyrolactone Butyl 4-oxopentanoate	
Empirical formula	$C_9H_{16}O_3$	$C_9H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	
Molecular weight	172.23	158.23
Boiling point	238°C	
Specific gravity	0.9735 (0.9745) at 20°C	
Refractive index	1.4283 (1.4290) at 20°C	
Solubility	Slightly soluble in water; soluble in ether, alcohol, chloroform, and other organic solvents	
Organoleptic characteristics	Characteristic burning, bitter taste	
Synthesis	By esterification of levulinic acid with *n*-butyl alcohol in the presence of HCl[6–8]	
Natural occurrence	Not reported found in nature	Reported found in strawberry[9,10]
Reported uses[3]	Non-alcoholic beverages 0.20–1.0 ppm Ice cream, ices, etc. 2.1 ppm Candy 4.6 ppm Baked goods 4.6 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 3.0 ppm Jellies, preserves, spreads 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2207	FEMA No. 3393

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

6. **Sah and Ma,** *J. Am. Chem. Soc.*, 52, 4881, 1930.
7. **Cox and Doods,** *J. Am. Chem. Soc.*, 55, 3392, 1933.
8. Niacet Chemical Corp., U.S. Patent 2,029,412, 1934.
9. **McFadden et al.,** *J. Chromatogr.*, 18, 10, 1965.
10. **Nursten and Williams,** *Chem. Ind.* (London), p. 486, 1967.

	Butyl phenylacetate	3-N-Butylphthalide
Other names	Butyl α-toluate	
Empirical formula	$C_{12}H_{16}O_2$	$C_{12}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Almost colorless oily liquid
Assay	98% min	
Molecular weight	192.26	190.24
Melting point		
Boiling point	260°C	177–178°C at 15 mm Hg 106–108°C at 0.1 mm Hg
Congealing point		
Flash point	74°C	
Specific gravity	0.991–0.994 at 25°C	1.0672 at 20°C
Refractive index	1.4880–1.4910 at 20°C	1.5260 at 20°C
Optical rotation		−57° (c = 1.96 in chloroform)
Acid value	1.0 max	
Solubility	1:2 in 80% alcohol	Slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics	Pleasant rose and honey-like odor	Herbaceous celery-like odor reminiscent of concentrated vegetable soup
Synthesis	By direct esterification of the acid with *n*-butyl alcohol in the presence of gaseous HCl	From celery oil;[6] from phthalide via bromination and subsequent reaction of the resulting phthaldeidic acid with *n*-butyl magnesium bromide[7]
Natural occurrence	Not reported found in nature	Reported found in *Levisticum officinale* and *L. acutilobum*; also in celery oil
Reported uses[3]	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 2.1 ppm Candy 4.5 ppm Baked goods 4.6 ppm Gelatins and puddings 5.0 ppm	Alcoholic beverages 0.5 ppm Gelatins and puddings 2.0 ppm Condiments, pickles 2.0 ppm Meats, meat sauces 1.0 ppm Soups 1.0 ppm Preserves and spreads 2.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2209	FEMA No. 3334

REFERENCES

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

6. Barton and de Vries, *J. Chem. Soc.*, 1916, 1963.
7. Naves, *Helv. Chim. Acta*, 26, 1281, 1943.

	Butyl propionate	Butyl stearate
Other names		Butyl octadecanoate Butyl octadecylate
Empirical formula	$C_7H_{14}O_2$	$C_{22}H_{44}O_2$
Structure	$CH_3-CH_2-\overset{\overset{O}{\|\|}}{C}-O-(CH_2)_3-CH_3$	$CH_3-(CH_2)_{16}-\overset{\overset{O}{\|\|}}{C}-O-(CH_2)_3-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Waxy or oily (>20 C), colorless material
Assay	96% min	
Molecular weight	130.18	340.35
Melting point		19–20 C
Boiling point	145–146 C	220–225°C at 25 mm Hg
Flash point	32 C	Approx. 172°C
Specific gravity	0.8795–0.8825 at 15 C; 0.8750 at 20 C	0.855–0.860 at 20 C
Refractive index	1.4000–1.4020 at 20 C; 1.4010 at 20 C	1.4430 at 20 C
Acid value	0.2 max	
Solubility	Slightly soluble in water; miscible with alcohol and ether	Insoluble in water; soluble in alcohol, ether, and mineral or vegetable oils
Organoleptic characteristics	Characteristic earthy, faintly sweet odor and apricot-like taste	Odorless or faintly fatty odor
Synthesis	By esterification of propionic acid with *n*-butyl alcohol in the presence of concentrated H_2SO_4[6] or *p*-toluene sulfonic acid[7]	By reacting silver stearate with *n*-butyl iodide at 100 C according to Whitly; by transesterification of glyceryl tristearate (tristearin) with *n*-butyl alcohol
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 4.0 ppm Ice cream, ices, etc. 5.2 ppm Candy 25 ppm Baked goods 27 ppm	Non-alcoholic beverages 1.0 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 190 ppm Baked goods 340 ppm Chewing gum 330 ppm
Regulatory status	FDA 121.1164; FEMA No. 2211	FDA 121.1164; FEMA No. 2214

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.

	Butyl sulfide	Butyl 10-undecenoate
Other names	Dibutyl sulfide	Butyl 10-hendecenoate Butyl undecylenoate
Empirical formula	$C_8H_{18}S$	$C_{15}H_{28}O_2$
Structure	$CH_3-(CH_2)_3-S-(CH_2)_3-CH_3$	$CH_2=CH-(CH_2)_8-\overset{\overset{O}{\|}}{C}-O-(CH_2)_3-CH_3$
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	146.30	240.39
Boiling point	182°C or 190–230°C (with decomposition)	125–128°C (252°C) at 3 mm Hg
Specific gravity	0.8386 at 20°C	0.8751 at 20°C
Refractive index	1.4530 at 20°C	1.4426 at 20°C
Solubility	Readily soluble in ether	
Organoleptic characteristics		Slightly fatty, buttery, wine-like, unpleasant odor
Synthesis	From butyl bromide and sodium sulfide in boiling ethanol.[6] According to some authors two forms exist, exhibiting different boiling points but identical solubilities in various solvents. Both forms are insoluble in water.[7]	By esterification of the acid with *n*-butyl alcohol at the boil in the presence of concentrated H_2SO_4[8] or in benzene solution[9]
Natural occurrence	Reported found in several natural products	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.02–1.0 ppm Ice cream, ices, etc. 0.01–1.0 ppm Candy 0.03–1.0 ppm Baked goods 0.03–1.0 ppm	Non-alcoholic beverages 0.90 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 6.6 ppm Baked goods 7.8 ppm Chewing gum 0.40–60 ppm Icings 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2215	FDA 121.1164; FEMA No. 2216

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

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7. Hinsberg, *Ber. Dtsch. Chem. Ges.*, 62, 2167, 1929.
8. Dankowa and Céll, *Zh. Obshch. Khim.*, 15, 191, 1945.
9. Jeffery and Vogel, *J. Chem. Soc.*, p. 662, 1948.

	n-Butyl valerate	Butyraldehyde
Other names	*n*-Butylpentanoate *n*-Butyl-*n*-valerianate	*n*-Butanal Butyl aldehyde Butyric aldehyde
Empirical formula	$C_9H_{18}O_2$	C_4H_8O
Structure	$C_4H_9-O-\overset{\overset{O}{\|\|}}{C}-(CH_2)_3-CH_3$	$CH_3-CH_2-CH_2-CHO$
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless liquid
Molecular weight	158.24	72.10
Melting point		−99°C
Boiling point	186.5°C (175°C)	75–76°C
Specific gravity	0.8680 at 20°C; 0.865 at 15.5°C	0.817 at 20°C
Refractive index	1.4118 at 20°C	1.3843 at 20°C
Solubility	Slightly soluble in water; soluble in propylene glycol	1:27 in water
Organoleptic characteristics	Characteristic fruity (apple-raspberry) odor and corresponding sweet taste	Characteristic pungent odor
Synthesis	By esterification of the acid with *n*-butyl alcohol in the presence of concentrated H_2SO_4 at the boil[6]	By dry distillation of calcium butyrate and calcium formate[7]
Natural occurrence	Reported found in several natural products	Reported found in the essential oils from flowers, fruits, leaves, or bark of: *Monarda fistulosa*,[8] *Litsea cubeba*,[9] Bulgarian clary sage,[10] cajeput, *Eucalyptus cinerea*,[11] *E. globulus*,[12] and others, as well as in apple and strawberry aromas[13,14]
Reported uses[3]	Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 2.6 ppm Candy 8.0 ppm Baked goods 6.8 ppm	Non-alcoholic beverages 0.71 ppm Alcoholic beverages 0.50 ppm Ice cream, ices, etc. 4.8 ppm Candy 2.9 ppm Baked goods 5.4 ppm Icings 0.25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2217	FDA 121.1164; FEMA No. 2219

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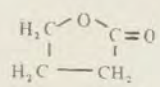
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7. **Lieben and Rossi,** *Justus Liebigs Ann. Chem.*, 158, 137, 1871.
8. **Miller et al.,** *Chem. Zentralbl.*, 2, 453, 1920.
9. **Fürst and Fenstel,** *Z. Chem.*, 1, 22, 1961.
10. *Perfum. Essent. Oil Rec.*, 49, 233, 1958.
11. **Baker and Smith,** *Research Eucalyptus E.O.*, Sydney, 1920.
12. *Schimmel Ber.*, 4, 47, 1904.
13. **Meigh,** *J. Sci. Food Agric.*, 7, 396, 1956.
14. **McGlamphy,** *Perfum. Essent. Oil Rec.*, 44, 352, 1953.

	n-Butyric acid
Other names	Butanoic acid Ethylacetic acid
Empirical formula	$C_4H_8O_2$
Structure	$CH_3-CH_2-CH_2-COOH$
Physical/chemical characteristics[5]	
Appearance	Colorless liquid
Molecular weight	88.10
Melting point	−5.55°C
Boiling point	163.55°C
Flash point	76 C
Specific gravity	0.960 at 15°C
Refractive index	1.3983–1.3984 at 20°C
Solubility	Soluble in water, alcohol, and ether
Organoleptic characteristics	Persistent, penetrating, rancid, butter-like odor and burning, acid taste
Synthesis	Obtained by fermentation of starches and molasses with selective enzymes (*Granulo saccharobutyricum*). It is subsequently isolated as the calcium salt.
Natural occurrence	Normally occurs in butter as a glyceride. It has been reported found in the essential oils of: citronella Ceylon, *Eucalyptus globulus*, *Araucaria cunninghamii*, *Lippia scaberrima*, *Monarda fistulosa*, cajeput, *Heracleum giganteum*, lavender, *Hedeoma pulegioides*, valerian, nutmeg, hops, *Pastinaca sativa*, Spanish anise, and others. It has been identified in strawberry aroma.[6]
Reported uses[3]	Non-alcoholic beverages 5.5 ppm Ice cream, ices, etc. 6.5 ppm Candy 82 ppm Baked goods 32 ppm Gelatins and puddings 0.19–45 ppm Chewing gum 60–270 ppm Margarine 18 ppm
Regulatory status	FDA GRAS; FEMA No. 2221

REFERENCES

For References 1–5, see end of Part III.
6. Willhalm et al., *Helv. Chim. Acta*, 49, 66, 1966.

	γ-Butyrolactone
Other names	4-Hydroxybutanoic acid, lactone 3 (or 4)-Hydroxybutyric acid, lactone 1,2-Butanolide 1,4-Butanolide
Empirical formula	$C_4H_6O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless to pale yellow, oily liquid
Molecular weight	86.09
Melting point	−44°C
Boiling point	206°C 89°C at 12 mm Hg
Specific gravity	1.1286 at 15°C 1.1441 at 0°C
Refractive index	1.4341 at 20°C
Solubility	Soluble in water in all proportions; very soluble in alcohol, ether, acetone, and benzene
Organoleptic characteristics	Faint, sweet, aromatic slightly buttery odor
Synthesis	From acetylene and formaldehyde;[6] also from a number of alternative sources: ethylene chlorohydrin, glutamic acid, γ-hydroxybutyric acid solutions, tetrahydrofuran, vinylacetic acid[7]
Natural occurrence	Reported found as a constituent in coffee aroma;[8,9] also a volatile flavor component in roasted filberts[10]
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 20.0 ppm Meat, meat sauces, soups 10.0 ppm Milk, dairy products 10.0 ppm Cereals 20.0 ppm
Regulatory status	FEMA No. 3291

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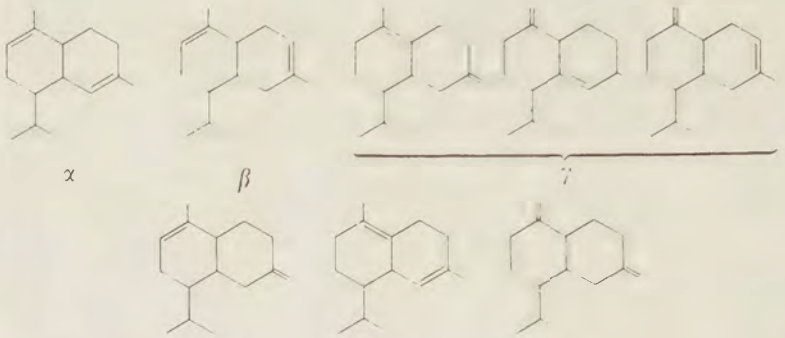
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7. Whitmore, *Organic Chemistry*, 2nd ed., Dover Publ., New York, 1951.
8. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.
9. Viani et al., *Helv. Chim. Acta*, 48, 1809, 1965.
10. Sheldon et al., *J. Food Sci.*, 37(2), 313, 1972.

Cadinene

Empirical formula $C_{15}H_{24}$

Structure



α β γ

γ_1 δ ε

Physical/chemical characteristics[5]	α and β	γ	γ_1	δ	ε
Molecular weight	204.34	204.34	204.34	204.34	204.34
Boiling point at 9 mm Hg			120–121°C		
Flash point					
Specific gravity at 20°C	0.9239	0.9125[a] 0.9146[b] 0.9087[c]		0.9175[a] 0.9146[c] 0.9162[b]	0.9107
Refractive index at 20°C	1.5059	1.5075[a] 1.5080[b] 1.5056[c]	1.5152[d]	1.5086[a] 1.5085[c] 1.5090[b]	1.5090
Optical rotation at 20°C	−251°	+148°[a] +3°4′[b] +56°7′[c]	−18°9′	+94°[a] +77°[e] +84°6′[b]	47°2′

Organoleptic characteristics

Synthesis The relative position of the two double bonds characterizes the stereoisomers of cadinene; these have been identified.[6]

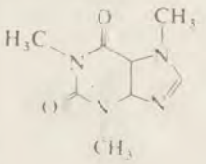
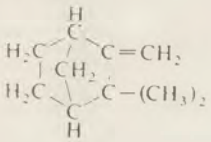
Natural occurrence Wallach confirmed the presence of cadinene in several essential oils:[7] α- and β-cadinene in the oil of *Dacrydium colensoi*; γ-cadinene in the oils of Java citronella, ylang-ylang, and *Populus balsamifera*; γ_1-cadinene in the oil of lemongrass Malabar; δ-cadinene in the oils of citronella, calamus, and ylang-ylang; ε-cadinene in the oil of ylang-ylang. See reference 8 for a tabular summary of essential oils containing cadinene and the corresponding plant and botanical family derivation.

[a] Citronella.
[b] Ylang-ylang.
[c] *Populus balsamifera.*
[d] At 26.5°C.
[e] Calamus.

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

6. Campbell and Soffer, *J. Am. Chem. Soc.*, 64, 417, 1942.
7. Wallach, *Annalen*, 238, 78, 1887.

	Caffeine	Camphene
Other names	Coffeine Guaramine Methyltheobromine Theine 1,3,7-Trimethyl-2,6-dioxopurine 1,3,7-Trimethylxanthine	3,3-Dimethyl-2-methylene norcamphane 2,2-Dimethyl-3-methylene norbornane
Empirical formula	$C_8H_{10}N_4O_2$	$C_{10}H_{16}$
Structure		
Physical/chemical characteristics[5]		
Appearance	Prism-like crystals	Crystalline solid
Assay		Commercial product may contain approximately 20% tricyclene.
Molecular weight	194.19	136.23
Melting point	238 C; sublimes at 178 C	*d*, 45–46°C; *l*, 51–52°C; sublimes when heated
Boiling point		159 C
Optical rotation		*d*, +104°; *l*, −85°
Solubility	One gm soluble in 46 ml water, 66 ml alcohol, 22 ml of 60% alcohol, 50 ml acetone. Solubility in water increases with increasing temperature or by adding alkali benzoates, cinnamates, citrates, or salicylates.	Insoluble in water; moderately soluble in alcohol; soluble in ether and chloroform
Organoleptic characteristics		Terpene, camphoraceous taste
Synthesis	Usually obtained from tea dust in which it is present up to 1.5–3.5% or as a by-product from the manufacture of caffeine-free coffee. Synthetically prepared starting with dimethylurea and malonic acid[6]	From pinene by catalytic isomerization or from bornyl chloride by heating with alkali in the presence of abietenesulfonic acid[7,8]
Natural occurrence	Occurs in tea, coffee, and maté leaves; also in guarana paste and cola nuts	The *l*-form was isolated in 1888 by Gobolow in the oil *Abies sibirica*; its structure was described by G. Wagner.[9] It also occurs in the oils of: *Tsuga canadensis*, *Thuja occidentalis*, *Artemisia herba alba*, and others. The *d*-form is present in several essential oils: orange flowers, camphor, lavender, calamus, *Curcuma aromatica*, and others.
Reported uses[3]	Non-alcoholic beverages 120 ppm	Non-alcoholic beverages 40–90 ppm Ice cream, ices, etc. 20 ppm Candy 160 ppm Baked goods 27 ppm
Regulatory status	FDA GRAS: 0.02% in cola-type beverages; FEMA No. 2224	FDA 121.1164; FEMA No. 2229

REFERENCES

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

6. **Fischer and Ach,** *Berichte*, 28, 2473, 3135, 1895.
7. **Dupont, Dulou and Thuet,** *Bull. Soc. Chim. Fr.*, 8, 891, 1941.
8. **Tischchenko and Rudakov,** *Chem. Abstr.*, p. 4052, 1934.
9. **Wagner,** *Ber. Dtsch. Chem. Ges.*, 23, 2311, 1890.

	d-Camphor	Caramel
Other names	*d*-2-Bornanone; *d*-2-Camphanone	
Empirical formula	$C_{10}H_{16}O$	
Structure		
Physical/chemical characteristics[5]	(The following values refer to synthetic camphor.)	
Appearance	Crystalline, white solid	Dark-brown, thick liquid
Molecular weight	152.23	
Melting point	>170 C	
Boiling point	209 C	
Flash point	Vapor mixtures of camphor and air are explosive	
Specific gravity	0.990–0.995 at 15 C	Approx. 1.35
Optical rotation	+2° to +5° at 20 C (This measurement is utilized to differentiate between the synthetic and the natural product.)	
Solubility	Readily soluble in alcohol (1:1), ether, chloroform, acetone, acetic acid, essential oils, and benzene; insoluble in alkali and glycerol. A solution of synthetic camphor in pet ether must be absolutely clear with a residue after evaporation of less than 1.0%.	Soluble in water and dilute alcohol
Organoleptic characteristics	Characteristic penetrating odor; burning, bitter, fresh taste	Odor of burnt sugar and pleasant, bitter taste
Synthesis	Natural camphor is obtained by distillation from the plants of *Cinnamomum* or *Laurus camphora* from China and Japan, together with the corresponding essential oils. The raw camphor contains several impurities. It is separated from the water and the essential oil by pressure or by centrifugation and subsequently purified by sublimation or crystallization. Synthetic camphor is prepared from pinene isolated by fractional distillation of turpentine oil. Pinene is reacted to bornyl chloride with gaseous HCl under pressure and then to camphene. The distilled and purified camphene is then oxidized to camphor with Na or K bichromate in the presence of H_2SO_4.	Made by heating sugar or glucose, adding small amounts of alkali, alkaline carbonate, or a trace of mineral acid during the heating
Natural occurrence	Frequently occurring in nature as the *d*- or *l*-form; the optically inactive form is seldom encountered. The *d*-form has been reported found in *Cinnamomum camphora* Nees. (*Laurus camphora* L.) from China, Japan, and the East Indies; in *Sassafras officinale*, *Lavandula spica*, and in other *Labiatae*. The *l*-form is reported found in the essential oils of *Salvia grandiflora*, *Matricaria parthenium*, *Artemisia herba alba*. The optically inactive form is found in *Chrysanthemum japonicum sinense*. For additional information see reference 6.	
Reported uses[3]	Ice cream, ices, etc., 0.10 ppm; candy, 1.1–25 ppm; baked goods, 11 ppm; condiments, 20 ppm	Non-alcoholic beverages, 2,200 ppm; ice cream, ices, etc., 590 ppm; candy, 180 ppm; baked goods, 220 ppm; meats, 2,100 ppm; syrups, 2,800 ppm
Regulatory status	FDA 121.1164; FEMA No. 2230	FDA GRAS; FEMA No. 2235

REFERENCES

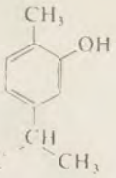
For References 1–5, see end of Part III.

6. **Gildemeister and Hoffmann,** *Die Aetherischen Oele*, Vol. 3c, Akademie Verlag, 1963, 291.

For further information on *d*-camphor see the following:

Gilman, H. (Ed.), *Organic Chemistry*, Vol. 4, John Wiley & Sons, 1953, 2907 ff.

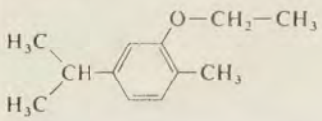
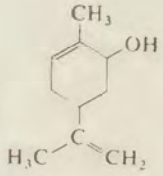
Simonsen, *The Terpenes*, Vol. 2, Cambridge University Press, 1947, 373 ff.

	Carvacrol
Other names	2-*p*-Cymenol 2-Hydroxy-*p*-cymene Isopropyl-*o*-cresol Isothymol 2-Methyl-5-isopropyl phenol
Empirical formula	$C_{10}H_{14}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless or yellowish, thick liquid
Molecular weight	150.22
Melting point	0–1°C
Boiling point	236–237°C
Flash point	100°C
Specific gravity	0.9743 at 21°C; 0.974–0.979 at 25°C
Refractive index	1.5209 at 21°C; 1.5210–1.5260 at 20°C
Solubility	Insoluble in water; soluble in alcohol and ether
Organoleptic characteristics	Characteristic pungent, warm odor. The commercial product consists of a mixture of isomers differing because of the position of the isopropyl radical. The technical and pure quality are different because of the odor characteristics.
Synthesis	From *p*-cymene by sulfonation and subsequent alkali fusion[6,7]
Natural occurrence	Occurs in the bark oil of *Thuja articulata*,[8] camphor oil,[9] in the oils of *Monarda citriodora*[10] and *Monarda fistulosa*,[11] in some species of *Satureja*,[12–14] in the oil of various species of *Origanum*,[15–17] *Thymus*,[18–20] *Thymbra spicata* L.,[21] in the seed oil of *Ptychotis ajowan* D.C.,[22] and others
Reported uses[3]	Non-alcoholic beverages 26 ppm Ice cream, ices, etc. 34 ppm Candy 92 ppm Baked goods 120 ppm Condiments 37 ppm
Regulatory status	FDA 121.1164; FEMA No. 2245

REFERENCES

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

6. **Hixson and McKee,** *Chem. Zentralbl.*, 2, 851, 1919.
7. **Gibbs and Phillips,** *J. Ind. Eng. Chem.*, 12, 145, 1920.
8. **Grimal,** *Compt. Rend.*, 139, 927, 1904.
9. *Schimmel Ber.*, October 1902.
10. **Prandel,** *Pharm. Rev.*, 22, 153, 1904.
11. **Kremers,** *Chem. Zentralbl.*, 2, 41, 1897.
12. **Jahns,** *Chem. Ber.*, 15, 816, 1882.
13. **Haller,** *Compt, Rend.*, 94, 132, 1882.
14. Schimmel and Co., *Chem. Zentralbl.*, 2, 1804, 1911.
15. **Jahns,** *Arch. Pharm.*, 215, 1, 1870.
16. **Umney and Bennett,** *Chem. Zentralbl.*, 1, 360, 1906.
17. **Pickles,** *J. Chem. Soc.*, 93, 866, 1908.
18. **Jahns,** *Arch. Pharm.*, 216, 277, 1880.
19. **Palazzo and Lutri,** *Ann. Chim.* (Rome), 14, 105, 1924.
20. **Puxeddu,** *Ann. Chim.* (Rome), 16, 329, 1926.
21. Schimmel and Co., *Chem. Zentralbl.*, (81), 1755, 1910.
22. **Sobt and Singh,** *Perfum. Essent. Oil Rec.*, 14, 399, 1923.

	Carvacryl ethyl ether	Carveol	
Other names	2-Ethoxy-*p*-cymene Ethyl carvacrol Ethyl carvacryl ether	*p*-Mentha-6,8-dien-2-ol 1-Methyl-4-isopropenyl-6-cyclohexen-2-ol	
Empirical formula	$C_{12}H_{18}O$	$C_{10}H_{16}O$	
Structure			
Physical/chemical characteristics[5]		*cis*-**Carveol**[7]	*trans*-**Carveol**[7]
Appearance	Oily, light liquid		
Molecular weight	178.27		
Boiling point	235°C	101°C (*dl*- at 10 mm Hg) 108°C (*dl*- at 16 mm Hg)	102.2–102.4°C (*d*- at 10 mm Hg) 108°C (*dl*- at 16 mm Hg)
Specific gravity		*dl*-, 0.9521 at 25°C	*d*-, 0.9484; *dl*-, 0.9510 at 18°C
Refractive index		*dl*-, 1.4959 at 25°C *dl*-, 1.4972 at 18°C	*d*-, 1.4942; *dl*-, 1.4956 at 19°C
Optical rotation		*d*-, +23°9′ at 25°C; *l*-, −23°9′	*d*-, +213°1′
Organoleptic characteristics	Odor similar to carrot		
Synthesis	By passing vapors of ethyl alcohol and carvacrol over a catalyst (ThO_2) at 400–500°C[6]	The various *d*-, *l*-, and *dl*- (*cis*- and *trans*-, respectively) forms have been prepared synthetically and isolated by means of the dinitrobenzoates according to Amvers's law. They are prepared by oxidation of limonene or, better, from carvone.	
Natural occurrence	Not reported found in nature	In small amounts, sometimes esterified, it has been reported present in nature (caraway, spearmint).	
Reported uses[3]	Non-alcoholic beverages 2.0–13 ppm Ice cream, ices, etc. 10 ppm Candy 21 ppm Baked goods 3.0–39 ppm	Non-alcoholic beverages 1.5–13 ppm Ice cream, ices, etc. 3.0 ppm Candy 3.0–39 ppm Baked goods 3.0–5.0 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2246	FDA 121.1164; FEMA No. 2247	

REFERENCES

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

6. Sabatier and Maibhe, *Compt. Rend.*, 158, 611, 1914.
7. Johnston and Read, *J. Chem. Soc.* (London), p. 233, 1934.

4-Carvomenthenol

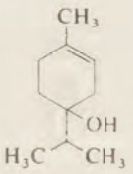
Other names

1-*p*-Menthen-4-ol
1-Methyl-4-isopropyl-1-cyclohexen-4-ol
Origanol
4-Terpinenol

Empirical formula

$C_{10}H_{18}O$

Structure



Physical/chemical characteristics[5]

	dextro	*levo*	*racemic*
Molecular weight	154.24	154.24	154.24
Boiling point	208–212°C	70–71°C (at 3 mm Hg)	92–97°C (at 14 mm Hg)
Specific gravity	0.9265 at 19°C	0.9266 at 20°C	0.9210 at 24°C
Refractive index	1.4785 at 19°C	1.47604 at 20°C	1.4778 at 24°C
Optical rotation	Approx +25°	−24°32′ at 20°C	—

Synthesis

One of several terpinenol isomers, depending on the position of the double bond and that of the hydroxyl group. This terpene, whose structure has been defined by Wallach, can be isolated by fractional distillation. It exists in nature as the *dextro*, *levo*, and racemic isomer. The synthetic product is always optically inactive. The 1-terpinenol or 1-methyl-4-isopropyl-3-cyclohexen-1-ol has been prepared by Wallach.[6]

Natural occurrence

4-Carvomenthenol (*dextro*) has been reported present in the oil of *Cupressus macrocarpa*, lavender, Spanish origanum, *Ledum palustre*, *Eucalyptus australiana* var. *A.*, *Thuja occidentalis*, etc. The *levo* form is present in the oil of *Eucalyptus dives* and in some other essences such as *Xanthoxylum rhetsa*, together with the racemic form. The racemic form is found in camphor oil.

Reported uses[3]

Non-alcoholic beverages	1.0–21 ppm
Ice cream, ices, etc.	1.0–84 ppm
Candy	7.0–63 ppm
Baked goods	7.0 ppm

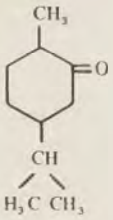
Regulatory status

FDA 121.1164; FEMA No. 2248

REFERENCES

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

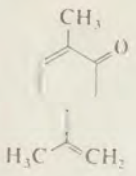
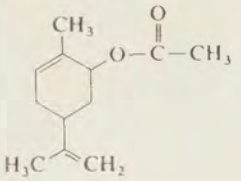
6. **Wallach**, *Annalen*, 356, 218, 1907; 362, 269, 1908.

	Carvomenthone
Other names	*p*-Menthan-2-one Tetrahydrocarvone 1-Methyl-4-isopropylcyclohexan-2-one 5-Isopropyl-2-methylcyclohexanone
Empirical formula	$C_{10}H_{18}O$
Structure	
Physical/chemical characteristics[5]	
Molecular weight	154.24
Melting point	
Boiling point	80 100°C at 12 mm Hg *l*-, *trans*-, 218–219°C at 705 mm Hg *dl*-, 220–221°C
Specific gravity	*l*-, *trans*-, 0.9001 at 30°C *dl*-, 0.900 at 20°C *l*-iso-0.9102 at 20°C *d*-, 0.9075 at 15°C
Refractive index	*l*-, *trans*- 1.4531 at 30°C *dl*-, 1.4554 at 20°C *l*-iso-1.4558 at 20°C *d*-, 1.4544 at 20°C
Optical rotation	*l*-, *trans*-, -9.33 at 30°C *l*-iso–56.5 at 20°C *d*-, +17.15 at 21°C
Solubility	Very soluble in alcohol; soluble in benzene and chloroform
Synthesis	By oxidation of carvomenthol;[6,7] from α-methyl-β′-isopropyl pimelic acid, dimethyl ester[8]
Natural occurence	Reported found in the oil of *Blumea malcomii* and *Blumea eriantha*;[9,10] a flavor component in cognac[11]
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm
Regulatory status	FEMA No. 3176

REFERENCES

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

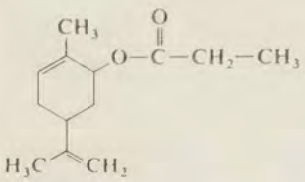
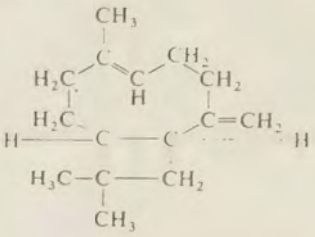
6. Bayer, *Berichte*, 26, 882, 1893.
7. Wallach, *Annalen*, 226, 133, 1893.
8. Ruzička and Trebler, *Helv. Chim. Acta*, 3, 779, 1920.
9. Simonsen and Rao, *J. Chem. Soc.*, 121, 876, 1922.
10. *Schimmel Ber.*, 8, 1937.
11. Schaefer and Timmer, *J. Food Sci.*, 35(1), 10, 1970.

	Carvone		Carvyl acetate
Other names	Carvol 6,8(9)-*p*-Menthadien-2-one 1-Menthyl-4-isopropenyl-6-cyclohexen-2-one		
Empirical formula	$C_{10}H_{14}O$		$C_{12}H_{18}O_2$
Structure			
Physical/chemical characteristics[5]	*/*-Carvone	*d*-Carvone	
Appearance	Colorless to pale straw-colored liquid[2]	Colorless to light yellow liquid	Colorless liquid
Assay	97% min[2] (as ketone content)	95% min[2]	
Molecular weight	150.21	150.21	194.27
Boiling point	230 C at 755 mm Hg	230–231 C at 763 mm Hg	115–116°C
Specific gravity	0.956–0.960 at 25 C[2]	0.956–0.960 at 25 C[2]	0.9755 at 15°C
Refractive index	1.4950–1.4990 at 20 C[2]	1.4965–1.4990 at 20 C[2]	
Optical rotation	−57.0 to −62.0[2]	50 to +60[2]	
Solubility	1:2 in 70% alcohol[4]	1:5 in 60% alcohol[2]	
Organoleptic characteristics	*/*-Carvone exhibits odor of spearmint;[2] *d*-carvone exhibits odor reminiscent of caraway[2]		Characteristic odor reminiscent of spearmint
Synthesis	Carvone occurs in the *dextro*, *levo*, and racemic form. */*-Carvone can be isolated from the essential oil of spearmint or is commercially synthesized from *d*-limonene.[2] *d*-Carvone is usually prepared by fractional distillation of oil caraway; also from dillseed and dillweed oils, but this type differs in odor and flavor.[2]		By boiling carveol with acetic anhydride and sodium acetate[6]
Natural occurrence	The optically active and inactive forms have been reported among the constituents of about 70 essential oils. The *dextro* form is present in carvi, *Anethum graveolens*, *Anethum sowa*, *Lippia carviodora*, *Mentha arvensis*, etc. The *levo* form is present in *Mentha viridis* var. *crispa*, *Mentha longifolia* from South Africa, *Eucalyptus globulus*, and several mint species. The racemic form is present in ginger grass, *Litsea guatemaleusis*, lavender, and *Artemisia fergan-ensis*.		In *Mentha crispa* and *Mentha aquatica*
Reported uses[3]	Non-alcoholic beverages 850 ppm Alcoholic beverages 130 ppm Ice cream, ices, etc. 120 ppm Candy 180 ppm Baked goods 110 ppm		Non-alcoholic beverages 1.5–11 ppm Ice cream, ices, etc. 3.0–44 ppm Candy 20 ppm Baked goods 20 ppm
Regulatory status	FDA GRAS; FEMA No. 2249		FDA 121.1164; FEMA No. 2250

REFERENCES

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

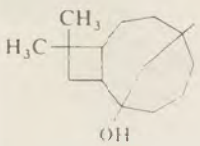
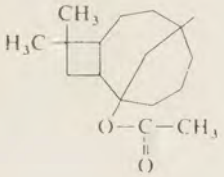
6. **Blumann and Zeitschel,** *Chem. Ber.*, 47, 2627, 1914.

	l-Carvyl propionate	β-Caryophyllene
Other names	*l-p*-Mentha-6,8-dien-2-yl propionate	Commercially known as caryophyllene
Empirical formula	$C_{13}H_{20}O_2$	$C_{15}H_{24}$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless oil
Molecular weight	208.30	204.34
Boiling point	239 C	254–257 C[6]
Specific gravity	0.95	0.909–0.910 at 16 C[6]
Refractive index		1.5004–1.5027[6]
Optical rotation		−22 C[6]
Solubility	Insoluble in water; soluble in alcohol	Soluble in alcohol; insoluble in water
Organoleptic characteristics	Sweet, warm, minty, and fruity odor; sweet, fruity, minty taste	Terpene odor, midway between that of cloves and turpentine
Synthesis	By esterification of *l*-carveol with propionic anhydride; also from α-terpinyl propionate	Isolated from oil of clove stems and separated from eugenol by treating the oil with a 7% sodium carbonate solution, extracting with ether, repeating the carbonate treatment on the concentrated extracts, and finally steam distilling[7]
Natural occurrence	Not reported found in nature	Three isomers (α-, β-, and γ-caryophyllene) are found in nature. The β-isomer is the most frequently encountered and most abundant. This sesquiterpene hydrocarbon naturally occurs in approximately 60 essential oils, mainly in that of cloves, from which it was originally isolated.[8] The chemical structure has been thoroughly studied.[9–11] Other studies have been conducted on the isolation and the dipolar moment,[12,13] as well as on its oxide.[14]
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 2.0–24 ppm Baked goods 2.0–24 ppm	Non-alcoholic beverages 14 ppm Ice cream, ices, etc. 2.0 ppm Candy 34 ppm Baked goods 27 ppm Chewing gum 200 ppm Condiments 50 ppm
Regulatory status	FDA 121.1164; FEMA No. 2251	FDA 121.1164; FEMA No. 2252

REFERENCES

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

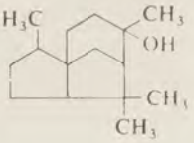
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	Caryophyllene alcohol	Caryophyllene alcohol acetate
Other names		Caryophyllene acetate
Empirical formula	$C_{15}H_{26}O$	$C_{17}H_{28}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Isomers are white crystalline solids	Crystalline solid
Molecular weight	222.36	264.41
Melting point	α-, 117 C; β-, 94–96 C	40 C
Boiling point	α-, 143–152 C at 10 mm Hg; β-, 287–297°C	149–152 C at 10 mm Hg
Specific gravity	α-, 0.9860 at 17 C	1.003 at 17°C
Refractive index	α-, 1.5010 at 17 C	1.4919 at 17 C
Optical rotation	α-, none; β-, −5.8 (alcohol)	
Solubility	Soluble in alcohol; insoluble in water	Rather soluble in alcohol and pet ether; insoluble in water
Organoleptic characteristics	Warm, moss-like, spicy odor; slightly minty, earthy flavor	Mild fruity and woody odor
Synthesis	Both isomers are obtained from caryophyllene. An ether solution of caryophyllene is treated with an ether solution of sulfuric acid monohydrate under cooling to prevent the temperature from raising above 10 C. After alkalinization of the solution, the β-caryophyllene alcohol is distilled off; from the residue where it is present as an ester, the α-caryophyllene alcohol is distilled after the ether solution has been made acid once again.	The β-caryophyllene alcohol acetate is prepared from chlordihydrocaryophyllene by boiling with acetic acid and sodium acetate[11]
Natural occurrence	The β-form occurs in the high boiling fraction of the oils of *Mentha arvensis* and *Mentha piperita*. The chemical structure of these compounds has been the subject of various investigations.[6–8] The structures of the α- and β-form are reported in references 9 and 10, respectively.	
Regulatory status	FDA 121.1164	FDA 121.1164

REFERENCES

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

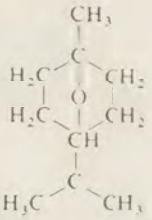
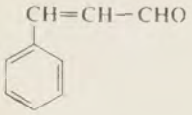
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9. *J. Am. Chem. Soc.*, 86, 1437, 1652, 1964.
10. **Robertson and Todd,** *Chem. Ind.*, p. 437, 1953.
11. **Henderson, Robertson and Kerr,** *J. Chem. Soc.*, p. 64, 1926.

	Cedarwood oil alcohols	Cedarwood oil terpenes	
Other names	Cedarwood camphor Cedrenol* Cedrol	Cedrene (indicates the terpene fraction obtained by distillation from the wood of various cedar species)	
Empirical formula	$C_{15}H_{26}O$	$C_{15}H_{24}$	
Structure			
Physical/chemical characteristics	*Note*: The physical constants refer to the purest grade of cedrol obtained by recrystallization; they do not cover the many grades obtained by distillation or fractional solidification.		
		Natural	Synthetic
Appearance	White crystals		
Molecular weight	222.36[2]	204.34	204.34
Melting point	77–80 C[2] (86 C)		
Boiling point		262–263 C	—
Specific gravity	0.98	0.9320–0.9390 at 20 C	
Refractive index		1.4989–1.5021 at 20 C	1.4983–1.4989
Optical rotation		52.8° to 71.3°	−77.67′ to 85.35′
Solubility	Soluble in benzyl benzoate; slightly soluble in glycol and mineral oil[2]	Soluble in alcohol; insoluble in water	
Organoleptic characteristics	Mild odor of cedarwood		
Synthesis	Usually obtained from cedarwood oil by fractional distillation, followed by recrystallization from suitable solvents of the appropriate solid fractions[2]	See reference 7. The natural product is also prepared from distillation of cedarwood.	
Natural occurrence	Cedrol is found in the wood of several conifers, particularly cypresses and cedars: *Cedrus atlantica*, *Cupressus sempervirens*, *Juniperus virginiana*, and others. It exhibits a positive optical rotation.[6]	A constituent of the oil of *Juniperus virginiana* and other junipers. It exists in nature in the α- and β- forms. Also found in the oils of clary sage, costus, lavender, and others. For ample description of these types of hydrocarbons, see reference 8.	
Reported uses[3]			
Regulatory status	FDA 121.1164	FDA 121.1164	

REFERENCES

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

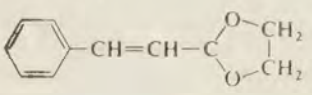
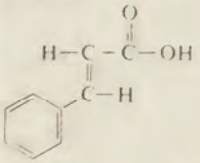
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	1,4-Cineole	Cinnamaldehyde
Other names	1,4-Epoxy-*p*-menthane	Cinnamal Cinnamic aldehyde *β*-Phenylacrolein 3-Phenylpropenal
Empirical formula	$C_{10}H_{18}O$	C_9H_8O
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Greenish-yellow liquid
Assay		98% min[2]
Molecular weight	154.24	132.15
Melting point		7.5 C
Boiling point	109–112 C (173 C) at 100 mm Hg	252 C
Flash point		120 C
Specific gravity	0.90	1.046–1.050 at 25/25 C;[2] 1.050–1.058 at 15 C
Refractive index		1.6190–1.6230 at 20 C;[2] 1.61949 at 20 C
Acid value		5 max[2]
Solubility	Almost insoluble in water; soluble in alcohol	1:5 in 60% alcohol;[2] 1:25 in 50% alcohol; 1:2.5 in 70% alcohol; almost insoluble in water
Organoleptic characteristics	Light and mild camphoraceous odor; cool, mildly spice-like flavor	Pungent, spicy note and burning taste
Synthesis	Its structure has been confirmed through synthesis.[6] For its description see reference 8.	By isolation from natural sources. Synthetically, by condensation of benzaldehyde with acetaldehyde in the presence of sodium or calcium hydroxide.[9]
Natural occurrence	Reported present in *Piper cubeba*.[7] It is also present in various essential oils: *Boldea fragrans* Juss., *Xanthoxylum rhetsa* DC, and *Ormenis multicaulis*.	It has been identified in the essential oils of: Ceylon and Madagascar cinnamon leaves, Ceylon, Seychelles, and Japanese (*Cinnamomum laureirii*) cinnamon bark, and in other cinnamon species in varying amounts (0.1–76%); also in the essential oils of: hyacinth, myrrh, Bulgarian rose, patchouli, and others.
Reported uses[3]		Non-alcoholic beverages 9.0 ppm Ice cream, ices, etc. 7.7 ppm Candy 700 ppm Baked goods 180 ppm Chewing gum 4,900 ppm Condiments 20 ppm Meats 60 ppm
Regulatory status	FDA 121.1164	FDA GRAS; FEMA No. 2286

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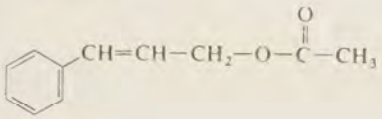
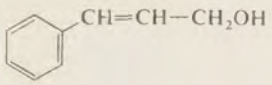
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	Cinnamaldehyde ethylene glycol acetal	Cinnamic acid
Other names	Cinnamic aldehyde ethylene glycol acetal "Cinncloval" 2-Styryl-1,3-dioxolane 2-Styryl-*m*-dioxolane	β-Phenylacrylic acid 3-Phenylpropenoic acid
Empirical formula	$C_{11}H_{12}O_2$	$C_9H_8O_2$
Structure		 *trans*-Cinnamic acid
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	White, colorless, crystalline powder
Molecular weight	176.22	148.16
Melting point		136°C; *cis*-, 57°C
Boiling point	265°C (approx.)	300°C
Specific gravity		1.2450 at 15°C; 1.285 at 15.5°C
Solubility	Insoluble in water; soluble in alcohol	Almost insoluble in water; slightly soluble in alcohol; soluble in benzene, chloroform, acetone, and essential oils
Organoleptic characteristics	Soft, warm, spicy odor reminiscent of cinnamon; sweet, spicy cinnamon-allspice flavor	Almost odorless with a burning taste, then turning sweet and reminiscent of apricot
Synthesis	From cinnamic aldehyde and ethylene glycol	Two isomers, *trans*- and *cis*-, exist. The *trans*-isomer is of interest for use in flavoring. In addition to the extraction from natural sources (storax), it can be prepared as follows: 1. From benzaldehyde, anhydrous sodium acetate, and acetic anhydride in the presence of pyridine (Perkin reaction) 2. From benzaldehyde and ethyl acetate (Claisen condensation) 3. From benzaldehyde and acetyl chloride 4. By oxidation of benzylidene acetone with sodium hypochlorite
Natural occurrence	Not reported found in nature	The *trans*-form has been found among the constituents of the essential oils of: basil, Chinese cinnamon, *Melaleuca bracteata*, *Alpinia galanga*, and in Peru balsam, Asian and American storax, cocoa leaves, etc. The *cis*-form is present in the oil of *Alpinia malacensis*.
Reported uses[3]	Candy 0.06–2.0 ppm Baked goods 2.0 ppm Condiments 5.0 ppm	Non-alcoholic beverages 31 ppm Ice cream, ices, etc. 40 ppm Candy 30 ppm Baked goods 36 ppm Chewing gum 10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2287	FDA 121.1164; FEMA No. 2288

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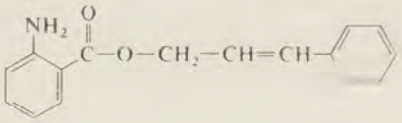
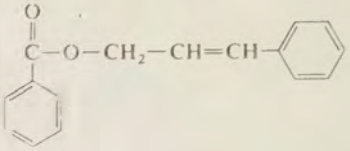
For References 1–5, see end of Part III.

	Cinnamyl acetate	Cinnamyl alcohol
Other names		Cinnamic alcohol γ-Phenylallyl alcohol 3-Phenyl-2-propen-1-ol Styryl carbinol
Empirical formula	$C_{11}H_{12}O_2$	$C_9H_{10}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to yellowish liquid	White to yellowish solid
Assay	98% min	98% min[2]
Molecular weight	176.22	134.17
Melting point		33°C
Boiling point	265°C (114°C at 3 mm Hg)	257.5°C
Freezing point		>31°C[2]
Flash point	118°C	126°C
Specific gravity	1.047–1.051 at 25°C; 1.050 at 15.5°C	1.0440 at 20°C
Refractive index	1.5400–1.5430 at 20°C; 1.5300 at 20°C	1.5819 at 20°C
Aldehyde content		Not more than 1.5%[2] (as cinnamic aldehyde)
Solubility	Insoluble in water; 1:5 in 70% alcohol; soluble in most organic solvents	Somewhat soluble in water; 1:2 in 60% alcohol; soluble in most organic solvents
Organoleptic characteristics	Characteristic balsamic-floral odor and burning, sweet taste reminiscent of pineapple. The ester obtained from natural cinnamyl alcohol exhibits a more delicate (hyacinth, jasmine-like) note.	Pleasant, floral odor and bitter taste
Synthesis	By acetylation of cinnamyl alcohol with acetic acid[6]	Obtained originally by saponification of cinnamyl cinnamate (styracin). This method of extraction from storax is still usable. Synthetically, by reduction of cinnamaldehyde with sodium or potassium hydroxide
Natural occurrence	Reported in the essential oil of mimosa (black wattle)	Occurring as an ester or in the free state in several natural products: cinnamon leaves, hyacinth, *Aristolochia clematis*, and *Xanthorrhoea hastilis*; also in the essence of daffodil flowers[7]
Reported uses[3]	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 6.5 ppm Candy 16 ppm Baked goods 11 ppm Chewing gum 8.7 ppm Condiments 2.0 ppm	Non-alcoholic beverages 8.8 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 8.7 ppm Candy 17 ppm Baked goods 33 ppm Gelatins and puddings 22 ppm Chewing gum 720 ppm
Regulatory status	FDA 121.1164; FEMA No. 2293	FDA 121.1164; FEMA No. 2294

REFERENCES

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

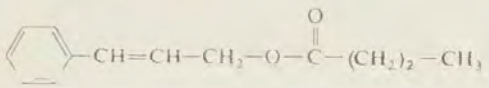
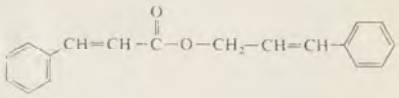
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7. Igolen, *Chem. Abstr.*, 43, 2373, 1949.

	Cinnamyl anthranilate	Cinnamyl benzoate
Other names	Cinnamyl 2-aminobenzoate Cinnamyl *o*-aminobenzoate	
Empirical formula	$C_{16}H_{15}NO_2$	$C_{16}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Brownish powder	White, crystalline powder
Assay	96% min	
Molecular weight	253.30	238.29
Melting point	>60°C	31°C
Boiling point	332°C	209°C (335°C) at 13 mm Hg
Specific gravity	1.180 at 15.5°C	1.04 (liquid)
Refractive index		
Solubility	1 gm dissolves in 20 ml of 95% alcohol	Soluble in alcohol; insoluble in water
Organoleptic characteristics	Balsamic, fruity odor somewhat reminiscent of grape	Characteristic balsamic, aromatic, spicy odor
Synthesis	By esterification of anthranilic acid with cinnamyl alcohol	From cinnamyl alcohol and benzoyl chloride in pyridine[6]
Natural occurrence	Not reported found in nature	In Siam benzoin[7,8]
Reported uses[3]	Non-alcoholic beverages 6.8 ppm Ice cream, ices, etc. 1.7 ppm Candy 4.3 ppm Baked goods 5.3 ppm Gelatins and puddings 28 ppm Chewing gum 46–730 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2295	FDA 121.1164

REFERENCES

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

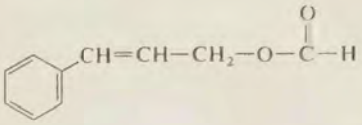
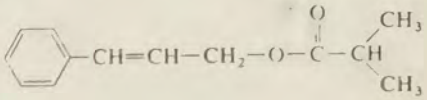
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8. Reinitzer, *Arch. Pharm.* (Wernheim), 264, 132, 1926.

	Cinnamyl butyrate	Cinnamyl cinnamate
Other names	Phenyl propenyl-*n*-butyrate	Cinnamyl β-phenyl acrylate Cinnamyl 3-phenyl propenoate Phenylallyl cinnamate Styracin
Empirical formula	$C_{13}H_{16}O_2$	$C_{18}H_{16}O_2$
Structure		
Physical chemical characteristics[2]		
Appearance	Colorless to yellowish liquid	Low-melting, crystalline solid
Assay	98% min	
Molecular weight	204.27	264.31
Melting point		44 C
Boiling point	300 C	
Flash point	>100 C	
Specific gravity	1.010-1.015 (1.02) at 25/25 C	1.1565 at 4 C
Refractive index	1.525-1.528 at 20 C	
Acid value	3 max	
Solubility	1:5 in 80% alcohol; insoluble in water	Insoluble in water; 1:20 in cold alcohol; 1:3 in boiling alcohol and in ether
Organoleptic characteristics	Fruity, slightly floral odor and sweet taste reminiscent of honey; used in orange and citrus flavors	Characteristic, faintly sweet, resinous odor
Synthesis	By esterification of cinnamic alcohol with *n*-butyric acid	It can be extracted from storax; synthetically, by prolonged reaction of aluminum ethylate with cinnamic aldehyde in absolute ether[6]
Natural occurrence	Not reported found in nature	One of the most important constituents of storax: *Liquidambar orientale*,[7-9] *Liquidambar styraciflua* L.;[10,11] also in white Peru and Honduras balsams[12-14]
Reported uses[3]	Non-alcoholic beverages 1.6 ppm Ice cream, ices, etc. 8.5 ppm Candy 7.6 ppm Baked goods 11 ppm Gelatins and puddings 1.2 ppm	Non-alcoholic beverages 0.81 ppm Ice cream, ices, etc. 1.5 ppm Candy 10 ppm Baked goods 7.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2296	FDA 121.1164; FEMA No. 2298

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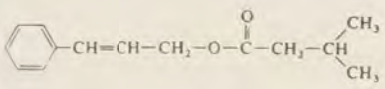
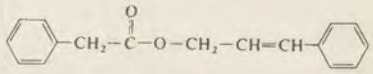
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13. Hellstrom, *Arch. Pharm.*, 243, 234, 1905.
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	Cinnamyl formate	Cinnamyl isobutyrate
Other names		
Empirical formula	$C_{10}H_{10}O_2$	$C_{13}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to yellowish liquid	Colorless to yellowish liquid
Assay	92% min	96% min
Molecular weight	162.18	204.27
Boiling point	250°C	254°C
Flash point	100°C	>100°C
Specific gravity	1.074–1.079 at 25°C; 1.040 at 15.5°C	1.008–1.014 (1.01) at 25°C
Refractive index	1.5500–1.5560 (1.5680) at 20°C	1.5230–1.5280 at 20°C
Acid value	3 max	3 max
Solubility	1:10 in 70% alcohol; 1:2 in 80% alcohol; insoluble in water; soluble in most organic solvents	1:2 in 70% alcohol; insoluble in water; poorly soluble in propylene glycol
Organoleptic characteristics	Balsamic, fruital-floral odor and bittersweet taste reminiscent of apple	Sweet, balsamic, fruital odor and sweet taste reminiscent of apple and banana
Synthesis	By esterification of cinnamyl alcohol with formic acid	By esterification of cinnamic alcohol with isobutyric 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. 9.1 ppm Candy 6.9 ppm Baked goods 8.0 ppm Chewing gum 0.60 ppm	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 5.0 ppm Candy 7.7 ppm Baked goods 8.5 ppm Gelatins and puddings 0.02–1.2 ppm Chewing gum 140 ppm Toppings 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2299	FDA 121.1164; FEMA No. 2297

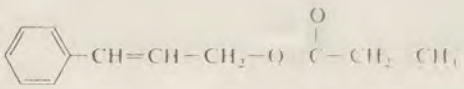
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For References 1–5, see end of Part III.

	Cinnamyl isovalerate	Cinnamyl phenylacetate
Other names		Cinnamyl α-toluate
Empirical formula	$C_{14}H_{18}O_2$	$C_{17}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to yellowish liquid	Colorless liquid
Assay	95% min	
Molecular weight	218.29	252.32
Melting point		
Boiling point	313°C	333–335°C
Flash point	>100°C	
Specific gravity	0.991–0.995 (1.00) at 25°/25°C	1.086 (1.09) at 15.5°C
Refractive index	1.5180–1.5240 at 20°C	
Acid value	3 max	
Solubility	1:1 in 90% alcohol; insoluble in water; poorly soluble in propylene glycol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Characteristic rose-like odor; apple-like taste	Deep, rich, chrysanthemum-like odor; spicy, honey-like flavor
Synthesis	By esterification of cinnamic alcohol with isovaleric acid	From cinnamylchloride and sodium phenylacetate; also by esterification
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.2 ppm Ice cream, ices, etc. 2.6 ppm Candy 4.1 ppm Baked goods 3.6 ppm Gelatins and puddings 11 ppm Chewing gum 19–30 ppm	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 0.25–2.0 ppm Candy 7.3 ppm Baked goods 7.3 ppm
Regulatory status	FDA 121.1164; FEMA No. 2302	FDA 121.1164; FEMA No. 2300

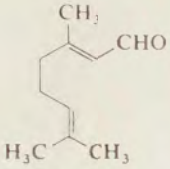
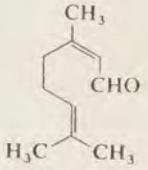
REFERENCES

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

	Cinnamyl propionate
Other names	γ-Phenylallyl propionate 3-Phenyl-2-propenyl propanoate
Empirical formula	$C_{12}H_{14}O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless to yellowish liquid
Assay	95% min (98%)
Molecular weight	190.24
Melting point	
Boiling point	289°C
Flash point	>100°C (95°C)
Specific gravity	0.991–0.995 at 25°/25°C; 1.0370–1.0410 at 15°C
Refractive index	1.5180–1.5240 (1.5330–1.5360) at 20°C
Acid value	3 max (0.9)
Solubility	1:1 in 90% alcohol; 1:2.5–3.5 in 80% alcohol; insoluble in water
Organoleptic characteristics	Spicy, fruital odor with a woody, balsamic undernote; sweet, warm, powerful, spicy taste
Synthesis	By esterification of cinnamic alcohol with propionic acid
Natural occurrence	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 4.3 ppm Candy 7.5 ppm Baked goods 8.8 ppm Gelatins and puddings 2.4–4.0 ppm Chewing gum 20–53 ppm
Regulatory status	FDA 121.1164; FEMA No. 2301

REFERENCES

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

	Citral (Neral)
Other names	Geranial: 2-*trans*-3,7-dimethyl-2,6-octadien-1-al Neral: 2-*cis*-3,7-dimethyl-2,6-octadien-1-al
Empirical formula	$C_{10}H_{16}O$
Structure	 Geranial  Neral
Physical/chemical characteristics[5]	
Appearance	Mobile, pale-yellow liquid
Assay	Not less than 96%[2] (88%)
Molecular weight	152.23
Boiling point	103–104°C at 12 mm Hg from lemon; 106–107°C at 12 mm Hg from lemongrass
Flash point	92°C (>100°C)
Specific gravity	0.885–0.891[2] (0.881–0.889) at 25°/25°C
Refractive index	1.4860–1.4900[2] (1.4820–1.4910) at 20°C
Acid value	5.0 max
Solubility	1:7 in 60% alcohol;[2] nearly insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Strong, lemon-like odor; characteristic bittersweet taste
Synthesis	Citral is usually isolated from the citral-containing oil by chemical means or by chemical synthesis (from β-pinene, isoprene, etc.)
Natural occurrence	Commercially, the product is a mixture of two geometric isomers—α-citral and β-citral, each exhibiting *cis*- and *trans*-isomers because of the position of the double bond. Originally reported found in lemongrass oil (*Cymbopogon flexuosus* (Nees.) Stapf.) in amounts up to 75%.[6–9] Also reported found in: *Litsea citrata* (approx. 90%), *Litsea cubeba* Blume. (approx. 70%), *Lindera citriodora* (approx. 65%), *Backhousia citriodora* (approx. 95–97%), *Calypranthes parriculata* (approx. 62%), *Leptospermum liversidgei* var. *A.* leaves (approx. 70–80%), and *Ocimum gratissimum* (approx. 66.5%). Also present in lemon (2–5%), lime (6–9%), and *Citrus aurantifolia* leaves (petitgrain, approx. 36%).[10]
Reported uses[3]	Non-alcoholic beverages 9.2 ppm Ice cream, ices, etc. 23 ppm Candy 41 ppm Baked goods 43 ppm Chewing gum 170 ppm
Regulatory status	FDA GRAS; FEMA No. 2303

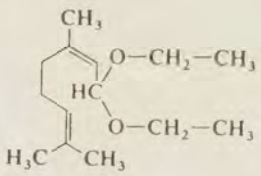
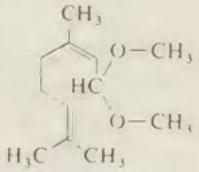
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For References 1–5, see end of Part III.

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7. **Dodge,** *J. Am. Chem. Soc.*, 12, 553, 1890.
8. **Barbier and Bouveault,** *C. R. Hebd. Séances Acad. Sci. Paris*, 131, 1159, 1895.
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10. **Payron,** *Fr. Ses Parfums*, 2(12), 41, 1959.

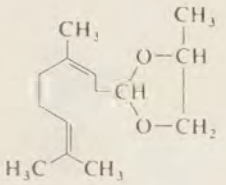
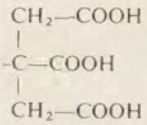
For further information on citral see the following:

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Hibbert and Cannon, *J. Am. Chem. Soc.*, 46, 119, 1924.
Yamashita and Matsumura, *J. Chem. Soc. Jap.*, 64, 506, 1943.
Lauchenauer and Schinz, *Helv. Chim. Acta*, 32, 1273, 1949.
Stoll and Commarmont, *Helv. Chim. Acta*, 32, 1354, 1949.
Wagner and Jauregg, *Annalen*, 488, 176, 1931; 496, 52, 1932.
Lennartz, *Ber. Dtsch. Chem. Ges.*, 76, 831, 1943.
Lebedewa et al., *J. Gen. Chem. USSR*, 28, 904, 1958.
Sancy et al., *Chimia*, 12, 326, 1958; *Helv. Chim. Acta*, 42, 1945, 1959.
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Mitchell and Strauss, *Perfum. Essent. Oil Rec.*, 39, 312, 1948.
Tiemann, *Ber. Dtsch. Chem. Ges.*, 32, 117, 1899; 33, 880, 1900.
Naves, *Bull. Soc. Chim. Fr.*, p. 521, 1952.
Nadal, Chapel and Lecumberry, *Am. Chem. Perfum. Cosmet.*, 79(4), 43, 1964.

	Citral diethyl acetal	Citral dimethyl acetal
Other names	1,1-Diethoxy-3,7-dimethyl-2,6-octadiene 3,7-Dimethyl-2,6-octadienal diethylacetal	1,1-Dimethoxy-3,7-dimethyl-2,6-octadiene 3,7-Dimethyl-2,6-octadienal dimethylacetal
Empirical formula	$C_{14}H_{26}O_2$	$C_{12}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to yellowish liquid
Assay		93% min
Molecular weight	226.36	198.31
Melting point		
Boiling point	230°C	Approx 198°C
Flash point	79°C	70°C
Specific gravity	0.8745–0.8790 at 15°C	0.883–0.888 at 25°/25°C
Refractive index	1.4520–1.4545 at 20°C	1.4560–1.4630 at 20°C
Aldehyde content	11% max	
Solubility	1:2–2.6 in 80% alcohol; almost insoluble in water; soluble in propylene glycol	1:5 in 70% alcohol and 1:1 in 80% alcohol
Organoleptic characteristics	Mild, green, citrus odor; green, oily, citrus-peel flavor	Fresh, lemon-like odor. The commercial product consists of a mixture of *cis*- and *trans*-isomers.
Synthesis	From ethyl orthoformate and citral	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.03 ppm Candy 0.13 ppm Condiments 110 ppm	Non-alcoholic beverages 6.3 ppm Ice cream, ices, etc. 11 ppm Candy 60 ppm Baked goods 60 ppm Chewing gum 15 ppm
Regulatory status	FDA 121.1164; FEMA No. 2304	FDA 121.1164; FEMA No. 2305

REFERENCES

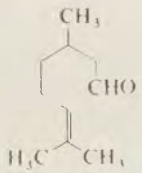
For References 1–5, see end of Part III.

	Citral propylene glycol acetal	Citric acid
Other names		2-Hydroxy-1,2,3-propanetricarboxylic acid
Empirical formula	$C_{13}H_{22}O_2$	$C_6H_8O_7$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	White solid
Molecular weight	210.32	192.12
Melting point		153° C (anhydrous)
Solubility	Slightly soluble in water (with some decomposition); soluble in propylene glycol, alcohol, and oils	Extremely soluble in water and alcohol; slightly soluble in ether
Organoleptic characteristics	Sweet, citrus, lemon-orange odor; mild, lemony flavor changing to a lemon flavor in aqueous media	Pleasant acid taste; odorless
Synthesis	Condensation of citral with propylene glycol using a catalyst	By mycological fermentation using molasses and strains of *Aspergillus niger*; from citrus juices and pineapple wastes
Natural occurrence	Not reported found in nature	Extremely widespread in nature; also identified in the flowers of *Hibiscus subdariffa*[6]
Reported uses[3]		Non-alcoholic beverages 2,500 ppm Ice cream, ices, etc. 1,600 ppm Candy 4,300 ppm Baked goods 1,200 ppm Chewing gum 3,600 ppm
Regulatory status		FDA GRAS; FEMA No. 2306

REFERENCES

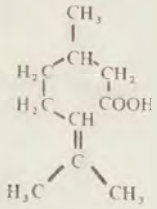
For References 1–5, see end of Part III.

6. **Indovina and Capotummino,** *Chem. Zentralbl.*, 2, 1295, 1939.

	Citronellal
Other names	3,7-Dimethyl-6-octenal 3,7-Dimethyl-6-octen-1-al Rhodinal (*dextro*-rotatory form)
Empirical formula	$C_{10}H_{18}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless to slightly yellow liquid
Assay	Not less than 85%[2]
Molecular weight	154.24
Boiling point	*d*-, 69–71°C at 5 mm Hg *l*-, 88°C at 10.5 mm Hg *dl*-, 106–108°C at 15 mm Hg
Flash point	77°C
Specific gravity	0.850–0.860 at 25°/25°C[2]
Refractive index	1.4460–1.4560 at 20°C[2]
Optical rotation	−1° to +11°[2]
Acid value	<3.0[2]
Solubility	1:5 in 70% alcohol;[2] insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Intense lemon-, citronella-, rose-type odor
Synthesis	Can be prepared by chemical synthesis or by fractional distillation of natural oils, such as citronella. Industrially prepared by hydrogenation of β-citronellol or by catalytic hydrogenation of citral;[b] also in the laboratory by dehydration of hydroxydihydrocitronellal.
Natural occurrence	The *d*-form of citronellal has been reported in the oil of citronella (Ceylon, Jammus, Kaschmis), in the oil from leaves of *Barosma pulchella*, in the oil from roots of *Phebalium nudum*, in the oils of *Eucalyptus citriodora*, *Leptospermum citratum*, and *Baeckea citriodora*. The *l*-form is present in the oils of: *Backhousia citriodora* var. *A*, *Eucalyptus citriodora*, *Litsea cubeba* (fruits), and lemongrass. Citronellal in general also is present in the oils of lemon, mandarin, *Lavandula delphinensis*, *Ocimum canum* f. *citrata*, and others.
Reported uses[3]	Non-alcoholic beverages 4.0 ppm Ice cream, ices, etc. 1.3 ppm Candy 4.5 ppm Baked goods 4.7 ppm Gelatins and puddings 0.60 ppm Chewing gum 0.30 ppm
Regulatory status	FDA 121.1164; FEMA No. 2307

REFERENCES

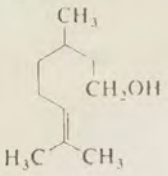
For References 1–5, see end of Part III.
6. Paal, German Patent 298,193.

	Citronellic acid
Other names	3,7-Dimethyl-6-octenoic acid; Rhodinic acid; Rhodinolic acid
Empirical formula	$C_{10}H_{18}O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid
Molecular weight	170.25
Boiling point	*d*-, 139–140°C at 10 mm Hg; *l*-, 117–119°C at 0.6 mm Hg; *dl*-, 126°C at 4 mm Hg
Specific gravity	*d*-, 0.9308 at 20°C; *l*-, 0.9274 at 25°C; *dl*-, 0.9557 at 15°C
Refractive index	*d*-, 1.4561 at 21.5°C; *l*-, 1.4563 at 24°C; *dl*-, 1.4606 at 20°C
Optical rotation	*d*-, +2.48; *l*-, −2.49
Solubility	Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Green-grassy odor
Synthesis	By oxidation of citronellal; also by the conversion of pulegone[6]
Natural occurrence	The *d*-form is reportedly a constituent of Java citronella,[7] geranium, *Borosma pulchellum*, *Xanthoxylum piperitum*,[8] bitter-orange leaves,[9] lemon grass,[10] *Calytrix virgata*,[11] and *Calytrix tetragona*[12] leaves; the *l*-form has been reportedly identified in cypress oil (*Callitris glauca* R. Br.),[13] *Callitris intratropica*,[14] in the oil of *Chamaecyparis obtusa*,[15] and of *Thujopsis dolabrata*;[16] the *dl*-form is isolated from camphor oil[17]
Reported uses[3]	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	FEMA No. 3142

REFERENCES

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

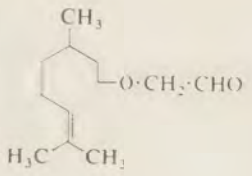
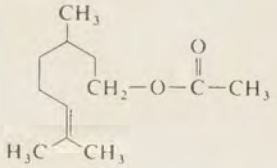
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7. Liu, *cfr.*, *Schimmel Ber.*, 32, 1955.
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9. Uchida, *Chem. Zentralbl.*, 2, 2197, 1928.
10. Naves, *Chem. Zentralbl.*, 2, 329, 1931.
11. Penfold and Morrison, *Chem. Zentralbl.*, 2, 2300, 1934.
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13. Neuhaus and Reuter, *Schimmel Ber.*, 12, 1951.
14. Trikojus and White, *Chem. Zentralbl.*, 2, 1456, 1935.
15. Nozoe, *Chem. Zentralbl.*, 2, 3142, 1936.
16. Nozoe et al., *Chem. Abstr.*, 46, 11585, 1952.
17. Rochussen, *J. Prakt. Chem.*, 105(2), 124, 1922.

	Citronellol
Other names	*d*-Citronellol 3,7-Dimethyl-6-octen-1-ol For the *l*-form see Rhodinol
Empirical formula	$C_{10}H_{20}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid[2]
Assay	90% min[2]
Molecular weight	156.26
Melting point	
Boiling point	*l*-, 103°C at 5 mm Hg *d*-, 105–105.5°C at 15 mm Hg
Flash point	102°C
Specific gravity	0.850–0.860 at 25°/25°C[2]
Refractive index	1.4540–1.4620 at 20°C[2]
Optical rotation	−1° to +5°[2]
Ester content	Not more than 1% (as citronellyl acetate)[2]
Aldehyde content	Not more than 1% (as citronellal)[2]
Solubility	1:2 in 70% alcohol;[2] very slightly soluble in water; soluble in most organic solvents
Organoleptic characteristics	Rose-like odor. Because odor plays such an important part in selecting this material, there may be special grades of citronellol that do not meet the E.O.A. specification. These limits have been broadened enough to include best qualities of commercial citronellol and chemically pure citronellol. *l*-Citronellol has a sweet, peach-like flavor; *d*-citronellol has a bitter taste.
Synthesis	It is generally accepted to distinguish rhodinol as the product isolated from geranium consisting of a mixture of *l*-citronellol and geraniol, whereas the name *l*-citronellol should be used to indicate the corresponding synthetic product with the highest level of purity. *dl*-Citronellol can be prepared by catalytic hydrogenation of geraniol[6] or by oxidation of allo-cymene.[7] *l*-Citronellol is prepared from (−) *d*-pinene via (±) *cis*-pinene to (−) 2,6-dimethyl-2,7-octadiene and finally isolating *l*-citronellol by hydrolysis of the aluminum-organo compound.
Natural occurrence	*l*-Citronellol has been found in nature in the plants of the *Rosaceae* family; *d*- and *dl*-citronellol have been identified in: *Verbenaceae*, *Labiatae*, *Rutaceae*, *Geraniaceae*, and others. Citronellol has been reported in about 70 essential oils and in the oil of *Rosa bourbonia*.[8] The Bulgarian rose oil has been reported to contain more than 50% *l*-citronellol, whereas East African geranium contains more than 80% of the *d*-isomer.[9] The natural product is always optically active. For identification see references 10, 11, 12, and 13.
Reported uses[5]	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 4.1 ppm Candy 16 ppm Baked goods 18 ppm Gelatins and puddings 5.8 ppm Chewing gum 29–52 ppm
Regulatory status	FDA 121.1164; FEMA No. 2309

REFERENCES

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

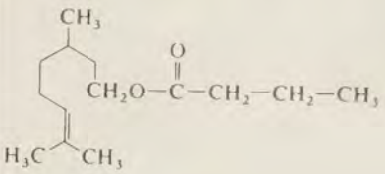
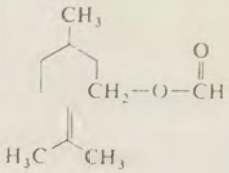
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9. Glichitch et al., *Parfums Fr.*, 5, 361, 1927.
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11. Naves, *C. R. Hebd. Séances Acad. Sci. Paris*, 237, 146, 1953.
12. Carrol et al., *J. Chem. Soc.* (London), p. 3457, 1950.
13. Nave, *Perfum. Essent. Oil Rec.*, 49, 290, 1958.

	Citronellyl oxyacetaldehyde	Citronellyl acetate
Other names		3,7-Dimethyl-6-octen-yl acetate
Empirical formula	$C_{12}H_{22}O_2$	$C_{12}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Assay		92% min[2]
Molecular weight	198.28	198.31
Boiling point	130°C at 12 mm Hg	240°C; 119–121°C at 15 mm Hg
Specific gravity		0.883–0.890 at 25°/25°C[2]
Refractive index		1.4400–1.4500 at 20°C[2]
Optical rotation		−1° to +4°[2]
Acid value		Not more than 1[2]
Solubility		1:9 in 70% alcohol;[2] soluble in most organic solvents
Organoleptic characteristics	Strong, rose odor	Fresh, fruity odor reminiscent of rose; pungent taste at the beginning, turning to sweet, apricot-like taste afterwards
Synthesis	Interaction of bromoacetals with sodium or potassium alcoholates[6–10]	By direct acetylation of citronellol (natural or synthetic). Its physical-chemical characteristics vary, depending on the quality of the starting alcohol.
Natural occurrence	Not reported found in nature	Reported in the oil of citronella and, more recently, in *Chamaecyparis lawsoniana* Parl.
Reported uses[3]	Non-alcoholic beverages 0.005–1.0 ppm Ice cream, ices, etc. 1.4 ppm Candy 4.1 ppm Baked goods 4.3 ppm	Non-alcoholic beverages 3.4 ppm Ice cream, ices, etc. 4.2 ppm Candy 7.5 ppm Baked goods 9.7 ppm Gelatins and puddings 0.71–3.7 ppm Chewing gum 6.9–600 ppm
Regulatory status	FDA 121.1164; FEMA No. 2310	FDA 121.1164; FEMA No. 2311

REFERENCES

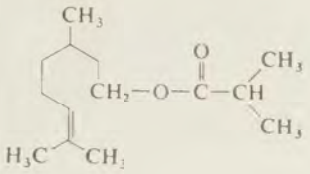
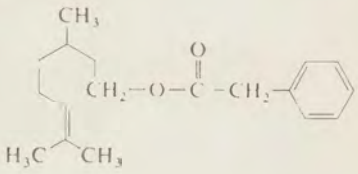
For References 1–5, see end of Part III.

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7. Sabetay, *Bull. Soc. Chim. Fr.*, 45, 1161, 1929.
8. Sabetay et al., *Compt. Rend.*, 194, 617, 1932; 196, 1508, 1933.
9. Rothart, *Compt. Rend.*, 196, 2013, 1933; 197, 1225, 1933.
10. Shoruigin and Korshak, *Berichte*, 68, 838, 1935; *Maslob. Zhir. Delo*, 11, 275, 1935; *Chem. Abstr.*, 29, 7941, 1935.

	Citronellyl butyrate	Citronellyl formate
Other names	3,7-Dimethyl-6-octen-l-yl butyrate	3,7-Dimethyl-6-octen-l-yl formate
Empirical formula	$C_{14}H_{26}O_2$	$C_{11}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Assay	90% min (97% min)	86% min[2] (95% min)
Molecular weight	226.36	184.28
Boiling point	134–135°C at 12 mm Hg	97–98°C at 11 mm Hg; 235°C at 760 mm Hg
Flash point	>100°C (119°C)	92°C (93°C)
Specific gravity	0.873–0.883 at 25°/25°C; 0.880–0.886 at 15°C	0.890–0.903 at 25°/25°C;[2] 0.898–0.902 at 15°C
Refractive index	1.444–1.448 (1.4400–1.4440) at 20°C	1.4430–1.4490[2] (1.4400–1.4440) at 20°C
Optical rotation	+1°30′	±1°30′
Acid value	Not more than 1 (0.06)	Not more than 3 (0.2)
Solubility	1:6 to 1:9 in 80% alcohol (1:5 to 1:6.5)	1:2–1:3 in 80% alcohol;[2] insoluble in water
Organoleptic characteristics	Strong, fruity, and rose-like odor with sweet, plum-like taste	Strong, fruity, rose-like odor with a sweet, fruity taste
Synthesis		By direct esterification of citronellol with formic acid
Natural occurrence	Reported in Ceylon citronella oil	Reported present in geranium essential oil and in the oils of *Rosa borbonica*, *Cupressus lusitanica*, and others
Reported uses[3]	Non-alcoholic beverages 3.8 ppm Ice cream, ices, etc. 11 ppm Candy 13 ppm Baked goods 11 ppm Gelatins and puddings 3.1–4.2 ppm Chewing gum 2.3 ppm	Non-alcoholic beverages 14 ppm Ice cream, ices, etc. 13 ppm Candy 19 ppm Baked goods 32 ppm Chewing gum 63–100 ppm
Regulatory status	FDA 121.1164; FEMA No. 2312	FDA 121.1164; FEMA No. 2314

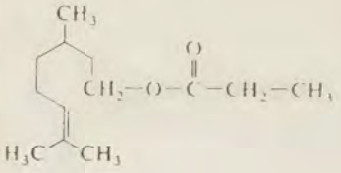
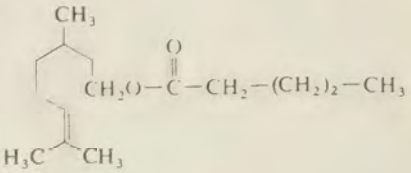
REFERENCES

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

	Citronellyl isobutyrate	Citronellyl phenylacetate
Other names	3,7-Dimethyl-6-octen-l-yl isobutyrate	Citronellyl α-toluate 3,7-Dimethyl-6-octen-l-yl phenylacetate
Empirical formula	$C_{14}H_{26}O_2$	$C_{18}H_{26}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Assay	92% min (96%)	
Molecular weight	226.36	274.41
Boiling point	249°C	342°C
Flash point	100 C (95 C)	
Specific gravity	0.870–0.880 at 25°/25°C; 0.8760–0.8830 at 15 C	0.992 at 15.5°C
Refractive index	1.4400–1.4480 (1.4375–1.4440) at 20°C	1.5100 at 20°C
Optical rotation	±1.30°	
Acid value	1 max (0.09)	
Solubility	1:6 in 80% alcohol (1:4.5–1:5.5); 1:1 in 90% alcohol; almost insoluble in water and propylene glycol	
Organoleptic characteristics	Sweet, fruity, and rose-like odor with a slightly sweet, apricot-like taste	Sweet, faintly honey, rose-like odor with a definite waxy undertone
Synthesis	By direct esterification of citronellol with isobutyric acid via azeotropic conditions or using isobutyric anhydride	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.3 ppm Ice cream, ices, etc. 1.7 ppm Candy 8.2 ppm Baked goods 12 ppm Gelatins and puddings 3.1 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 0.95 ppm Candy 2.4 ppm Baked goods 17 ppm
Regulatory status	FDA 121.1164; FEMA No. 2313	FDA 121.1164; FEMA No. 2315

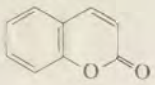
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For References 1–5, see end of Part III.

	Citronellyl propionate	Citronellyl valerate
Other names	3,7-Dimethyl-6-octen-l-yl propionate	3,7-Dimethyl-6-octen-l-yl valerate
Empirical formula	$C_{13}H_{24}O_2$	$C_{15}H_{28}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid
Assay	90% min (97%)	
Molecular weight	212.33	240.39
Boiling point	120–124°C (242°C) at 14 mm Hg	237°C (195°C at 31 mm Hg)
Flash point	>100°C (99°C)	
Specific gravity	0.877–0.883 at 25°/25°C; 0.8810–0.8840 at 20°C	0.890 at 15.5°C
Refractive index	1.4430–1.4490 (1.4400–1.4425) at 20°C	1.4435 at 20°C
Optical rotation	±1.50°	
Acid value	1 max (0.2)	
Solubility	1:3 in 80% alcohol (1:2.5 to 1:4)	Characteristic rose, herb, honey-like odor
Organoleptic characteristics	Rose-like odor; bittersweet, plum-like taste	
Synthesis	By direct esterification of citronellol with propionic acid under azeotropic conditions on using propionic anhydride	
Natural occurrence	In tomato	Reported in the essence of *Boronia citriodora*
Reported uses[3]	Non-alcoholic beverages 3.1 ppm Ice cream, ices, etc. 9.0 ppm Candy 18 ppm Baked goods 19 ppm Chewing gum 0.80–15 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 2.5 ppm Candy 3.0 ppm Baked goods 7.7 ppm
Regulatory status	FDA 121.1164; FEMA No. 2316	FDA 121.1164; FEMA No. 2317

REFERENCES

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

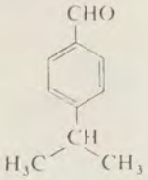
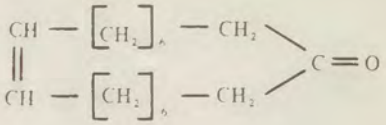
	Coumarin	*p*-Cresol
Other names	1,2-Benzopyrone; 5,6-Benzo-α-pyrone; *cis-o*-Coumaric acid anhydride; *o*-Hydroxycinnamic acid, lactone	4-Cresol *p*-Hydroxytoluene *p*-Methyl phenol
Empirical formula	$C_9H_6O_2$	C-H_8OS
Structure		
Physical/chemical characteristics[5]		
Appearance	White, crystalline solid (leaflets or rhomboids)	Low-melting, crystalline solid
Molecular weight	146.15	108.13
Melting point	68–70°C	35–36°C
Boiling point	297–299°C* (161–162°C at 14 mm Hg)	201–202°C
Congealing point	68.0°C min[1]	
Specific gravity		1.004 at 58°C
Refractive index		1.5395 at 20°C
Solubility	8% in alcohol; 0.3% in water; soluble in boiling water, alcohol, ether, and chloroform	Slightly soluble in water; soluble in alkali solutions and most organic solvents
Organoleptic characteristics	Sweet, fresh, hay-like, odor similar to vanilla seeds; burning taste with bitter undertone; nut-like flavour on dilution	Phenol-like odor
Synthesis	May be extracted from tonka beans.[6] From salicylaldehyde and acetic anhydride in the presence of sodium acetate.[7] Also from *o*-cresol and carbonyl chloride followed by chlorination of the carbonate and fusion with a mixture of alkali acetate, acetic anhydride, and a catalyst	It can be prepared by fractional distillation of coal tar, where it occurs together with the *ortho*- and *para*-isomers.
Natural occurrence	Reported in tonka bean (*Dipteryx odorata*) seed,[8,9] the flowers of *Melilotus officinalis*,[10–12] the leaves of *Melilotus albus*,[13] in *Liatris odoratissima*,[14] *Asperula odorosa*,[15] wild vanilla (*Achlys triphylla*),[16] lavender oil,[17] and several varieties of orchid[18]	Reported in *Acacia farnesiana*,[19] ylang-ylang oil (probably as *p*-cresyl acetate),[20] jasmine absolute,[21] orange oil from leaves,[22] the essence from flowers of *Lilium candidum*,[23] anise-seed oil,[24] the essence of *Artemisia santolinoffia*,[25] and some sea algae[26]
Reported uses[3]		Non-alcoholic beverages, 0.67 ppm; ice cream, ices, etc., 0.01–1.0 ppm; candy, 0.01–2.0 ppm; baked goods, 0.01–2.0 ppm
Regulatory status	Use in foods not permitted in USA	FDA 121.1164; FEMA No. 2337

*Sublimes; not volatile in steam except when superheated.

REFERENCES

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

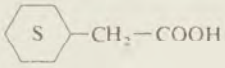
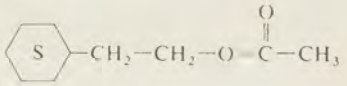
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22. **Igolen,** *Chem. Zentralbl.*, 2, 750, 1939.
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26. **Kamayama,** *Chem. Abstr.*, 50, 13184, 1956.

	Cuminaldehyde	Cycloheptadeca-9-en-1-one
Other names	Cumaldehyde Cuminal Cuminic aldehyde *p*-Isopropyl benzaldehyde	Civettone
Empirical formula	$C_{10}H_{12}O$	$C_{17}H_{30}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	From colorless to yellowish liquid	Colorless crystals
Assay	95% min	
Molecular weight	148.20	250.4
Melting point		32.5°C
Boiling point	232°C	342°C at 742 mm Hg 158–160°C at 2 mm Hg
Specific gravity	0.976–0.980 at 25°C; 0.9818 at 15°C	0.917 at 33°C
Refractive index	1.5290–1.5340 at 20°C; 1.5301 at 20°C	1.4830 at 33.4°C
Solubility	1:4 in 70% alcohol; soluble in most organic solvents	
Organoleptic characteristics	Strong, pungent, cumin-like odor and similar taste	Disgustingly obnoxious animal-gland odor; pleasant at extreme dilutions
Synthesis	Prepared synthetically by heating *p*-isopropylbenzoyl chloride with an aqueous or alcoholic hexamethylenetetraamine solution	From aleuritic acid, the *trans*-form only;[6,7] the *cis*- and *trans*-forms from ethyl-9-keto hepta-decanedioate[8]
Natural occurrence	Reported in a large number of essential oils: cumin, *Acacia farnesiana*, cinnamon, bitter orange, Mexican lime, *Eucalyptus globulus*, rue, boldus, *Artemisia hausiliensis*, and others	In civet (*cis*-form).
Reported uses[3]	Non-alcoholic beverages 3.1 ppm Ice cream, ices, etc. 3.2 ppm Candy 4.0 ppm Baked goods 4.0 ppm Chewing gum 0.40–0.50 ppm Condiments 3.0 ppm	Non-alcoholic beverages 0.03 ppm Ice cream, ices, etc. 0.02 ppm Candy 0.03 ppm Baked goods 0.05 ppm Gelatins and puddings 0.02 ppm
Regulatory status	FDA 121.1164; FEMA No. 2341	FEMA No. 3425

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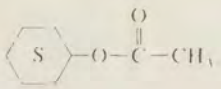
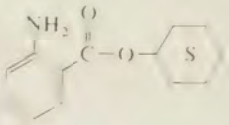
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7. **Mathur et al.,** *J. Chem. Soc.*, 114, 1963.
8. **Stoll et al.,** *Helv. Chim. Acta*, 31, 543, 1948.

	Cyclohexaneacetic acid	Cyclohexaneethyl acetate
Other names	Cyclohexylacetic acid	Cyclohexylethyl acetate Hexahydrophenethyl acetate
Empirical formula	$C_8H_{14}O_2$	$C_{10}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Crystalline solid	Liquid
Molecular weight	142.19	170.25
Melting point	27–33°C	
Boiling point	244–246°C (116–117°C at 4 mm Hg)	104°C at 15 mm Hg
Specific gravity	1.007 at 20°C	
Refractive index	1.4558 at 30°C	
Solubility	Slightly soluble in water; soluble in most organic solvents	
Organoleptic characteristics	Waxy, fatty odor reminiscent of phenylacetic acid	
Synthesis	By catalytic reduction of phenylacetic acid	From the corresponding alcohol by acetylation with sodium acetate in acetic acid solution[6]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Baked goods 2.0 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 6.0 ppm Baked goods 20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2347	FDA 121.1164; FEMA No. 2348

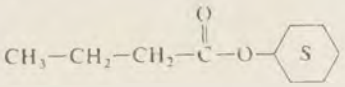
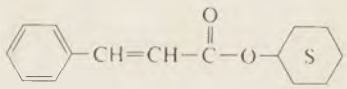
REFERENCES

For References 1–5, see end of Part III.
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	Cyclohexyl acetate	Cyclohexyl anthranilate
Other names		Cyclohexyl 2-aminobenzoate Cyclohexyl *o*-aminobenzoate
Empirical formula	$C_8H_{14}O_2$	$C_{13}H_{17}NO_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	Pale-yellow liquid
Assay	99% min	
Molecular weight	142.19	219.28
Boiling point	175–177°C; 61–62°C at 12 mm Hg	318°C
Flash point	58–64°C	
Specific gravity	0.9750–0.9790 at 15°C; 0.981 at 12°C	1.018 (1.01) at 15.5°C
Refractive index	1.4400–1.4410 (1.4390) at 20°C	
Acid value	0.2 max	
Solubility	1:1.2–1:1.6 in 70% alcohol; insoluble in water; miscible with alcohol and ether	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Odor reminiscent of amyl acetate	Faint, neroli-like, orange blossom odor; sweet, fruity, grape-like taste
Synthesis	By heating the corresponding alcohol with acetic anhydride or acetic acid in the presence of traces of sulfuric acid	From isatoic anhydride and cyclohexanol
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 20 ppm Ice cream, ices, etc. 15 ppm Candy 100 ppm Baked goods 110 ppm	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 3.7 ppm Candy 3.7 ppm Baked goods 2.0–10 ppm Gelatins and puddings 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2349	FDA 121.1164; FEMA No. 2350

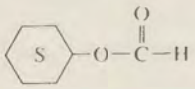
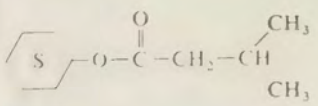
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For References 1–5, see end of Part III.

	Cyclohexyl butyrate	Cyclohexyl cinnamate
Other names		Cyclohexyl β-phenylacrylate Cyclohexyl 3-phenylpropenoate
Empirical formula	$C_{10}H_{18}O_2$	$C_{15}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, viscous liquid; solidifies when cold
Molecular weight	170.25	230.31
Melting point		28°C
Boiling point	212°C	195°C at 12 mm Hg
Specific gravity	0.957 at 15.5°C	1.054 at 14°C (supercooled liquid)
Refractive index	1.4490 at 20°C	
Solubility	Almost insoluble in water; soluble in alcohol	Insoluble in water; poorly soluble in propylene glycol; soluble in alcohol
Organoleptic characteristics	Fresh, floral odor reminiscent of benzyl butyrate; intense, sweet taste	Fruity, peach-, cherry-, and almond-like odor; similar flavor notes
Synthesis	By esterification of cyclohexanol with isobutyric acid	From cyclohexanol and cinnamic acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.9 ppm Ice cream, ices, etc. 5.7 ppm Candy 9.2 ppm Baked goods 28 ppm Gelatins and puddings 0.54 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 1.0–5.0 ppm Candy 4.0–10 ppm Baked goods 4.0–20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2351	FDA 121.1164; FEMA No. 2352

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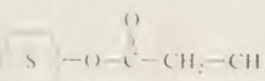
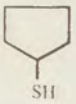
For References 1–5, see end of Part III.

	Cyclohexyl formate	Cyclohexyl isovalerate
Other names		
Empirical formula	$C_7H_{12}O_2$	$C_{11}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Light, colorless liquid	Liquid
Molecular weight	128.17	184.28
Boiling point	162–163°C (158–160°C)	58–62°C at 0.5 mm Hg
Specific gravity	1.0057 at 0°C	
Refractive index	1.4417 at 24°C	1.4410 at 21°C
Solubility	Soluble in alcohol and acetic and formic acids; insoluble in water	
Organoleptic characteristics	Pleasant, cherry-like odor	Apple- and banana-like aroma
Synthesis	From cyclohexyl alcohol and concentrated formic acid in the presence of sulfuric acid;[6,7] by distilling the alcohol-acid mixture in the presence of excess acid	From cyclohexane and isovaleric acid[8] in the presence of perchloric acid[6]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 11 ppm Ice cream, ices, etc. 2.8 ppm Candy 8.0 ppm Baked goods 7.0–10 ppm	Non-alcoholic beverages 13 ppm Ice cream, ices, etc. 7.0–25 ppm Candy 9.3 ppm Baked goods 1.7–60 ppm
Regulatory status	FDA 121.1164; FEMA No. 2353	FDA 121.1164; FEMA No. 2355

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

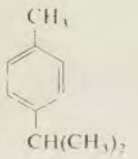
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	Cyclohexyl propionate	Cyclopentanethiol
Other names		Cyclopentyl mercaptan
Empirical formula	$C_9H_{16}O_2$	$C_5H_{10}S$
Structure		
Physical/chemical characteristics		
Appearance	Liquid	
Molecular weight	156.23	102.19
Boiling point	193°C at 750 mm Hg; 46–50°C at 0.7 mm Hg	129–131°C at 745 mm Hg
Specific gravity	0.9718 at 0°C	0.9550 at 20°C
Refractive index	1.4430 at 20°C	1.4880 at 20°C
Organoleptic characteristics	Apple- and banana-like aroma	
Synthesis	By direct esterification of the alcohol with the acid in the presence of concentrated sulfuric acid[10,11] or in the presence of benzene	From cyclopentyl bromide and potassium hydrosulfide;[6] by treating cycloalkanone dimethyl dithioacetals with four equivalents of an alkaline metal;[7] from cyclopentyl naphthyl sulfide and an aluminosilicate catalyst[8]
Natural occurrence	Not reported found in nature	Reported found in the 111–150°C boiling fraction of petroleum[9]
Reported uses[3]	Non-alcoholic beverages 2.4 ppm Ice cream, ices, etc. 2.7 ppm Candy 2.0–3.0 ppm Baked goods 3.0 ppm Gelatins and puddings 5.0 ppm	Baked goods 0.1 ppm Condiments, pickles 0.1 ppm Meat, meat sauces, soups 0.1 ppm Milk, dairy products 0.1 ppm Cereals 0.1 ppm
Regulatory status	FDA 121.1164; FEMA No. 2354	FEMA No. 3262

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

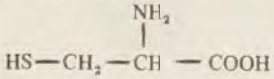
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9. Coleman, Thompson, Hopkins and Rall, *J. Chem. Eng. Data*, 10(1), 80, 1965.
10. Senderens and Aboulenc, *Compt. Rend.*, 155, 170, 1912.
11. Senderens and Aboulenc, *Ann. Chim.* (Paris), 9(18), 180, 1922.

	p-Cymene
Other names	*p*-Isopropyltoluene 1-Methyl-4-isopropyl benzene
Empirical formula	$C_{10}H_{14}$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid
Molecular weight	134.21
Boiling point	175–176°C (179 C)
Specific gravity	0.857 at 20 C
Refractive index	1.4917 at 20 C
Solubility	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Strong, characteristic odor reminiscent of carrot; tends to darken with aging
Synthesis	Obtained chiefly from the wash water of sulfite paper
Natural occurrence	Extensively widespread in nature, Reported in the oils of cypress,[6] *Artemisia cina* Bg.,[7] Ceylon cinnamon,[8,9] boldo leaf,[10] cascarilla,[11] *Cuminum cyminum* L.,[12,13] and lemon;[14] in the oils from seeds of coriander[15] and *Cicuta virosa*;[16] in the ether-extracted oils of *Monarda fisulosa*[17] and *Monarda punctata*;[18] in star anise and nutmeg essential oils.[19] Note that *p*-cymene reported in an essential oil may be formed from the conversion of a cyclic terpene. Its presence is indicative of aging in lemon essential oil.[20]
Reported uses[3]	Non-alcoholic beverages, 3.3 ppm; ice cream, ices, etc., 5.3 ppm; candy, 7.0 ppm; chewing gum, 250 ppm; condiments, 10 130 ppm
Regulatory status	FDA 121.1164; FEMA No. 2356

REFERENCES

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

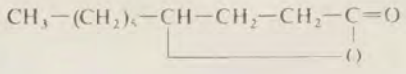
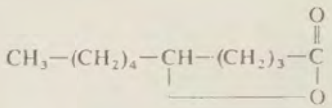
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11. **Fendler,** *Arch. Pharm.*, 238, 685, 1900.
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14. **Penfold,** *Chem. Zentralbl.*, 2, 753, 1927.
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16. **Trapp,** *Chem. Ann.*, 108, 386, 1858.
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18. **Schumann and Kremers,** *Chem. Zentralbl.*, 2, 42, 1897.
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	L-Cysteine	2-*trans*, 4-*trans*-Decadienal
Other names	α-Amino-β-mercaptopropionic acid 2-Amino-3-mercaptopropanoic acid *l*-β-Mercaptoalanine α-Amino-β-thiolpropionic acid	Heptenyl acrolein
Empirical formula	$C_3H_7O_2NS$	$C_{10}H_{16}O$
Structure		$CH_3-(CH_2)_4-CH=CH-CH=CH-CHO$
Physical/chemical characteristics[5]		
Appearance	Crystals; readily oxidizes to *l*-cystine	Colorless oily liquid
Molecular weight	121.16	152.23
Melting point	~ 240°C (decomposes)	
Boiling point		64–65°C at 0.1 mm Hg
Optical rotation	+6.5 at 25°C (c = 1 in 5*N* HCl) +9.8° at 30°C (c = 1.3 in water) +13° at 25°C (c = 1 in glacial acetic acid)	
Solubility	Very soluble in water, alcohol, and acetic acid; insoluble in ether, acetone, and benzene	Almost insoluble in water; soluble in alcohol; slightly soluble in propylene glycol; miscible with oils
Organoleptic characteristics		Powerful green odor; sweet, orange-like odor at high concentration; grapefruit/orange-like taste on dilution
Synthesis	By addition of a thiol compound to an unsaturated amino acid derivative;[6,7] by hydrolysis of proteins in the presence of carbon dioxide;[8] by treating an HCl hydrolysate of hair with CuO_2, followed by decomposition of the resulting copper-cysteine complex with hydrogen sulfide;[9] by the addition of thioacetic acid to α-acetamido acrylic acid;[10] by treatment of a keratine HCl hydrolysate with zinc to reduce the cystine present to cysteine;[11] by electrolytic reduction of cystine[12]	By autooxidation of methyl (*trans,trans*)-linoleate hydroperoxide[13]
Natural occurrence	Reported found in protein hydrolysates, with the exception of gelatin, in which only traces of cysteine are present	Reported as occurring in peanut oil and, as a volatile component, in fried potatoes,[14] the *trans,trans*-form is reported found among the volatile flavor components of potato chips[15] and tomato[16]
Reported uses[3]	Non-alcoholic beverages 100.0 ppm Baked goods 100.0 ppm Condiments, pickles 100.0 ppm Meat, meat sauces, soups 100.0 ppm Milk, dairy products 100.0 ppm Cereals 100.0 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 10.0 ppm Chewing gum 10.0 ppm Meat, meat sauces 10.0 ppm Cereals 10.0 ppm Vegetables 10.0 ppm
Regulatory status	FEMA No. 3263	FEMA No. 3135

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7. **Behringer,** *Chem. Ber.*, 81, 326, 1948.
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9. **Rapline,** U.S. Patent 2,376, 186, 1945.
10. **Farlow,** U.S. Patent 2,406,362, 1946.
11. **Holloway and Young,** U.S. Patent 2,414,303, 1947.
12. **Koperina and Gavrilov,** *J. Gen. Chem. USSR*, 17, 1651, 1947.
13. **Hoffman and Keppler,** *Nature*, 185, 310, 1960.
14. **Lefort and Sorba,** *Bull. Soc. Chim. Fr.*, p. 69, 1956.
15. **Deck, Pokorny and Chang,** *J. Food Sci.*, 38(2), 345, 1973.
16. **Kazeniac and Hall,** *J. Food Sci.*, 35(5), 519, 1970.

	γ-Decalactone	δ-Decalactone
Other names	4-Hydroxydecanoic acid, γ-lactone	Decanolide-1,4 γ-*n*-Hexyl-γ-butyrolactone 5-Hydroxy-decanoic acid, δ-lactone
Empirical formula	$C_{10}H_{18}O_2$	$C_{10}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Molecular weight	170.25	170.25
Boiling point	153°C at 15 mm Hg; 114–116°C at 0.5 mm Hg	281°C
Specific gravity		0.95
Refractive index	1.4610 at 21.5°C	
Solubility	Very slightly soluble in water	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Pleasant, fruity, peach-like odor	Oily, peach odor and taste
Synthesis	By heating γ-bromocapric acid in a sodium carbonate solution[7] by prolonged heating of 9-decen-1-oic acid with 80% H_2SO_4 at 90°C[8,9]	From hexylethylene oxide and sodium malonic ester; also from decanoic acid
Natural occurrence	Reported in peach and apricot aroma,[10] as well as in strawberry aroma[11]	Reported in coconut and raspberry[6]
Reported uses[3]	Non-alcoholic beverages, 2.0 ppm; ice cream, ices, etc., 4.5 ppm; candy, 5.7 ppm; baked goods, 7.1 ppm; gelatins and puddings, 0.08–8.0 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 10 ppm Candy 0.25–5.0 ppm Baked goods 0.25–8.0 ppm Toppings 50 ppm Margarine 10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2360	FDA 121.1164; tolerance 10 ppm in margarine. FEMA No. 2361

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9. Rochussen, *Schimmel Ber.*, p. 307, 1929.
10. Ruys, *Fr. Ses Parfums*, 47, 34, 1966.
11. Willhalm et al., *Helv. Chim. Acta*, 49, 65, 1966.

	Decanal	Decanal dimethyl acetal
Other names	Aldehyde C-10 Capric aldehyde Caprinaldehyde *n*-Decylaldehyde Decylic aldehyde	Aldehyde C-10 dimethyl acetal Capraldehyde dimethyl acetal Decylaldehyde dimethyl acetal 1,1-Dimethoxy decane 10,10-Dimethoxy decane
Empirical formula	$C_{10}H_{20}O$	$C_{12}H_{26}O_2$
Structure	$H_3C-(CH_2)_8-CHO$	$CH_3-(CH_2)_8-CH(OCH_3)(OCH_3)$
Physical/chemical characteristics[4]		
Appearance	Colorless to light-yellow liquid	Colorless liquid
Assay	92% min[2]	
Molecular weight	156.26	202.34
Melting point	17–18 C	
Boiling point	207–210 C	218 C; 77–79 C at 1 mm Hg
Flash point	84 C	
Specific gravity	0.823–0.832 at 25 /25 C;[2] 0.8502 at 20 C	0.830 at 15.5 C
Refractive index	1.4260–1.4300[2] (1.4287) at 20 C	1.4244 at 24 C
Acid value	Not more than 10[2]	
Solubility	Soluble 1:1 in 80% alcohol; almost insoluble in water; soluble in most organic solvents	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Pronounced, fatty odor that develops a floral character on dilution;[2] strong, orange-rose odor and fatty, citrus-like taste	Characteristic, herbaceous, citrus-floral odor; brandy, cognac flavor
Synthesis	Industrially prepared by oxidation of *n*-decanol or by reduction of the corresponding acid	From decanal and methyl alcohol
Natural occurrence	Among the aliphatic aldehydes, it has the largest natural occurrence in a variety of essential oils and extraction products: lemongrass, lavender, Taiwan citronella, sweet orange mandarin, grapefruit, orris, coriander, *Acacia farnesiana* Willd., lemon (from different sources), bitter orange, petitgrain bergamot, petitgrain lime, lime, and Bulgarian clary sage	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.3 ppm Ice cream, ices, etc. 4.1 ppm Candy 5.7 ppm Baked goods 6.6 ppm Gelatins and puddings 3.0 ppm Chewing gum 0.60 ppm	Non-alcoholic beverages 1.0–2.0 ppm Alcoholic beverages 8.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 8.0 ppm Baked goods 8.0 ppm Gelatins and puddings 3.0 ppm
Regulatory status	FDA GRAS; FEMA No. 2362	FDA 121.1164; FEMA No. 2363

REFERENCES

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

	1-Decanol	4-Decenal
Other names	Alcohol C-10 Capric alcohol Decyl alcohol Nonyl carbinol	
Empirical formula	$C_{10}H_{22}O$	$C_{10}H_{18}O$
Structure	$H_3C-(CH_2)_8-CH_2OH$	$CH_3-(CH_2)_4-CH=CH-CH_2-CH_2-CHO$
Physical/chemical characteristics[5]		
Appearance	Viscous, colorless liquid	
Assay	98% min[2]	
Molecular weight	158.28	154.24
Melting point	6–7°C	
Boiling point	231°C	
Flash point	> 5°C[2]	
Freezing point	> 86°C	
Specific gravity	0.826–0.831 at 25/25°C;[2] 0.8292 at 20°C	
Refractive index	1.4350–1.4390[2] (1.4378) at 20°C	
Acid value	Not more than 1[2]	
Solubility	1:3 in 60% alcohol;[2] almost insoluble in water; soluble in most organic solvents	
Organoleptic characteristics	Floral odor resembling orange flowers; slight, characteristic fatty taste	Strong orange-like odor
Synthesis	Synthetically prepared from coconut oil derivatives; by reduction of some capric esters, such as methyl caprate	From 1-octen-3-ol and vinyl ethyl ether in the presence of *p*-methylbenzene sulfonic acid[6]
Natural occurrence	Reported in the essential oils of ambrette seeds and almond flowers; also in citrus oils and fermented beverages	Reported formed in the autooxidation of lipids[7]
Reported uses[3]	Non-alcoholic beverages 2.1 ppm Ice cream, ices, etc. 4.6 ppm Candy 5.2 ppm Baked goods 5.2 ppm Chewing gum 3.0 ppm	Ice cream, ices, etc. 0.5 ppm Baked goods 1.0 ppm Condiments, pickles 0.5 ppm Meat, meat sauces, soups 0.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2365	FEMA No. 3264

REFERENCES

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

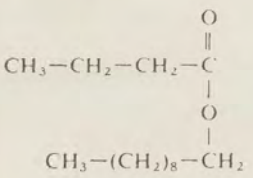
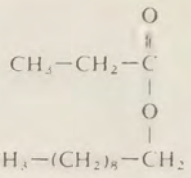
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	3-Decen-2-one	Decyl acetate
Other names	Heptylidene acetone Oenanthylidene acetone	Acetate C-10 Decanyl acetate
Empirical formula	$C_{10}H_{18}O$	$C_{12}H_{24}O_2$
Structure	$CH_3-(CH_2)_5-CH=CH-\overset{\overset{O}{\|}}{C}-CH_3$	$CH_3-(CH_2)_8-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_3$
Physical chemical characteristics[5]		
Appearance	Needles (almost colorless, mobile liquid)	Colorless liquid
Assay		98% min
Molecular weight	154.25	200.32
Melting point	16–17 C	
Boiling point	125–126 C at 12 mm Hg	125.6–125.8 C at 15.5 mm Hg; 272 C at 760 mm Hg; 244 C
Specific gravity		0.862–0.866 at 25° C; 0.873 at 15.5°C
Refractive index		1.4250–1.4300 at 20 C
Solubility	Almost insoluble in water; soluble in alcohol and perfume oils	1:2 in 80% alcohol; insoluble in water
Organoleptic characteristics	Fruity-floral, jasmine-like odor with orris notes	Floral, orange-rose odor and characteristic flavor; at high dilution, sweet flavor with a pineapple-like undertone; traces used in apple, orange, and rum flavors
Synthesis	From acetone and heptyl alcohol in 1% sodium hydroxide solution;[6] by dehydration upon heating of 4-decanol-2-one over pumice or clay;[7] also by condensation of heptaldehyde and acetone	By direct acetylation of *n*-decanol with acetic acid via azeotropic conditions or using acetic anhydride
Natural occurrence	In *Boletus edulis*	In orange, lemon, melon, and apple
Reported uses[3]		Non-alcoholic beverages 3.4 ppm Ice cream, ices, etc. 2.7 ppm Candy 6.1 ppm Baked goods 10 ppm Gelatins and puddings 1.2 ppm Chewing gum 12 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2367

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

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	Decyl butyrate	Decyl propionate
Other names		
Empirical formula	$C_{14}H_{28}O_2$	$C_{13}H_{26}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	Liquid
Assay		
Molecular weight	228.37	214.35
Melting point		
Boiling point	270°C; 135 C at 8 mm Hg	138/139 C at 15 mm Hg; 124 C at 8 mm Hg
Specific gravity	0.8617 at 20 C; 0.887 at 15.5 C	0.8639 at 20 C
Refractive index	1.43077 (1.4245) at 20 C	1.4291 at 20 C; 1.4280 at 22.5°
Solubility		
Organoleptic characteristics	Ethereal, apricot-like odor	Slightly fatty, aldehyde-like odor reminiscent of cognac
Synthesis	By esterification of the acid with the alcohol in the presence of concentrated H_2SO_4[6]	By direct esterification in the presence of benzene
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.18 ppm Ice cream, ices, etc. 1.4 ppm Candy 5.9 ppm Baked goods 7.5 ppm	Non-alcoholic beverages 0.81 ppm Ice cream, ices, etc. 1.4 ppm Candy 5.9 ppm Baked goods 7.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2368	FDA 121.1164; FEMA No. 2369

REFERENCES

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

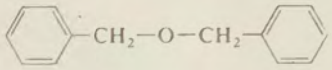
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	Diacetyl	Diallyl trisulfide
Other names	Biacetyl 2,3-Butanedione 2,3-Diketobutane Dimethylglyoxal "Dimethyl ketone" (incorrect)	Allyl trisulfide
Empirical formula	$C_4H_6O_2$	$C_6H_{10}S_3$
Structure	$H_3C-\overset{O}{\overset{\|}{C}}-\overset{O}{\overset{\|}{C}}-CH_3$	$CH_2=CH-CH_2-S-S-S-CH_2-CH=CH_2$
Physical chemical characteristics[5]		
Appearance	Yellow to greenish, mobile liquid	Liquid
Molecular weight	86.09	178.34
Melting point	3 to −4 C	
Boiling point	87-88 C	112–122°C at 16 mm Hg
Specific gravity	0.9734 at 22 C	1.0845 at 15°C
Refractive index	1.3933 at 18.5 C	
Solubility	Soluble in alcohol, carbitols, and many other organic solvents; miscible 1:4 with water	Insoluble in water and alcohol; miscible with ether
Organoleptic characteristics	Penetrating, very strong odor similar to butter on dilution; chlorine quinone-like odor when concentrated	Disagreeable odor
Synthesis	From methyl ethyl ketone by converting to the isonitroso compound and then decomposing to diacetyl by hydrolysis with HCl; by fermentation of glucose via methyl acetyl carbinol	
Natural occurrence	Reported in the oils of: Finnish pine, angelica, and lavender; in the flowers of *Polyalthia canangioides* Boerl. var. *angustifolia*[6] and *Fagroea racemosa* Jack. The following plants are also reported to contain diacetyl:[7] *Monodora grandiflora* Berth., *Magnolia tripetale* L., *Ximenia aegyptiaca* L., *Petasites fragrans* Presl., various narcissi, and tulips. It has been identified in certain types of wine,[8] the natural aromas of raspberry and strawberry, and the oils of lavender, lavandin, Reunion geranium, and Java citronella; finally, in *Cistus ladaniferus* L.[9] J. Pien has described its identification in butter.[10] Good quality butter should not contain less than 1.2 mg diacetyl, but a level up to 2.5 mg does not spoil the aroma (Holwerde and Van der Geest, 1948).	Reported found in garlic oil[11]
Reported uses[3]	Non-alcoholic beverages, 2.5 ppm; ice cream, ices, etc., 5.9 ppm; candy, 21 ppm; baked goods, 44 ppm; gelatins and puddings, 19 ppm; chewing gum, 35 ppm; shortening, 11 ppm	Baked goods 1.0 ppm Condiments, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm
Regulatory status	FDA GRAS; FEMA No. 2370	FEMA No. 3265

REFERENCES

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

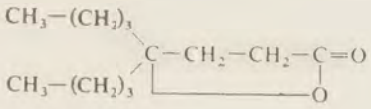
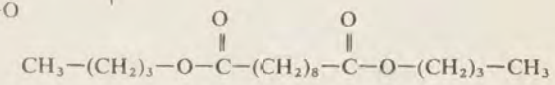
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7. **Maurer,** *Ind. Parfum.,* p. 9, 1954.
8. **Peynaud and Lafon,** *Bull. Soc. Chim. Fr.,* 44, 263, 1951.
9. **Fesan,** *Ind. Parfum.,* p. 5, 1950.
10. **Pien,** *Ann. Falsif. Fraudes,* p. 41, 1948.
11. **Semmler,** *Arch. Pharm.,* 231, 434, 1892.

	Di (butan-3-one-1-yl) sulfide		Dibenzyl ether
Other names			Benzyl ether
Empirical formula	$C_8H_{14}O_2S$		$C_{14}H_{14}O$
Structure	$CH_3-CO-CH_2-CH_2-S-CH_2-CH_2-CO-CH_3$		
Physical/chemical characteristics			
Appearance			Colorless liquid
Molecular weight	174.25		198.25
Melting point			3–4 C
Boiling point			170 C at 16 mm Hg
Specific gravity			1.0428 at 20 C
Refractive index			1.561 at 20 C
Solubility			Insoluble in water; miscible with alcohol and ether
Organoleptic characteristics			Slightly earthy, mushroom-like odor with a rosy undertone
Synthesis			As a by-product in the preparation of benzyl alcohol by hydrolysis of benzyl chloride; by using a concentrated caustic instead of carbonate, yields can be improved to 50% or higher[6]
Natural occurrence			Not reported found in nature
Reported uses	Non-alcoholic beverages	1.0 ppm	Non-alcoholic beverages, 8.3 ppm; ice cream, ices, etc., 5.6 ppm; candy, 23 ppm; baked goods, 25 ppm; chewing gum, 85–160 ppm
	Ice cream, ices, etc.	1.0 ppm	
	Candy	2.0 ppm	
	Baked goods	2.0 ppm	
	Gelatins and puddings	2.0 ppm	
	Other uses	1.0 ppm	
Regulatory status	FEMA No. 3335		FDA 121.1164; FEMA No. 2371

REFERENCES

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

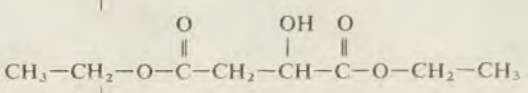
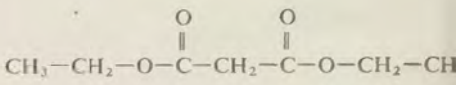
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	4,4-Dibutyl-γ-butyrolactone	Dibutyl sebacate
Other names	4-Butyl-4-hydroxyoctanoic acid, γ-lactone Dibutyl butyrolactone 4,4-Dibutyl-4-hydroxybutyric acid, γ-lactone	Butyl sebacate Dibutyl decanedioate Dibutyl 1,8-octanedicarboxylate
Empirical formula	$C_{12}H_{22}O_2$	$C_{18}H_{34}O_4$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Liquid
Molecular weight	198.31	314.47
Boiling point		349°C; 211–212°C at 11 mm Hg
Specific gravity		0.9405 at 15°C
Refractive index		1.4433 at 15°C
Solubility	Insoluble in water; poorly soluble in propylene glycol; soluble in alcohol	
Organoleptic characteristics	Oily, coconut-butter odor and creamy, coconut-like flavor	
Synthesis	From butyl pentanol and methylacrylate using a catalyst	By distillation of sebacic acid with butyl alcohol in the presence of concentrated HCl in benzene solution[6] or by reacting butyl alcohol and sebacyl chloride[7]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Ice cream, ices, etc. 2.8–3.5 ppm Candy 4.4–15 ppm Baked goods 15 ppm	Non-alcoholic beverages 1.0–5.0 ppm Ice cream, ices, etc. 2.0–5.0 ppm Candy 15 ppm Baked goods 15 ppm
Regulatory status	FDA 121.1164; FEMA No. 2372	FDA 121.1164; FEMA No. 2373

REFERENCES

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

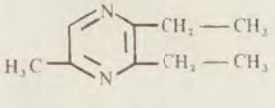
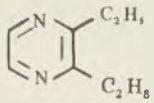
6. **Kawaii et al.**, *Chem. Zentralbl.*, 2, 1694, 1931.
7. **Boissonnos**, *Helv. Chim. Acta*, 20, 776, 1937.

	Diethyl malate	Diethyl malonate
Other names	Diethylhydroxysuccinate Ethyl malate	Ethyl malonate Malonic ester
Empirical formula	$C_8H_{14}O_5$	$C_7H_{12}O_4$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	190.20	160.17
Boiling point	91–92°C at 1 mm Hg	199–200°C; 82–83°C at 11 mm Hg
Specific gravity	1.4361 at 20°C	1.0551 at 20°C
Refractive index		1.4139 at 20°C
Optical rotation	−15.9° at 24°C (acetone; C = 6)	
Solubility		Insoluble in water; miscible with alcohol and ether
Organoleptic characteristics		Faint, pleasant, aromatic odor
Synthesis	The *l*-isomer can be prepared by esterification of the *l*-isomer of the acid with alcohol in the presence of HCl.[6]	Reacting chloroacetic acid to cyanoacetic acid using sodium cyanide and subsequent saponification. Malonic acid is finally esterified by azeotropic distillation with ethanol in benzene.[8]
Natural occurrence	It exhibits two optically active isomers in addition to the optically inactive form; the most common is the *l*-isomer. Reported present in the cultures of certain fungi (*Rhizopus*).[7]	Reported found in several natural products
Reported uses[3]	Non-alcoholic beverages 5.5 ppm Ice cream, ices, etc. 6.5 ppm Candy 18 ppm Baked goods 44 ppm Gelatins and puddings 1.5 ppm	Non-alcoholic beverages 5.6 ppm Ice cream, ices, etc. 17 ppm Candy 20 ppm Baked goods 19 ppm Gelatins and puddings 20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2374	FDA 121.1164; FEMA No. 2375

REFERENCES

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

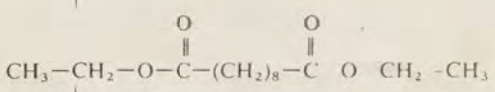
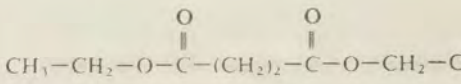
6. D'Ianni and Adkins, *J. Am. Chem. Soc.*, 61, 1680, 1939.
7. Mirocha et al., *Phytopathology*, 51, 274, 1961.
8. Kirk and Othmer, *Encyclopedia of Chemical Technology*, Vol. 2, John Wiley & Sons, 1948, 301.

	2,3-Diethyl-5-methylpyrazine	2,3-Diethylpyrazine
Other names		
Empirical formula	$C_9H_{14}N_2$	$C_8H_{12}N_2$
Structure		
Physical/chemical characteristics		
Appearance		
Assay	C: 71.96%; H: 9.39%; N: 18.65%	C: 70.55%; H: 8.88%; N: 20.57%
Molecular weight	150.23	136.20
Mass spectra	39(37), 41(14), 54(10), 55(51), 66(9), 67(8), 79(4), 80(3), 93(3), 94(7), 106(1), 107(2), 121(23), 122(9), 135(62), 136(7), 149(64), 150(100)[8]	39 (16), 41 (12), 54 (12), 56 (13), 65 (4), 66(3), 80(22), 81 (18), 93 (3), 94 (2), 107 (17), 108 (11), 119 (7), 121 (83), 135 (46), 136 (100)[11]
IR spectra	S (3.4, 6.9, 8.5, 9.5) M (7.6, 7.9, 8.8, 9.9, 10.2, 10.3, 11.1) W (5.6, 6.4, 6.5, 8.1, 10.8, 11.6, 11.8, 11.9)[8]	7.07, 3.36, 11.71, 6.82, 8.59, 9.67, 3.28 μ[11]
UV spectra	278.5[8]	
NMR spectra[10]		τ = 1.84 (s, ring protons, 2H), 7.24 (q, CH_2 4H), 8.75 (t, chain CH_3 6H)[13]
Synthesis	By condensation of 3,4-hexanedione with propylene diamine[7]	By condensation of 3-4-hexanedione with ethylenediamine[12]
Natural occurrence	Reported to be present in coffee, filberts, and potato products[6]	
Reported uses[3]	Non-alcoholic beverages 0.1 ppm Ice cream, ices, etc. 0.2 ppm Candy 0.5 ppm Baked goods 1.0 ppm Gelatins and puddings 0.2 ppm Meat, meat sauces, soups 0.2 ppm Cereals 1.0 ppm	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0 ppm Gelatins and puddings 1.0 ppm Used to modify the flavor of natural substances[9] and as a flavor additive to chocolate fudge candy[10]
Regulatory status	FEMA No. 3336	FEMA No. 3136

REFERENCES

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

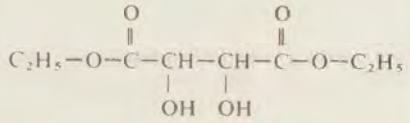
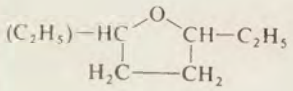
6. **Maga and Sizer,** *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
7. **Ishiguro and Matsumura,** *Yakugaku Zasshi*, 78, 229, 1958.
8. **Bondarovich et al.,** *J. Agric. Food Chem.*, 15, 1093, 1967.

	Diethyl sebacate	Diethyl succinate
Other names	Diethyl decanedioate Diethyl 1,8-octanedicarboxylate Ethyl sebacate	Diethyl butanedioate Diethyl ethanedicarboxylate Ethyl succinate
Empirical formula	$C_{14}H_{26}O_4$	$C_8H_{14}O_4$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to yellowish liquid	Colorless to yellowish, clear liquid
Assay		98% min[2]
Molecular weight	258.36	174.20
Melting point	1–3°C	
Boiling point	297°C; 151–153°C at 3 mm Hg	216°C; 105°C at 15 mm Hg
Specific gravity	0.9640 at 15°C	1.031–1.041[2] at 25°/25°C; 1.0416 at 20°C
Refractive index	1.4367 at 15°C	1.4190–1.4230[2] (1.4198) at 20°C
Acid value		Not more than 1.0[2]
Solubility	Partially water soluble; miscible with alcohol, ether, and other organic solvents	1:1 or more in 60% alcohol[2]
Organoleptic characteristics		Faint, pleasant odor
Synthesis	By heating sebacic acid and ethanol in the presence of concentrated H_2SO_4 or of other acid catalysts[6]	By direct esterification of the acid in the presence of concentrated H_2SO_4 in benzene solution;[7] from succinic anhydride and ethyl alcohol[2]
Natural occurrence	Not reported found in nature	In apple and cocoa
Reported uses[3]	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 9.1 ppm Candy 21 ppm Baked goods 41 ppm Gelatins and puddings 3.2–19 ppm Chewing gum 2.7–450 ppm	Non-alcoholic beverages 7.3 ppm Ice cream, ices, etc. 11 ppm Candy 38 ppm Baked goods 45 ppm
Regulatory status	FDA 121.1164; FEMA No. 2376	FDA 121.1164; FEMA No. 2377

REFERENCES

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

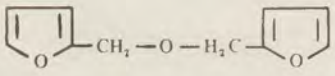
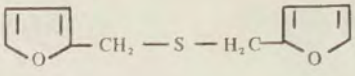
6. Vogel, *J. Chem. Soc.*, p. 632, 1948.
7. Commercial Solvents Corp., U.S. Patent 2,076,111, 1934.

	Diethyl tartrate	2,5-Diethyltetrahydrofuran
Other names	Diethyl 2,3-dihydroxybutanedioate Diethyl 2,3-dihydroxysuccinate Ethyl tartrate	
Empirical formula	$C_8H_{14}O_6$	$C_8H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, thick, oily liquid	Colorless liquid
Molecular weight	206.19	128.21
Boiling point	153°C at 12 mm Hg	116°C (approx)
Specific gravity	1.204 at 20°C	
Refractive index	1.4476 at 20°C	
Optical rotation	+7°5′ at 20 C	
Solubility	Insoluble in water; miscible with alcohol and ether	Slightly soluble in water; soluble in alcohol and propylene glycol
Organoleptic characteristics		Sweet, herbaceous, caramellic odor
Synthesis	By direct esterification of the acid in the presence of various catalysts, including Twitchell's reagent and HCl[6–8]	
Natural occurrence	The *d*-isomer has not been reported found in nature. The *l*-isomer and the racemic form are of little importance.	In mint
Reported uses[3]	Non-alcoholic beverages 50 ppm Ice cream, ices, etc. 200 ppm Candy 200 ppm Baked goods 200 ppm	The compound has been used in reconstructing mint flavors.
Regulatory status	FDA 121.1164; FEMA No. 2378	FDA 121.1164

REFERENCES

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

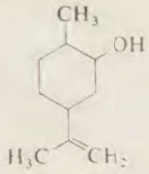
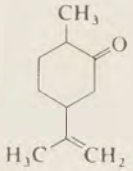
6. **Zaganiaris and Varvoglis,** *Ber. Dtsch. Chem. Ges.*, p. 69, 1936.
7. **Badoche,** *Ann. Chim.* (Paris), 11(18), 146, 1943.
8. **Bretschneider,** *Monatsh. Chem.*, 80, 258, 1949.

	Difurfuryl ether	Difurfuryl sulfide
Other names	Furfuryl ether	Furfuryl sulfide Bis-(2-furfuryl)-sulfide
Empirical formula	$C_{10}H_{10}O_3$	$C_{10}H_{10}O_2S$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Molecular weight	178.19	194.25
Melting point		31 32°C
Boiling point	101°C at 2 mm Hg 88–89°C at 1 mm Hg	135–143° at 14 mm Hg
Specific gravity	1.405 at 20°C	
Refractive index	1.5088 at 20°C	
Solubility	Insoluble in water	
Synthesis	By reacting furfuryl alcohol and furfuryl chloride[6] or furfuryl iodide[7] in boiling ether in the presence of KOH	By reacting furfuryl mercaptan and furfuryl bromide in ether solution in the presence of KOH[8]
Natural occurrence	Reported found as a constituent in coffee aroma[8]	Reported found as a constituent in coffee aroma[8]
Reported uses[3]	Baked goods 1.0 ppm Meat, meat sauces, soups 1.0 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 Chewing gum 5.0 ppm Condiments 5.0 ppm Meat, meat sauces, soups 5.0 ppm
Regulatory status	FEMA No. 3337	FEMA No. 3258

REFERENCES

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

6. Kirner, *J. Am. Chem. Soc.*, 50, 1960, 1928.
7. Zanetti, *J. Am. Chem. Soc.*, 49, 1064, 1927.
8. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.

	Dihydrocarveol	Dihydrocarvone
Other names	8-*p*-Menthen-2-ol 6-Methyl-3-isopropenylcyclohexanol Tuberyl alcohol	*cis-l*-Dihydrocarvone 8-*p*-Menthen-2-one *cis-p*-Menthen-8(9)-one (2) 1-Methyl-4-isopropenyl cyclohexan-2-one
Empirical formula	$C_{10}H_{18}O$	$C_{10}H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Almost colorless, straw-colored liquid (somewhat viscous)	Colorless to straw-yellow liquid
Assay	Commercial products usually are a mixture of several stereoisomers; the *dextro* form is a more desirable product	
Molecular weight	154.24	152.23
Boiling point	*d*, 222.5–223°C at 749 mm Hg *l*, 107°C at 14 mm Hg	*l*, 220°C at 750 mm Hg
Specific gravity	*d*, 0.9204 at 20°C; *l*, 0.9202 at 23°C	*l*, 0.929 at 15°C
Refractive index	*d*, 1.47818 at 20°C; *l*, 1.4748 at 23°C	*l*, 1.47348 at 20°C
Optical rotation	*d*, +33.86°; *l*, −33.25° at 23°C	*l*, −15.6° (−18 to −19° at 20°C for synthetic product)
Solubility	Soluble in alcohol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Floral, woody odor; sweet, somewhat spicy flavor (peppery)	Warm, powerful, herb-like odor; spearmint-like flavor
Synthesis	By reducing carvone and separating the resulting isomers	By isomerization of limonene oxide; by oxidation of dihydrocarveol or reduction of carvone
Natural occurrence	For determination of structure see reference 6. Because of the presence of 3 asymmetric carbons, 8 optically active isomers are possible. The *d*-, *l*-, and *dl*-forms are known. Reported found (free or esterified) in the essential oils of: *Mentha longifolia*,[6] *Mentha verticillata*, *Artemisia juncea*, caraway, and others. Also identified in the essential oil of *Mentha viridis* var. *sativa* cultivated in Calabria.[7]	The following stereoisomers are known: *dl*- and *l*-dihydrocarvone and the *l*-isodihydrocarvone. The optically inactive form is usually prepared by synthesis. The *l*-forms are reported found among the constituents of the essential oils of: caraway, anethum, *Mentha spicata* var. *longifolia*, angelica seeds, and others. For the identification of chemical structure, see references 8, 9, 10, and 11.
Reported uses[3]	Non-alcoholic beverages 84 ppm Alcoholic beverages 500 ppm Ice cream, ices, etc. 300 ppm Candy 10–250 ppm Baked goods 10–250 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2379	FDA 121.1164

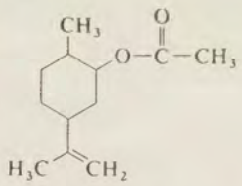
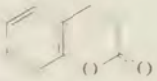
REFERENCES

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

6. **LaFace,** *Chem. Abstr.*, 48, 7261, 1954.
7. **Bonaccorsi,** *Chem. Zentralbl.*, 2, 1261, 1936.
8. **Wallach,** *Annalen*, 275, 114, 1893; *Ber. Dtsch. Chem. Ges.*, 28, 2704, 1895.
9. **Wallach and Schrader,** *Annalen*, 279, 377, 1894.
10. **Wagner,** *Ber. Dtsch. Chem. Ges.*, 27, 1652, 1894.

For further information on dihydrocarveol see the following:

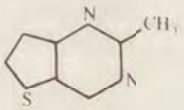
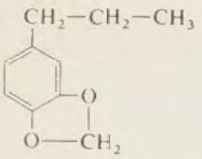
Schmidt, *Chem. Ber.*, 83, 193, 1950; B: *Schimmel Ber.*, p. 136, 1951; C: *Miltizer Ber.*, 122, 1956.

	Dihydrocarvyl acetate	Dihydrocoumarin
Other names	8-*p*-Menthen-2-yl acetate *p*-Menth-8-(9)-en-2-yl acetate 6-Methyl-3-isopropenyl cyclohexyl acetate	Benzodihydropyrone 3,4-Dihydrocoumarin Hydrocoumarin
Empirical formula	$C_{12}H_{20}O_2$	$C_9H_8O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Low-melting solid
Assay		98% min
Molecular weight	196.29	148.16
Melting point		25°C
Boiling point		272 C
Congealing point		23–23.6°C
Flash point		130°C
Specific gravity	0.96	1.955–1.980 at 15°C
Refractive index		1.5560–1.5575 at 20°C
Acid value		0.9
Solubility	Slightly soluble in water; soluble in alcohol	Slightly soluble in water; soluble in alcohol, ether, and especially in chloroform; 1:2.5–3.5 in 70% alcohol
Organoleptic characteristics	Sweet, floral, rose-like odor; slightly minty; used in imitation spearmint	Odor similar to coumarin at room temperature or reminiscent of nitrobenzene at higher temperature; burning taste
Synthesis	Acetylation of dihydrocarveol	By reduction of coumarin under pressure in the presence of nickel at 160–200 C[6] or in the presence of Pd-$BaSO_4$ in alcoholic solution[7]
Natural occurrence	In mint and celery	Reported found in *Melilotus officinalis*,[8] from which it may be extracted by water distillation
Reported uses[3]	Non-alcoholic beverages 2.0–5.0 ppm Ice cream, ices, etc. 20 ppm Candy 22 ppm Baked goods 22 ppm Condiments 10 ppm	Non-alcoholic beverages 7.8 ppm Ice cream, ices, etc. 21 ppm Candy 44 ppm Baked goods 28 ppm Gelatins and puddings 10 ppm Chewing gum 78 ppm
Regulatory status	FDA 121.1164; FEMA No. 2380	FDA status not fully defined; FEMA No. 2381

REFERENCES

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

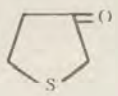
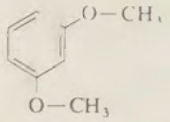
6. Tetralin Gesellschaft, German Patent 355,650.
7. Paal and Schiedewitz, *Ber. Dtsch. Chem. Ges.*, 63, 775, 1930.
8. Phipson, *Chem. News*, 32, 25, 1875.

	5,7-Dihydro-2-methylthieno(3,4d)pyrimidine		Dihydrosafrole
Other names	Thienyl pyrimidine; with the same number, FEMA also report *p*-tolylisovalevate		3,4-Methylenedioxy-propylbenzene
Empirical formula	$C_8H_{12}N_2S$		$C_{10}H_{12}O_2$
Structure			
Physical/chemical characteristics[5]			
Appearance			Colorless to yellowish liquid
Molecular weight	276.26		164.21
Boiling point			112°C at 15 mm Hg
Flash point			TCC 202°F
Specific gravity			1.063–1.070 at 25°C; 1.0759 at 15.6°C
Refractive index			1.5170–1.5200 at 20°C; 1.5228 at 15.6°C
Solubility			1:9 in 80% alcohol; 1:2 in 90% alcohol
Organoleptic characteristics			Odor reminiscent of sassafras
Synthesis	By reaction of acetamidine HCl with 3-carbomethoxytetrahydro-4-furanones[6]		From safrole or isosafrole by hydrogenation over nickel at 200°C;[6] by hydrogenation of either safrole in alcoholic solution in the presence of palladium or activated carbon[7] or of 3,4-methylenedioxy cinnamic aldehyde[8]
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	
	Baked goods	1.0 ppm	
	Gelatins and puddings	1.0 ppm	
	Chewing gum	1.0 ppm	
	Condiments, pickles	1.0 ppm	
	Meat, meat sauces, soups	1.0 ppm	
	Cereals	1.0 ppm	
	Milk, dairy products	1.0 ppm	
Regulatory status	FEMA No. 3338		Use in foods not permitted in USA

REFERENCES

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

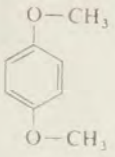
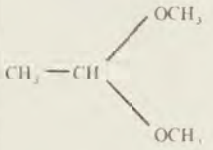
6. **Katz et al.**, (International Flavor and Fragrances), German Patent 2,141,916.
7. **Henrard,** *Chem. Zentralbl.*, 2, 1512, 1907.
8. **Spät and Quietensky,** *Ber. Dtsch. Chem. Ges.*, 60, 1887, 1927.
9. **Lohans,** *J. Prakt. Chem.*, 2(119), 259, 1928.

	4,5-Dihydro-3-(2H)thiophenone		*m*-Dimethoxybenzene	
Other names	3-Tetrahydrothiophenone-3-thiophanone		1,3-Dimethoxybenzene Dimethylresorcinol Resorcinol dimethyl ether	
Empirical formula	C_4H_6OS		$C_8H_{10}O_2$	
Structure				
Physical/chemical characteristics[5]				
Appearance			Liquid	
Molecular weight	102.15		138.16	
Melting point			−52 to −55°C	
Boiling point			215–217.5°C	
Specific gravity			1.0803 at 0°C	
Solubility			Slightly soluble in water; soluble in alcohol, ether, and benzene	
Organoleptic characteristics			Acrid, fruity odor reminiscent of nerolin with a similar taste	
Synthesis	From 4-methoxycarboxyl-3-oxothiophane treated with 10% sulfuric acid[6]		From resorcinol by methylation using dimethyl sulfate and alkali[7–9]	
Natural occurrence			Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages	1.0 ppm	Non-alcoholic beverages	3.0 ppm
	Ice cream, ices, etc.	1.0 ppm	Ice-cream, ices, etc.	5.0 ppm
	Candy	1.0 ppm	Candy	5.0 ppm
	Gelatins and puddings	1.0 ppm	Baked goods	8.0 ppm
	Chewing gum	1.0 ppm		
	Condiments, pickles	1.0 ppm		
	Meat, meat sauces, soups	1.0 ppm		
	Milk, dairy products	1.0 ppm		
	Cereals	1.0 ppm		
Regulatory status	FEMA No. 3266		FDA 121.1164; FEMA No. 2385	

REFERENCES

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

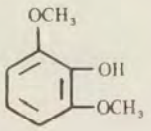
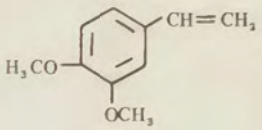
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	p-Dimethoxybenzene	1,1-Dimethoxyethane
Other names	Dimethyl hydroquinone Hydroquinone dimethyl ether	Dimethylacetal Acetaldehyde dimethylacetal Ethylidene dimethyl ether
Empirical formula	$C_8H_{10}O_2$	$C_4H_{10}O_2$
Structure		
Physical/chemical characteristics		
Appearance	Low-melting solid	Mobile liquid
Molecular weight	138.16	90.12
Melting point	53°C (56 C)	
Boiling point	109 C at 20 mm Hg	64–65°C
Specific gravity	1.036 at 66 C	0.8501 at 20°C
Refractive index		1.3668 at 20°C
Solubility	1:10 in 95% alcohol	Miscible with water, alcohol, chloroform, and ether
Organoleptic characteristics	Bitter taste	
Synthesis	By methylation of hydroquinone using dimethyl sulfate and alkali[17]	From acetaldehyde and methanal[6,7]
Natural occurrence	Reported found in hyacinth (*Hyacinthus orientalis* L.) essential oil[18] and in *Rhodophyllus icterius*	In raspberry and blackberry,[8] strawberry,[9-11] hop oil,[12,13] coffee,[14,15] tea[16]
Reported uses[3]	Non-alcoholic beverages 8.1 ppm Ice cream, ices, etc. 5.0 ppm Candy 4.7 ppm Baked goods 5.8 ppm	Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 6.0 ppm Baked goods 6.0 ppm Gelatins and puddings 3.0 ppm Jellies, preserves, spreads 3.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2386	FEMA No. 3426

REFERENCES

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

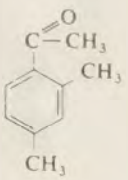
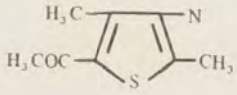
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16. Bondarovich et al., *J. Agric. Food Chem.*, 15, 36, 1967.
17. Dyson, George and Hunter, *J. Chem. Soc.*, p. 440, 1927.
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	2,6-Dimethoxyphenol	3,4-Dimethoxy-1-vinyl benzene
Other names	Pirogallol, 1,3-dimethyl ether	
Empirical formula	$C_8H_{10}O_3$	$C_{10}H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White or colorless crystals	
Molecular weight	154.17	164.20
Melting point	56–57°C	
Boiling point	262°C	
Solubility	Slightly soluble in water; soluble in alcohol and aqueous alkalis; very soluble in ether	
Organoleptic characteristics	Woody, medicinal odor	
Synthesis	By reacting pyrogallol with methyl iodide in alkaline aqueous medium;[6] by demethylation of pyrogallol trimethyl ether in aqueous alkali or in alcohol[7]	
Natural occurrence	Reported found in beech tar creosote	Reported found in coffee[8-10]
Reported uses[3]	Meat 3.0 ppm Soups 0.80 ppm Seafood 2.0 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm Gelatins and puddings 2.0 ppm Meat 2.0 ppm Soups 2.0 ppm
Regulatory status	FEMA No. 3137	FEMA No. 3138

REFERENCES

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

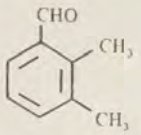
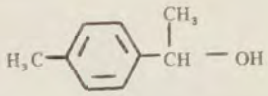
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	2,4-Dimethylacetophenone		2,4-Dimethyl-5-acetylthiazole	
Other names	Methyl 2,4-dimethylphenyl ketone			
Empirical formula	$C_{10}H_{12}O$		C_7H_9NOS	
Structure				
Physical/chemical characteristics[5]				
Appearance	Oily, colorless to yellowish liquid			
Assay	97% min			
Molecular weight	148.20		155.22	
Boiling point	228°C; 110°C at 13 mm Hg			
Flash point	208°F			
Specific gravity	0.993–0.996 at 25°/25°C			
Refractive index	1.533–1.535 at 20 C			
Acid value	1 max			
Solubility	1:6 in 60% alcohol; 1:2 in 70% alcohol			
Organoleptic characteristics	Odor reminiscent of peppermint or floral, sweet odor			
Synthesis	By condensation of acetyl chloride and *m*-xylene in the presence of aluminum chloride[6] or in the presence of ferric chloride[7,8]			
Natural occurrences	Not reported found in nature			
Reported uses[3]	Non-alcoholic beverages	0.78 ppm	Ice cream, ices, etc.	10.0 ppm
	Alcoholic beverages	1.0 ppm	Candy	10.0 ppm
	Ice cream, ices, etc.	0.77 ppm	Baked goods	6.0 ppm
	Candy	3.9 ppm	Meat, meat sauces, soups	10.0 ppm
	Baked goods	2.7 ppm		
Regulatory status	FDA 121.1164; FEMA No. 2387		FEMA No. 3267	

REFERENCES

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

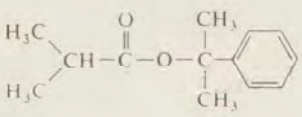
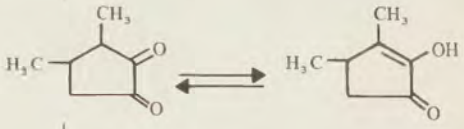
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	2,4-Dimethylbenzaldehyde		*p*, α-Dimethylbenzyl alcohol	
Other names	2,4-Xylylaldehyde 1-Formyl-2,4-dimethylbenzene		Methyl-*p*-tolyl carbinol 1-*p*-Tolyl-1-ethanol 4-(α-Hydroxyethyl)toluene 4-Methyl-α-phenethyl alcohol	
Empirical formula	$C_9H_{10}O$		$C_9H_{12}O$	
Structure				
Physical/chemical characteristics				
Appearance			Colorless, slightly oily liquid	
Molecular weight	134.17		136.19	
Melting point	−9°C			
Boiling point	212–215°C at 710 mm Hg		219°C	
Congealing point			134°C at 14 mm Hg	
Flash point			*dl*- 115–116°C at 11 mm Hg	
Specific gravity			0.9668 at 15.5°C	
Solubility			Sparingly soluble in water; miscible with alcohol and ether; soluble in isopropanol and liquid petrolatum	
Organoleptic characteristics			Odor reminiscent of menthol	
Synthesis	By passing HCl into a mixture of *o*-xylole, aluminum chloride, and sodium cyanide at 100°C[6]		From *p*-tolylmagnesium bromide and acetaldehyde in ether;[7,8] from 4-methylacetophenone with sodium metal in ethanol[9]	
Natural occurrence			Reported found as a constituent in the essential oil of *Curcuma longa* L. and related species (Zingiberaceae); the product obtained from natural sources is probably levorotatory	
Reported uses[3]	Non-alcoholic beverages	2.0 ppm	Non-alcoholic beverages	10.0 ppm
	Ice cream, ices, etc.	2.0 ppm	Ice cream, ices, etc.	10.0 ppm
	Candy	3.0 ppm	Candy	10.0 ppm
	Gelatins and puddings	2.0 ppm		
	Condiments	1.0 ppm		
	Jellies, preserves, spreads	1.0 ppm		
Regulatory status	FEMA No. 3427		FEMA No. 3139	

REFERENCES

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

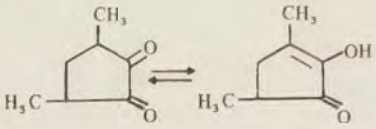
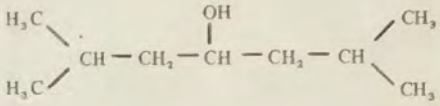
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9. Gastaldi and Cherchi, *Gazz. Chim. Ital.*, 45(2), 274, 1915.

	α,α-Dimethylbenzyl isobutyrate	3,4-Dimethyl-1,2-cyclopentanedione
Other names	Phenyldimethyl carbinyl isobutyrate 2-Phenylpropan-2-yl isobutyrate	
Empirical formula	$C_{13}H_{18}O_2$	$C_7H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Molecular weight	206.28	126.15
Melting point	71–72°C	
Solubility	Insoluble in water; soluble in alcohol	
Organoleptic characteristics	Sweet, fruity, apricot, peach, and plum odor; green, dry, banana-, peach-, plum-like flavor	
Synthesis	By esterification of dimethylphenylcarbinol with isobutyric acid	By alkylation of 3,5-dicarbetoxy-4-methylcyclopentane-1,2-dione followed by hydrolysis and decarboxylation of the resulting 3,5-dicarbetoxy-3,4-dimethylcyclopentane-1,2-dione[6]
Natural occurrence	Not reported found in nature	Reported found as a constituent in coffee[7]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 40 ppm Candy 30 ppm Baked goods 20 ppm	Ice cream, ices, etc. 0.3 ppm Candy 4.0 ppm Chewing gum 1.9 ppm Protein foods 3.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2388	FEMA No. 3268

REFERENCES

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

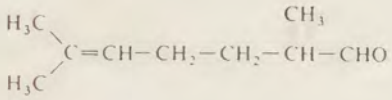
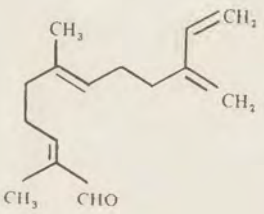
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	3,5-Dimethyl-1,2-cyclopentadione	2,6-Dimethyl-4-heptanol
Other names	3,5-Dimethyl-1,2-cyclopentadione	Diisobutyl carbinol 4-Hydroxy-2,6-dimethyl heptane
Empirical formula	$C_7H_{10}O_2$	$C_9H_{20}O$
Structure		
Physical/chemical characteristics[5]		
Molecular weight	126.15	144.26
Melting point	91–92°C	
Boiling point		178°C 79°C at 15 mm Hg
Specific gravity		0.8097 at 20°C
Refractive index		1.4238 at 20°C
Solubility		Insoluble in water; soluble in alcohol and ether
Synthesis	By direct alkylation of the methyl ester of the commercially available 3-methylcyclopent-2-en-2-ol-1-one, followed by the cleavage of the ether function[6]	By catalytic hydrogenation of diisobutyl ketone[8,9]
Natural occurrence	Reported found as a volatile constituent in coffee aroma[7]	
Reported uses[3]	Non-alcoholic beverages 2.4 ppm Ice cream, ices, etc. 6.0 ppm Candy 5.0 ppm	Non-alcoholic beverages 20.0 ppm Ice cream, ices, etc. 20.0 ppm Candy 20.0 ppm Gelatins and puddings 20.0 ppm Chewing gum 20.0 ppm
Regulatory status	FEMA No. 3269	FEMA No. 3140

REFERENCES

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

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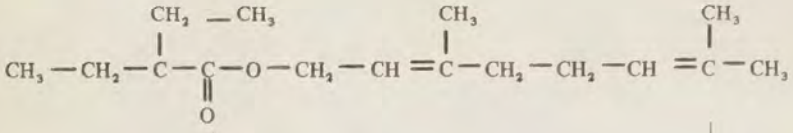
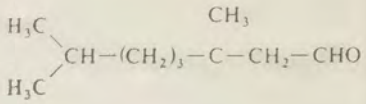
	2,6-Dimethyl-5-heptenal	2,6-Dimethyl-10-methylene-2,6,11-dodecatrienal
Other names	Melonal[4]*	β-Sinensal (Note: the old name of α-sinensal was recently changed to β-sinensal in agreement with the structure of α- and β-farnesene; α-sinensal is now 2,6,10-trimethyl-2,6,9,11-dodecatetraenal[6-8])
Empirical formula	$C_9H_{16}O$	$C_{15}H_{22}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellow liquid	Colorless liquid
Assay	85% min[2]	
Molecular weight	140.23	218.34
Boiling point		>300°C 180°C at 1 mm Hg 100°C at 0.1 mm Hg
Flash point	144°F	
Specific gravity	0.845–0.855 at 25/25°C[2]	
Refractive index	1.4410–1.4470 at 20°C[2]	1.5077 at 20°C
Acid value	Not more than 5.0[2]	
Organoleptic characteristics	Characteristic odor of melon and corresponding taste	
Synthesis		From myrcene by oxidation and other synthetic routes[7,8]
Natural occurrence	Not reported found in nature	Reported found in orange oil (*Citrus sinensis* L.)[9]
Reported uses[3]	Non-alcoholic beverages 2.8 ppm Ice cream, ices, etc. 1.7 ppm Candy 8.4 ppm Baked goods 19 ppm Gelatins and puddings 0.02–10 ppm Chewing gum 0.80 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2389	FEMA No. 3141

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REFERENCES

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

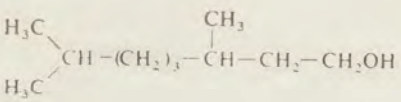
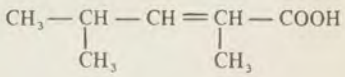
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	3,7-Dimethylocta-2,6-dienyl-2-ethyl butanoate		2,6-Dimethyl octanal
Other names	Geranyl 2-ethyl butyrate		2,6-Dimethyl octanoic aldehyde Isoaldehyde C-10 Isodecylaldehyde
Empirical formula	$C_{16}H_{27}O_2$		$C_{10}H_{20}O$
Structure			
Physical/chemical characteristics[5]			
Appearance			Colorless liquid
Molecular weight	251.38		156.26
Boiling point			*d*, 81°C at 12 mm Hg; *dl*, 82–84°C at 15 mm Hg
Specific gravity			*d*, 0.8253 at 20 C; *d*, 0.823 at 22°C
Refractive index			*d*, 1.4257 at 20 C; *d*, 1.4285 at 17°C
Optical rotation			*d*, +9°
Solubility			Insoluble in water; soluble in alcohol
Organoleptic characteristics			Powerful, sweet odor of fruit; somewhat green flavor
Synthesis			The *d*-isomer is prepared by heating *d*-dihydrocitronellol and isopropyl aluminate at 70–100 C and 14 mm Hg and subsequently adding cinnamaldehyde at 140–160 C;[6] or by hydrogenation of citronellal with palladium or strontium carbonate in methanol under pressure (3 atm).[7] The *dl*-form is prepared by hydrogenation of citral in ethanol under pressure in the presence of palladium and strontium carbonate[8] or of palladium and calcium carbonate.[9,10]
Natural occurrence	Reported found in geranium		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages	10.0 ppm	Non-alcoholic beverages 0.44 ppm
	Alcoholic beverages	40.0 ppm	Ice cream, ices, etc. 3.2 ppm
	Ice cream, ices, etc.	40.0 ppm	Candy 1.9 ppm
	Candy	75.0 ppm	Baked goods 1.9 ppm
	Baked goods	100.0 ppm	
	Gelatins and puddings	50.0 ppm	
	Preserves and spreads	50.0 ppm	
Regulatory status	FEMA No. 3339		FDA 121.1164; FEMA No. 2390

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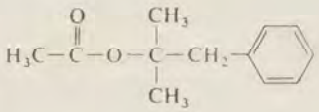
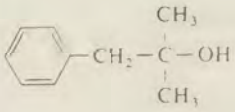
For References 1–5, see end of Part III.

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8. **Rydon,** *J. Chem. Soc.,* p. 1546, 1939.
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10. **Braum and Rudolph,** *Ber. Dtsch. Chem. Ges.,* 67, 1738, 1934.

	3,7-Dimethyl-1-octanol	2,4-Dimethyl-2-pentenoic acid
Other names	Dihydrocitronellol Tetrahydrogeraniol	
Empirical formula	$C_{10}H_{22}O$	$C_7H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Assay	90% min[2]	
Molecular weight	158.29	128.17
Boiling point	221–223 C; 81–82 C at 2.4 mm Hg	
Specific gravity	0.826–0.842 at 25 /25 C;[2] 0.8308 at 20 C	
Refractive index	1.4350–1.4450[2] (1.4360) at 20 C	
Acid value	Not more than 1[2]	
Solubility	1:3 and more in 70% alcohol;[2] insoluble in water	
Organoleptic characteristics	Sweet, rosy odor and bitter taste	
Synthesis	Usually prepared by hydrogenation of geraniol, citronellol, or citronellal	
Natural occurrence	Reported found in nature. Corresponds to the *dl*-form of dihydrocitronellol	
Reported uses[3]	Non-alcoholic beverages 4.3 ppm Ice cream, ices, etc. 2.0–44 ppm Candy 15 ppm Baked goods 19 ppm Chewing gum 2.9 ppm	Candy 1.0 ppm Baked goods 1.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2391	FEMA No. 3143

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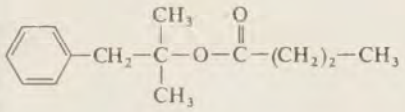
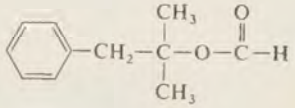
For References 1–5, see end of Part III.

	α,α-Dimethylphenethyl acetate	α,α-Dimethylphenethyl alcohol
Other names	Benzyldimethylcarbinyl acetate Benzylpropyl acetate	Benzyl dimethyl carbinol Dimethyl benzyl carbinol 1,1-Dimethyl-2-phenylethanol 2-Methyl-1-phenyl-propanol-2
Empirical formula	$C_{12}H_{16}O_2$	$C_{10}H_{14}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Watery, white liquid; solidifies at room temperature	Low-melting, white, crystalline solid. It may remain super-cooled as a white, oily liquid
Assay	98% min[2]	97%[2]
Molecular weight	192.26	150.22
Melting point	29.5°C	24°C
Boiling point		108°C at 11 mm Hg
Congealing point	>28.0°C[2]	>22°C[2]
Flash point	>100°C	92°C
Specific gravity	0.995–1.002 at 25°/25°C[2] (supercooled liquid)	0.972–0.977 at 25°/25°C;[2] 0.9790 at 16°C
Refractive index	1.4910–1.4950 at 20°C[2] (supercooled liquid)	1.5140–1.5170 at 20°C (supercooled liquid);[2] 1.5174 at 16°C
Acid value	Not more than 1.0[2]	Not more than 1.0[2]
Solubility	1:4 and more in 70% alcohol[2]	1:3 in 50% alcohol; 1:2 in 60% alcohol
Organoleptic characteristics	Floral, fruity odor reminiscent of pear[2]	Fresh, floral odor and bitter taste
Synthesis	By acetylation of dimethylbenzyl carbinol	From acetone and benzyl magnesium chloride[6] or benzyl magnesium bromide[7]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.8 ppm Ice cream, ices, etc. 8.0 ppm Candy 22 ppm Baked goods 19 ppm Chewing gum 2.9 ppm	Non-alcoholic beverages 3.3 ppm Ice cream, ices, etc. 3.2 ppm Candy 4.0 ppm Baked goods 4.9 ppm Gelatins and puddings 0.01 ppm Jellies 3.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2392	FDA 121.1164; FEMA No. 2393

REFERENCES

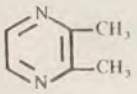
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	α,α-Dimethylphenethyl butyrate	α,α-Dimethylphenethyl formate
Other names	Benzyl dimethylcarbinyl butyrate Dimethylbenzylcarbinyl butyrate D.M.B.C. butyrate	Benzyl dimethylcarbinyl formate Dimethylbenzylcarbinyl formate
Empirical formula	$C_{14}H_{20}O_2$	$C_{11}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	220.31	178.23
Solubility	Insoluble in water; soluble in alcohol	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Mild, herbaceous, fruity (plum-prune) odor; apricot, peach, plum-like taste	Dry, herbaceous, green, lily-jasmine odor; spicy taste, quite warm and herbaceous
Synthesis	By esterification of dimethylbenzylcarbinol with *n*-butyric acid under catalysis or azeotropic conditions	From dimethylbenzylcarbinol and formic acid using acetic anhydride
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 20 ppm Candy 20 ppm Gelatins and puddings 20 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 10 ppm Candy 10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2394	FDA 121.1164; FEMA No. 2395

REFERENCES

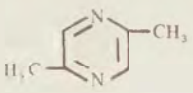
For References 1–5, see end of Part III.

	2,3-Dimethylpyrazine
Other names	2,3-Dimethyl-1,4-diazine
Empirical formula	$C_6H_8N_2$
Structure	
Physical/chemical characteristics	
Appearance	Liquid (volatile with steam)
Assay	C: 66.64%; H: 7.46%; N: 25.90%
Molecular weight	108.14
Boiling point	156°C
Congealing point	
Flash point	
Specific gravity	1.0218 at 0°C
Refractive index	
Mass spectra[8]	40 (20), 42 (23), 51 (6), 52 (11), 67 (100), 68 (6), 93 (4), 94 (1), 108 (97), 109 (6)
NMR spectra	
IR spectra[8]	S (6.9, 7.0, 7.1, 8.5, 10.1, 10.5, 11.8) M (3.3, 3.4, 7.3, 9.8, 11.3) W (5.2, 5.5, 6.5, 8.0, 8.3)
UV spectra[8]	(273.0, 269.5 nm)
Solubility	Soluble in water, alcohol, and ether
Organoleptic characteristics	Odor threshold: 2,500 ppb in water[9]
Synthesis	By heating the reaction product of diacetyl and ethlenediamine with potassium hydroxide in alcohol[6]
Natural occurrence	Reported to be present in the following foods: bakery products, roasted barley, cocoa products, coffee, dairy products, meat, peanuts, pecans, filberts, popcorn, potato products, rum and whisky, soy products[7]
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 10.0 ppm Meat, meat sauces, soups 10.0 ppm
Regulatory status	FEMA No. 3271

REFERENCES

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

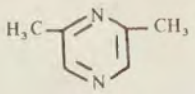
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7. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
8. Bondarovich et al., *J. Agric. Food Chem.*, 15, 1093, 1967.
9. Guadagni et al., *J. Sci. Food Agric.*, 23, 1435, 1972.

	2,5-Dimethylpyrazine
Other names	2,5-Dimethyl-1,4-diazine Glycoline Ketine
Empirical formula	$C_6H_8N_2$
Structure	
Physical/chemical characteristics	
Appearance	Colorless liquid; solidifies in cold weather
Assay	C: 66.64%; H: 7.46%; N: 25.90%
Molecular weight	108.14
Melting point	15°C
Boiling point	155°C
Specific gravity	0.9887 at 20°C
Refractive index	1.4980 at 20°C
Mass spectra[8]	39(35), 42(87), 51(4), 52(6), 64(1), 66(2), 80(3), 81(18), 93(1), 108(100), 109(6)
IR spectra[9]	S (6.7, 7.2, 7.5, 8.6, 9.6)
UV spectra[9]	(277.0, 272.0 nm)
Solubility	Soluble in water, alcohol, and ether in all proportions; also soluble in acetone
Organoleptic characteristics	Characteristic flavor reminiscent of potato chips; odor threshold: 1,800 ppb in water,[10] 1,000 ppb in water[11]
Synthesis	By the interaction of acrolein and ammonia when heated in glycerol in the presence of ammonium salts;[6] by self-condensation of aminoacetone, followed by oxidation with mercury chloride[7]
Natural occurrence	Reported to be present in the following foods: bakery products, roasted barley, cocoa products, roasted coffee, dairy products, meat, peanuts, pecans, filberts, popcorn, potato products, rum and whisky, soy products;[8] a volatile component in roasted filberts[12] and in potato chips;[13] reportedly identified in the fat of cooked beef;[14] also reported found in toasted off-flavors[15]
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 10.0 ppm Meat 10.0 ppm Mil, dairy products 10.0 ppm Cereals 10.0 ppm
Regulatory status	FEMA No. 3272

REFERENCES

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

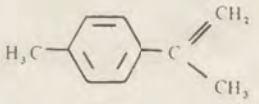
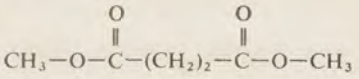
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13. Watanabe and Sato, *Agric. Biol. Chem.*, 35, 756, 1971.
14. Goldman et al., *Helv. Chim. Acta*, 50, 694, 1967.
15. Sapers et al., *J. Food Sci.*, 36(1), 93, 1971.

	2,6-Dimethylpyrazine
Other names	2,6-Dimethyl-1,4-diazine
Empirical formula	$C_6H_8N_2$
Structure	
Physical/chemical characteristics	
Appearance	White crystals
Assay	C: 66.64%; H: 7.46%; N: 25.90%
Molecular weight	108.14
Melting point	47–48°C
Boiling point	155.6°C
Specific gravity	0.9647 at 50°C
Mass spectra[8]	40(43), 42(74), 52(4), 54(2), 66(7), 67(8), 80(1), 81(7), 92(3), 93(1), 108(100), 109(7)
IR spectra[8]	S (6.8, 7.1, 7.2, 8.0, 8.6, 9.8, 11.6) M (3.3, 3.4, 6.5, 7.8, 8.4, 10.7) W (5.1, 5.3, 5.6, 5.8, 7.6, 10.2)
UV spectra[8]	(275.6, 271.0 nm)
Solubility	Soluble in water, alcohol, ether, and essential oils
Organoleptic characteristics	Sweet, "fried" odor; odor threshold: 54,000 ppb in water,[9] 1,500 ppb in water[10]
Synthesis	By condensation of 1,2-diaminopropane, followed by column chromatography to separate the 2,6-methylpyrazine from the 2,5-dimethylpyrazine[6]
Natural occurrence	Reported to be present in the following foods: cocoa products, coffee, dairy products, meat, peanuts, pecans, filberts, potato products, rum and whisky, soy products;[7] reported found in grilled beef;[11] also a volatile flavor component of potato chips[12,13]
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 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
Regulatory status	FEMA No. 3273

REFERENCES

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

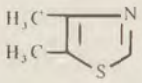
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7. Maga and Sizer, *Crit. Rev. Food Technol.,* 4(1), 39, 1973.
8. Bondarovich et al., *J. Agric. Food Chem.,* 15, 1093, 1967.
9. Koehler et al., *J. Food Sci.,* 36, 816, 1971.
10. Guadagni et al., *J. Sci. Food Agric.,* 23, 1435, 1972.
11. Flament and Ohloff, *Helv. Chim. Acta,* 54(7), 1911, 1971.
12. Deck, Pokorny and Chang, *J. Food Sci.,* 38(2), 345, 1973.
13. Watanabe and Sato, *Agric. Biol. Chem.,* 35, 756, 1971.

	p,α-Dimethyl styrene	Dimethyl succinate
Other names	*p*-Isopropenyl toluene 1-Methyl-4-isopropenyl benzene 2-*p*-Tolyl propene	Dimethyl butanedioate Methyl succinate
Empirical formula	$C_{10}H_{12}$	$C_6H_{10}O_4$
Structure		
Physical/chemical characteristics[3]		
Appearance	Liquid; oxidizes and slowly polymerizes in the presence of air	Colorless liquid (at room temperature); solidifies when cold
Molecular weight	132.18	146.15
Melting point	−20°C (−28°C)	18–19°C
Boiling point	186–189°C 82°C at 21 mm Hg	195–196°C; 80°C at 11 mm Hg
Specific gravity	0.9038 at 15.5°C	1.1198 at 20°C
Refractive index	1.5329 at 20°C (1.5350 at 20°C)	1.4196 at 20°C
Solubility		Soluble at 1% in water; 3% in alcohol
Organoleptic characteristics		Pleasant, ethereal, winey odor; fruity, winey, and burning flavor
Synthesis	By passing a stream of *p*-cymene and water vapors over activated aluminum oxide at 730°C[6]	By direct esterification of the acid with the alcohol in benzene solution at the boil in the presence of concentrated H_2SO_4[8]
Natural occurrence	Reported present in Indian hemp *(Cannabis indica)*[7]	In filbert nuts
Reported uses[3]	Non-alcoholic beverages 0.15 ppm Candy 2.8 ppm Gelatins and puddings 1.0 ppm	Non-alcoholic beverages 1.0–100 ppm Ice cream, ices, etc. 5.0 ppm Candy 15 ppm Baked goods 15 ppm Chewing gum 5.0 ppm
Regulatory status	FEMA No. 3144	FDA 121.1164; FEMA No. 2396

REFERENCES

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

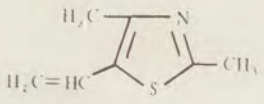
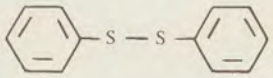
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	4,5-Dimethyl thiazole	Dimethyl trisulfide
Other names		Methyl trisulfide
Empirical formula	C_5H_7NS	$C_2H_6S_3$
Structure		$CH_3-S-S-S-CH_3$
Physical/chemical characteristics		
Appearance		Colorless to pale-yellow mobile, oily liquid
Molecular weight	113.18	126.27
Melting point	83–84°C	
Boiling point	158° 81–83°C at 59 mm Hg	165–170°C
Refractive index		n_D^{20} 1.6010
Solubility	Soluble in alcohol and ether	Slightly soluble in water; soluble in alcohol, propylene glycol, and oils
Organoleptic characteristics		Powerful, diffusive, penetrating odor reminiscent of fresh onion
Synthesis	From methyl-α-bromoethyl ketone;[6] by oxidation of 2-mercaptothiazoles with hydrogen peroxide in aqueous solution;[7] from 2-mercapto-4,5-dimethyl thiazole[8]	
Natural occurrence		Reported as occurring in the volatile portion of fresh onion juice; the major aroma component in cooked vegetables of the *Brassica* genus[9]
Reported uses[3]	Ice Cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 6.0 ppm Condiments, pickles 20.0 ppm Meat, meat sauces, soups 20.0 ppm	Baked goods 1.0 ppm Condiments, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm
Regulatory status	FEMA No. 3274	FEMA No. 3275

REFERENCES

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

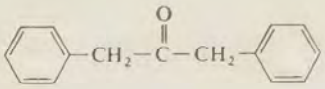
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7. **Russell,** U.S. Patent 2,509,453; *Chem. Abstr.*, 44, 7885, 1950.
8. **Hoffman-La Roche, A. G.,** British Patent 492,637; *Chem. Abstr.*, 33, 1760, 1939.
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	2,4-Dimethyl-5-vinylthiazole		Diphenyl disulfide	
Other names			Phenyl disulfide	
Empirical formula	C_7H_9NS		$C_{12}H_{10}S_2$	
Structure				
Physical/chemical characteristics				
Appearance			Needles (from alcohol)	
Molecular weight	139.21		218.34	
Melting point			61–62°C	
Boiling point			310°C	
			192°C at 15 mm Hg	
Specific gravity			1.353 at 20°C	
Solubility			Insoluble in water; soluble in alcohol, ether, benzene, and carbon disulfide	
Synthesis			By heating and passing a stream of air over an ammoniacal solution of thiophenol[7]	
Natural occurrence	In cooked beef[6]			
Reported uses[3]	Non-alcoholic beverages	0.10 ppm		
	Ice cream, ices, etc.	0.50 ppm	Non-alcoholic beverages	1.0 ppm
	Candy	0.50 ppm	Ice cream, ices, etc.	1.0 ppm
	Baked goods	0.50 ppm	Candy	1.0 ppm
	Gelatins and puddings	0.50 ppm	Gelatins and puddings	1.0 ppm
Regulatory status	FEMA No. 3145		FEMA No. 3225	

REFERENCES

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

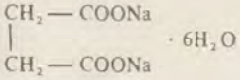
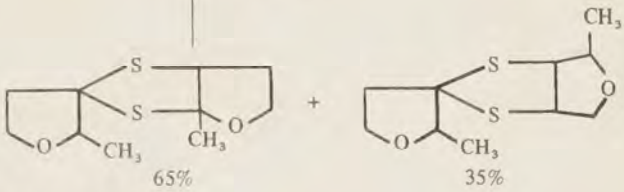
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	1,3-Diphenyl-2-propanone	Dipropyl trisulfide
Other names	Benzyl ketone Dibenzyl ketone	Propyl trisulfide
Empirical formula	$C_{15}H_{14}O$	$C_6H_{14}S_3$
Structure		$CH_3-CH_2-CH_2-S-S-S-CH_2-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance	Low-melting solid	Colorless to pale-yellow mobile liquid
Assay	98% min	
Molecular weight	210.28	182.38
Melting point	35°C	
Boiling point	331°C	68–69°C at 0.9 mm Hg
Refractive index		n_D^{20} 1.5424
Solubility	Soluble in ether; 1:2 in 95% alcohol; insoluble in water	Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Fruity odor reminiscent of bitter almond	Very powerful, diffusive garlic-like odor
Synthesis	By heating α,α′-phenyl benzyl ethylene glycol or α,α′-phenyl benzyl ethylene oxide in the presence of diluted H_2SO_4 or $ZnCl_2$;[7,8] also by dry distillation of phenylacetate and magnesium chloride ($C_6H_5CH_2COOMgCl$)[9] or other salts of phenylacetic acid	By an adaptation of Westlake's procedure[6]
Natural occurrence	Not reported found in nature	Reported found as a volatile constituent in onion oil
Reported uses[3]	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 4.5 ppm Candy 9.5 ppm Baked goods 13 ppm	Baked goods 1.0 ppm Condiments, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2397	FEMA No. 3276

REFERENCES

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

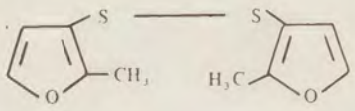
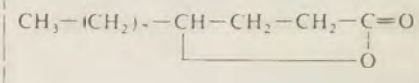
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8. McKenzie, Luis and Mitchell, *Chem. Ber.*, 65, 800, 1932.
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	Disodium succinate	spiro[2,4-Dithia-1-methyl-8-oxabicyclo [3.3.0] octane-3,3'-(1'-oxa-2'-methyl)cyclopentane] plus spiro [dithia-6-methyl-7-oxabicyclo[3.3.0] octane-3,3'-(1'-oxa-2-methyl)cyclopentane]
Other names	Sodium succinate Succinic acid, disodium salt	
Empirical formula	$C_4H_4Na_2O_4 \cdot 6H_2O$	$C_{10}H_{16}O_2S_2$
Structure		 65% + 35%
Physical/chemical characteristics[5]		
Appearance	Granules or crystalline powder; anhydrous when heated to 120°C	
Assay	Anhydrous, 59.99%; hydrate, 40.01%; as succinic acid, 43.71%	95% by VPC (65/35 mixture)
Molecular weight	270.16	232.2
Melting point		
Boiling point		135–140°C at 3 mm Hg
Refractive index		n_D^{20} 1.5619
Solubility	Soluble in about five parts of water; insoluble in alcohol	
Organoleptic characteristics		Meaty aroma
Synthesis	By a patented process[6]	
Natural occurrence	Reported found in condiments[7]	
Reported uses[3]	Non-alcoholic beverages 60.0 ppm Baked goods 60.0 ppm Meat, meat sauces, soups 60.0 ppm Milk, dairy products 60.0 ppm Cereals 60.0 ppm Extensively employed in the microencapsulation of flavoring oils[8]	Non-alcoholic beverages 0.045 ppm Ice cream, ices, etc. 0.25 ppm Candy 0.10 ppm Meat, meat sauces, soups 0.07 ppm Protein foods 0.40 ppm Mayonnaise 2.4 ppm
Regulatory status	FEMA No. 3277	FEMA No. 3270

REFERENCES

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

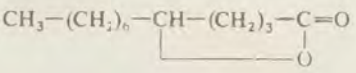
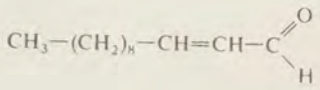
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8. Anonymous, *Fed. Regist.*, 33(232), 1968; *Chem. Abstr.*, 70, 27717w, 1969.

	3,3'-Dithio-bis- (2-methylforan)	γ-Dodecalactone
Other names	Bis(2-methyl-3-furyl) disulfide 2-Methyl-3-furyl disulfide	Dodecanolide-1,4 4-Hydroxydodecanoic acid, γ-lactone γ-Octyl-γ-butyrolactone γ-*n*-Octyl-γ-*n*-butyrolactone
Empirical formula	$C_{10}H_{10}O_2S_2$	$C_{12}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless, oily liquid
Molecular weight	226.31	198.31
Boiling point		170–171°C (258°C) at 11 mm Hg
Specific gravity		130°C at 5.1 mm Hg 0.9382 at 15°C
Refractive index		1.4522 at 20°C
Solubility		Insoluble in water; poorly soluble in propylene glycol; soluble in alcohol
Organoleptic characteristics		Fatty, peachy odor; buttery, peach-like flavor
Synthesis		From 1-dodecen-12-oic acid with H_2SO_4 at 90°C;[6] from 4-hydroxydodecanoic acid by lactonization; also from methyl-acrylate and octanol
Natural occurrence		Reported found in *Prunus persica*
Reported uses[3]	Baked goods 0.1 ppm Condiments, pickles 0.1 ppm Meat, meat sauces, soups 0.1 ppm	Non-alcoholic beverages 3.3 ppm Ice cream, ices, etc. 4.3 ppm Candy 13 ppm Baked goods 11 ppm Gelatins and puddings 0.15 ppm Jellies 0.01 ppm
Regulatory status	FEMA No. 3259	FDA 121.1164; FEMA No. 2400

REFERENCES

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

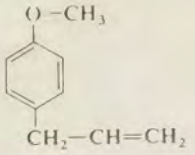
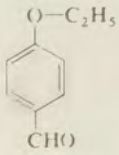
6. Chint et al., *Helv. Chim. Acta*, 10, 114, 1927.

	δ-Dodecalactone	2-Dodecenal
Other names	*n*-Heptyl-δ-valerolactone 5-Hydroxydodecanoic acid, δ-lactone	*n*-Dodecen-2-ol; *trans*-2-dodecen-l-ol; 3-nonyl acrolein
Empirical formula	$C_{12}H_{22}O_2$	$C_{12}H_{22}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to very pale straw-yellow, viscous liquid	Colorless, oily liquid
Molecular weight	198.31	182.31
Boiling point		108–109°C (272°C) at 1 mm Hg
Solubility	Insoluble in water; soluble in alcohol; poorly soluble in propylene glycol	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Powerful, fresh-fruit, oily odor; at low levels has peach, pear, plum-like flavor	Powerful, citrus, mandarin orange-like odor at low levels; mandarin taste
Synthesis	By lactonization of 5-hydroxydodecanoic acid	See Synthesis by R. Delaby;[6] by condensation of acetaldehyde with decanal; also from α-bromolauric acid by way of the ethyl ester and alcohol
Natural occurrence	Reported found in several natural products	Its presence has been reported in the essential oils of: *Eryngium factidum*,[7] *Achasma walang* Val.,[8] Guinea orange,[9] and bitter orange[10]
Reported uses[3]	Baked goods 0.06 ppm Gelatins and puddings 0.06 ppm Toppings 10 ppm	Non-alcoholic beverages, 2.9 ppm; ice cream, ices, etc., 3.1 ppm; candy, 2.8 ppm; baked goods, 2.8 ppm
Regulatory status	FDA 121.1164; tolerance 10 ppm in margarine; FEMA No. 2401	FDA 121.1164; FEMA No. 2402

REFERENCES

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

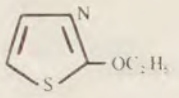
6. **Delaby**, *Bull. Soc. Chim. Fr.*, 5(3), 2375, 1936.
7. **Koolas**, *Chem. Zentralbl.*, 2, 630, 1932.
8. **Van Romburg**, *Chem. Zentralbl.*, 2, 2511, 1938.
9. **Naves**, *Perfum. Essent. Oil. Rec.*, 38, 237, 1947.
10. **Mehlitz and Minas**, *Ind. Obst Gemueseverwert.*, 50, 861, 1965.

	Estragole	*p*-Ethoxybenzaldehyde
Other names	*p*-Allyl anisole; chavicol methyl ether; methyl chavicol; *p*-methoxyallyl benzene	
Empirical formula	$C_{10}H_{12}O$	$C_9H_{10}O_2$
Structure		
Physical/chemical characteristics[2]		
Appearance	Colorless liquid	Colorless liquid; solidifies
Molecular weight	148.20	134.18
Melting point		14°C
Boiling point	214–216°C; 97–97.5°C at 12 mm Hg	140°C (249°C) at 20 mm Hg
Specific gravity	0.9600 at 25°C; 0.9645 at 20°C	
Refractive index	1.51372 at 22°C; 1.5230 at 17.5°C	
Solubility	Forms azeotropic mixtures with water (18%) and acetamide (18%); soluble in most organic solvents; 1:6 in 80% alcohol and 1:1 in 90% alcohol	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Odor reminiscent of anise with a corresponding sweet taste (differing from anethole)	Sweet and floral odor; sweet, floral taste
Synthesis	Obtained by fractional distillation of the oil of turpentine or by treating a solution of the same oil in ether with an aqueous solution of mercuric acetate and subsequently heating the aqueous phase with zinc and sodium hyydroxide;[6] from allyl bromide and magnesium *p*-methoxy phenate in ether[7,8]	By ethylation of *p*-hydroxybenzaldehyde using aluminum chloride catalyst
Natural occurrence	Isolated initially from the rind of *Persea gratissima* Gartn.[9] and subsequently from the oil of estragon.[10] It has been found in large amounts (as much as 60 – 90%) in the oils of: Chinese star anise, Russian anise, basil, fennel, turpentine, *Feronia elephatum* Corr., *Solidago odora*, *Agasnache rugosa*, and *Orthodon methylchavicoliferum*; obtained by steam distillation in the oil of *Fagara manishurica*[11]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages, 10 ppm; ice cream, ices, etc., 11 ppm; candy, 36 ppm; baked goods, 41 ppm; chewing gum, 50 ppm; condiments, 2.0 ppm	Non-alcoholic beverages 0.06–0.08 ppm Ice cream, ices, etc. 0.36–0.50 ppm Candy 1.0 ppm Baked goods 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2411	FDA 121.1164; FEMA No. 2413

REFERENCES

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

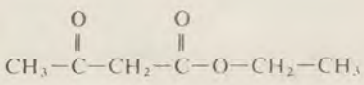
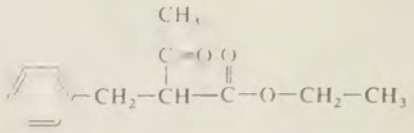
6. Hasselstroh and Hampton, *J. Am. Chem. Soc.*, 60, 3086, 1938.
7. Tiffeneau, *Compt. Rend.*, 139, 482, 1904.
8. Verley, German Patent 154,654.
9. *Schimmel Ber.*, 1892.
10. Grimand, *C. R. Séances Acad. Sci. Paris*, 117, 1089, 1893.
11. Goto, *J. Pharm. Jap.*, 61, 91, 1941.

	2-Ethoxythiazole	Ethyl acetate
Other names	Ethyl-2-thiazosyl ether	Acetic ether Vinegar naphtha
Empirical formula	C_5H_7OSN	$C_4H_8O_2$
Structure		$CH_3-C(=O)-O-CH_2-CH_3$
Physical/chemical characteristics		
Appearance		Colorless, mobile liquid
Assay		99–100%
Molecular weight	129.18	88.10
Melting point		−83.4°C
Boiling point		75–76°C (77.11°C)
Flash point		3°C
Specific gravity		0.9000–0.9040 (0.9065–0.9070) at 15°C
Refractive index		1.3723 (1.3470) at 20°C
Acid value		Not more than 0.01%
Solubility		Soluble in most organic solvents; soluble in alcohol, ether, and approximately 1:10 in water
Organoleptic characteristics		Characteristic ether-like odor reminiscent of pineapple with a bittersweet, wine-like, burning taste
Synthesis	2-Bromothiazole is treated with sodium alkoxides to give 2-alkoxythiazole[6]	By reacting acetic acid and ethanol in the presence of sulfuric acid; by distillation of sodium, potassium, or lead acetate with ethanol in the presence of sulfuric acid; by polymerization of acetaldehyde in the presence of aluminum ethylate or aluminum acetate as catalysts
Natural occurrence		Although it has been reported present in some natural fruital aromas and in some distillates (rum, rum ether),[7] it has not been reported yet as a constituent of essential oils. It has been identified also in the petals of *Magnolia fuscata*.[8]
Reported uses[3]	Ice cream, ices, etc. 0.2 ppm Candy 1.0 ppm Baked goods 1.0 ppm Meat, meat sauces, soups 0.5 ppm Cereals 2.0 ppm	Non-alcoholic beverages 67 ppm Alcoholic beverages 50–65 ppm Ice cream, ices, etc. 99 ppm Candy 170 ppm Baked goods 170 ppm Gelatins and puddings 200 ppm Chewing gum 1,400 ppm
Regulatory status	FEMA No. 3340	FDA GRAS; FEMA No. 2414

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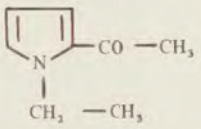
For References 1–5, see end of Part III.

6. Friedmann, *C. R. Acad. Sci. Ser. C*, 269(24), 1560, 1969; *Chem. Abstr.*, 72, 78934p, 1970.
7. Fenaroli et al., *Riv. Ital. EPPOS*, p. 9, 1965.
8. Goppert, *Justus Liebigs Ann. Chem.*, 111, 127, 1859.

	Ethyl acetoacetate	Ethyl 2-acetyl-3-phenylpropionate
Other names	Acetoacetic ester Ethyl β-ketobutyrate Ethyl-3-oxobutanoate	Ethyl α-acetylhydroxycinnamate Ethyl benzylacetoacetate Ethyl-3-oxo-2-benzylbutanoate
Empirical formula	$C_6H_{10}O_3$	$C_{13}H_{16}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	130.14	220.26
Melting point	−45°C	
Boiling point	180–184°C; 78°C at 13 mm Hg	290°C (with decomposition); 164°C at 18 mm Hg
Flash point	84.5°C (85°C)	
Specific gravity	1.0358 at 17°C; 1.0315–1.0350 at 15°/15°C	1.061 at 25°C
Refractive index	1.41696 at 25°C; 1.4180-1.4195 at 20°C	
Solubility	Slightly soluble in water; soluble in most organic solvents	Insoluble in water; completely miscible with alcohol and ether
Organoleptic characteristics	Characteristic ether-like, fruity, pleasant, refreshing odor	
Synthesis	Ethyl acetoacetate is a mixture of two tautomer forms: the enolic and the ketonic. The liquid ester at equilibrium contains approximately 70% of the enolic form. It is prepared by Claisen condensation of ethyl acetate in the presence of sodium ethylate; also by reacting diketene with ethanol in the presence of sulfuric acid or triethylamine and sodium acetate, with or without solvent.	By reacting benzyl chloride over hot sodium acetoacetate
Natural occurrence	Naturally occurring in strawberry and bread	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 17 ppm Ice cream, ices, etc. 24 ppm Candy 110 ppm Baked goods 120 ppm Gelatins and puddings 93 ppm Chewing gum 530 ppm	Non-alcoholic beverages 0.10–5.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 7.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2415	FDA 121.1164; FEMA No. 2416

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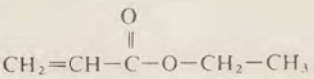
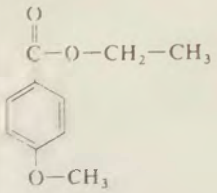
For References 1–5, see end of Part III.

	1-Ethyl-2-acetyl pyrrole	Ethyl aconitate, mixed esters
Other names		Ethyl-2-carboxyglutaconate Ethyl 1-propene-1,2,3-tricarboxylate A partially esterified product containing mono-, di-, and triethyl aconitate
Empirical formula	$C_8H_{11}NO$	$C_8H_{10}O_6$ $C_{10}H_{14}O_6$ $C_{12}H_{18}O_6$
Structure		$CH-COO-(C_2H_5)$ (3) $C-COO-(C_2H_5)$ (2) $CH_2-COO-(C_2H_5)$ (1)
Physical/chemical characteristics[5]		
Appearance		Oily, colorless liquid
Molecular weight	137.18	Mono- = 202.17; di- = 230.22; tri- = 258.28
Boiling point		172°C (260°C) at 18 mm Hg
Specific gravity		1.0961 at 25°C
Refractive index		1.45771 at 14.5°C
Solubility		Slightly soluble in water; soluble in alcohol
Organoleptic characteristics		Sweet, fruity, winey odor and flavor
Synthesis		By esterification of the acid with ethanol in the presence of acid catalysts; also by heating the citric acid triethyl ester Aconitic acid also yields the diethyl and the monoethyl esters upon esterification.
Natural occurrence	Reported found in roasted coffee[6-8]	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	Non-alcoholic beverages 3.6 ppm Ice cream, ices, etc. 12 ppm Candy 55 ppm Baked goods 66 ppm Gelatins and puddings 2.5 ppm
Regulatory status	FEMA No. 3147	FDA 121.1164; FEMA No. 2417

REFERENCES

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

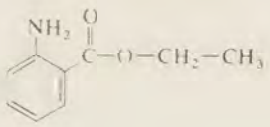
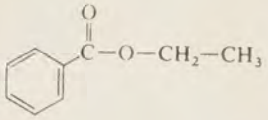
6. **Stoffelsma et al.,** *Recl. Trav. Chim.*, 87, 241, 1968.
7. **Stoffelsma et al.,** *J. Agric. Food Chem.*, 16, 1000, 1968.
8. **Walter et al.,** *Z. Ernährungswiss.*, 9, 123, 1969.

	Ethyl acrylate	Ethyl *p*-anisate
Other names	Ethyl propenoate	Ethyl *p*-methoxybenzoate
Empirical formula	$C_5H_8O_2$	$C_{10}H_{12}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid (at room temperature)
Molecular weight	100.12	180.21
Melting point	−71 to −75°C	7–8°C
Boiling point	99–100 C	263°C; 136–137°C at 13 mm Hg
Specific gravity	0.9234 at 20 C	1.1090 at 14.4°C
Refractive index	1.4068 at 20 C	1.5245 at 18.5°C
Solubility	Slightly soluble in water	Insoluble in water; soluble in alcohol and ether
Organoleptic characteristics	Characteristic penetrating and persistent odor	Sweet, fruity, anise-like taste and similar odor
Synthesis	By esterification of acrylic acid; by heating acetylene with HCl in alcoholic solution in the presence of $Ni(CO)_4$; also from ethyl-3-chloropropionate passed over activated carbon at high temperature	By esterification of anisic acid with ethanol in the presence of an acid catalyst
Natural occurrence	Reported found in the fruits of *Ananas sativus* Lindl.[6]	In guava
Reported uses[3]	Non-alcoholic beverages 0.13–0.26 ppm Ice cream, ices, etc. 0.06–1.0 ppm Candy 1.1 ppm Baked goods 1.1 ppm Chewing gum 0.10 ppm	Non-alcoholic beverages 2.6 ppm Ice cream, ices, etc. 0.96 ppm Candy 8.8 ppm Baked goods 7.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2418	FDA 121.1164; FEMA No. 2420

REFERENCES

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

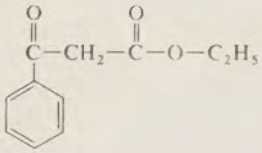
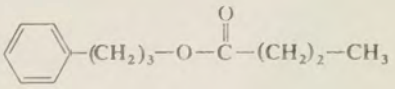
6. Haagen-Smit et al., *J. Am. Chem. Soc.*, 67, 1646, 1945.

	Ethyl anthranilate	Ethyl benzoate
Other names	Ethyl-2-aminobenzoate Ethyl *o*-aminobenzoate	Ethyl benzenecarboxylate
Empirical formula	$C_9H_{11}NO_2$	$C_9H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Liquid (at room temperature)	Colorless liquid
Assay		98% min[2]
Molecular weight	165.19	150.18
Melting point	13°C	−34 to −35°C
Boiling point	145–147°C at 15 mm Hg	213°C (94°C at 14 mm Hg)
Flash point		88°C
Specific gravity	1.1174 at 20°C	1.043–1.046 at 25°/25°C;[2] 1.0458 at 25°C
Refractive index	1.56455 at 20°C	1.5030–1.5060 at 20°C;[2] 1.5068 at 18°C
Acid value		Not more than 1[2]
Solubility	1:7 in 60% alcohol; 1:2 in 70% alcohol	1:6 in 60% alcohol;[2] 1:3 in 70% alcohol; almost insoluble in water
Organoleptic characteristics	Faint, orange-flowers odor and similar taste	Somewhat fruity odor similar to ylang-ylang but milder than methyl benzoate
Synthesis	By esterification of anthranilic acid with ethanol in the presence of acid catalysts; by reacting sodium hypochlorite with an alkaline alcoholic solution of phthalimide	By esterification of ethyl alcohol and benzoic acid in the presence of anhydrous aluminum sulfate and a trace of sulfuric acid;[6] by transesterification of methyl benzoate with ethanol in the presence of potassium ethylate[7]
Natural occurrence	In grapes	Reported found in volatiles from hard, mature peaches;[8] also found in pineapple and currant's
Reported uses[3]	Non-alcoholic beverages 5.9 ppm Ice cream, ices, etc. 7.6 ppm Candy 19 ppm Baked goods 23 ppm Gelatins and puddings 14 ppm Chewing gum 79 ppm	Non-alcoholic beverages 2.8 ppm Alcoholic beverages 0.50 ppm Ice cream, ices, etc. 2.8 ppm Candy 9.0 ppm Baked goods 10 ppm Gelatins and puddings 0.06 ppm Chewing gum 59 ppm
Regulatory status	FDA 121.1164; FEMA No. 2421	FDA 121.1164

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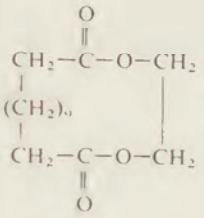
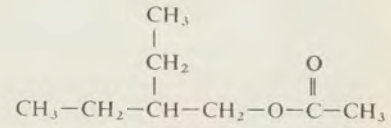
For References 1–5, see end of Part III.

6. **Kotake and Fujita,** *Chem. Zentralbl.*, 2, 1545, 1928.
7. **Reimer and Downes,** *J. Am. Chem. Soc.*, 43, 948, 1921.
8. **Do et al.,** *J. Food Sci.*, 34, 618, 1969.

	Ethyl benzoylacetate	α-Ethylbenzyl butyrate
Other names	Benzoyl acetic ester Ethyl β-keto-β-phenylpropionate Ethyl 3-phenyl-3-oxopropanoate	Ethyl phenyl carbinyl butyrate α-Phenylpropyl butyrate
Empirical formula	$C_{11}H_{12}O_3$	$C_{15}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid; turns yellow on storage and/or exposure to sunlight	Liquid
Assay		97% min
Molecular weight	192.22	206.28
Boiling point	147–149°C at 11 mm Hg (270°C)	282°C; 146–148°C at 15 mm Hg
Flash point		118°C
Specific gravity	1.12	0.9875–0.9905 at 15°C
Refractive index	1.5338 at 20°C	1.4875–1.4895 at 20°C
Acid value		0.06 max
Solubility	Insoluble in water; miscible with alcohol and ether	
Organoleptic characteristics	Brandy-like odor; bitter, whisky-like taste	Floral-fruity odor reminiscent of jasmine and apricot; sweet, plum-like taste
Synthesis	By condensation of ethyl benzoate with ethyl acetate (via Claisen condensation) using sodium ethoxide; another method also known	
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.70 ppm Ice cream, ices, etc. 5.0 ppm Candy 10 ppm Baked goods 10 ppm	Non-alcoholic beverages 0.13–1.0 ppm Ice cream, ices, etc. 0.12–0.20 ppm Candy 1.0 ppm Baked goods 0.14 ppm
Regulatory status	FDA 121.1164; FEMA No. 2423	FDA 121.1164; FEMA No. 2424

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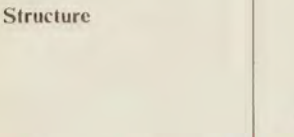
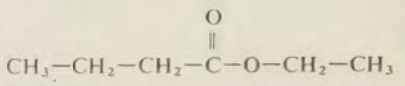
For References 1–5, see end of Part III.

	Ethyl brassylate	2-Ethylbutyl acetate
Other names	Cyclo-1,13-ethylenedioxytridecane-1,13-dione Ethylene brassylate Tridecanedioic acid, cyclic ethylene glycol diester	
Empirical formula	$C_{15}H_{26}O_4$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	White to light-yellow liquid[2]	Liquid
Assay	97% min[2]	
Molecular weight	270.37	144.21
Melting point	332 C	
Congealing point	0–7°C	
Boiling point		160–163°C; 64–65°C at 20 mm Hg
Specific gravity	1.040–1.047[2] (1.05) at 25°/25°C	0.8784 at 20°C
Refractive index	1.4690–1.4730 at 20°C[2]	1.4109 at 20°C
Acid value	Not more than 1.0[2]	
Solubility	Soluble in alcohol and most organic solvents; insoluble in water; poorly soluble in propylene glycol	
Organoleptic characteristics	Musk-like character;[2] sweet odor	
Synthesis	Esterification of brassylic acid[2]	By reacting 2-ethylbutanol with acetic anhydride or acetic acid in the presence of sulfuric acid[6,7]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]		Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 0.03–7.0 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2425

REFERENCES

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

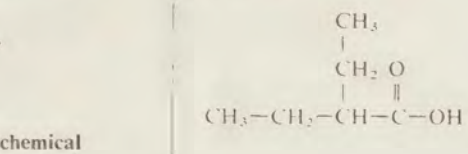
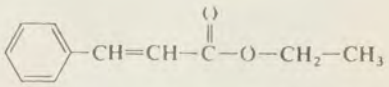
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	2-Ethylbutyraldehyde	Ethyl butyrate
Other names		
Empirical formula	$C_6H_{12}O$	$C_6H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, flammable liquid	Colorless liquid
Assay		98% min[2] (97.5%)
Molecular weight	100.16	116.16
Melting point	−89°C	
Boiling point	116–117°C; 80–135°C for commercial product	121–122 C
Flash point		26 C
Specific gravity	0.814 (0.817–0.823) at 20°C	0.870–0.877 at 25 /25 C;[2] 0.8825–0.8860 at 15 C
Refractive index	1.40398	1.3910–1.3940[2] (1.3910–1.3935) at 20 C
Acid value	Not more than 2%	Not more than 1 (0.06)
Solubility	Slightly soluble in water; soluble in alcohol and ether	1:3 in 60% alcohol;[2] 1:1–1.5 in 70% alcohol
Organoleptic characteristics		Fruity odor with pineapple undernote and sweet, analogous taste
Synthesis	From diethyl carbinol and anhydrous oxalic acid according to Béhal and Sommelet or with sulfuric acid according to Stoernier. A more recent synthetic route (Zeisel-Neuwirth method) calls for the reduction of α-vinylcrotonaldehyde using iron dust and acetic acid.	By esterification of *n*-butyric acid with ethyl alcohol in the presence of Twitchells reagent[6] or $MgCl_2$;[7] also by heating *n*-butyl alcohol and ethanol over $CuO + UO_3$ catalyst at 270 C[8]
Natural occurrence	Not reported found in nature	Reported found in strawberry juice;[9] also identified by gas chromatography in olive oil and other vegetable oils[10]
Reported uses[3]	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 40 ppm Candy 0.12–25 ppm Baked goods 0.20–20 ppm	Non-alcoholic beverages 28 ppm Ice cream, ices, etc. 44 ppm Candy 98 ppm Baked goods 93 ppm Gelatins and puddings 54 ppm Chewing gum 1,400 ppm
Regulatory status	FDA 121.1164; FEMA No. 2426	FDA GRAS; FEMA No. 2427

REFERENCES

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

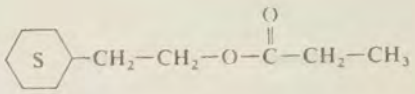
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7. Petjumin, *Zh. Obshch. Khim.*, 10, 37, 1940.
8. Iwannikiow, *Chem. Zentralbl.*, p. 7846, 1940.
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10. Ratay, *J. Assoc. Of. Agric. Chem.*, 4(47), 780, 1964.

	2-Ethylbutyric acid	Ethyl cinnamate
Other names	α-Ethylbutyric acid	Ethyl β-phenylacrylate Ethyl-3-phenylpropenoate
Empirical formula	$C_6H_{12}O_2$	$C_{11}H_{12}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Liquid	Oily, almost colorless liquid
Assay		98% min
Molecular weight	116.16	176.22
Melting point	32 C	7 C;[7] 12 C[8]
Boiling point	193 C; 99–101 C at 18 mm Hg	271–272°C; 158–159°C at 24 mm Hg
Flash point		>100 C
Specific gravity	0.9243 at 20 C	1.045–1.048 at 25°/25°C
Refractive index	1.4132 at 20 C	1.5590–1.5610 at 20°C
Acid value		Not more than 1
Solubility		1:5 in 70% alcohol; insoluble in water; soluble in ether
Organoleptic characteristics	Faint, somewhat pleasant odor	Pleasant, cinnamon-like, balsamic, honey-like odor and sweet, peach/apricot-like taste
Synthesis	By catalytic oxidation of diethylacetaldehyde or by decarboxylation of diethylmalonic acid	By heating to 100°C cinnamic acid, alcohol, and sulfuric acid in the presence of aluminum sulfate;[6] also by Claisen condensation of benzaldehyde and ethyl acetate
Natural occurrence		Normally occurring in the *trans*-form; a *cis*-form also exists. Reported found in Oriental styrax,[9,10] in the oil of *Campheria galanga*,[11–13] and in the rhizomes of *Hedychium spicatum*[14]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 20 ppm Candy 20–35 ppm Baked goods 20 ppm	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 8.8 ppm Candy 9.5 ppm Baked goods 12 ppm Gelatins and puddings 2.4 ppm Chewing gum 11–40 ppm
Regulatory status	FDA 121.1164; FEMA No. 2429	FDA 121.1164; FEMA No. 2430

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	Ethyl crotonate	Ethyl cyclohexanepropionate
Other names	*trans*-2-Butenoic acid ethyl ester Ethyl *trans*-2-butenoate Ethyl β-methylacrylate	Cyclohexane ethyl propionate Ethyl-3-cyclohexylpropanoate Ethyl cyclohexylpropionate Hexahydro phenylethyl propionate
Empirical formula	$C_6H_{10}O_2$	$C_{11}H_{20}O_2$
Structure	$CH_3-CH=CH-\overset{\overset{O}{\|}}{C}-O-CH_2-CH_3$	
Physical/chemical characteristics[5]		
Appearance	Liquid	Colorless, oily liquid
Molecular weight	114.15	184.28
Boiling point	136°C	
Specific gravity	0.9183 at 20°C	
Refractive index	1.4247 at 20°C	
Solubility		Insoluble in water; soluble in alcohol
Organoleptic characteristics		Powerful, fruity, sweet odor resembling pineapple; sweet, pineapple-like taste at high dilutions
Synthesis	By esterification of crotonic acid with ethyl alcohol in the presence of concentrated H_2SO_4[6-8]	By esterification of ethyl cyclohexanol with propionic acid or anhydride
Natural occurrence	Reported found in *Fragaria vesca*	Not reported found in nature
Reported uses[3]		Non-alcoholic beverages 9.0 ppm Candy 0.03–30 ppm Baked goods 24 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2431

REFERENCES

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

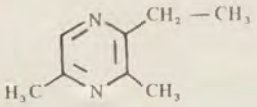
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	Ethyl-*trans*-2,*cis*-4-decadienoate	Ethyl decanoate
Other names		Ethyl caprate Ethyl decylate
Empirical formula	$C_{12}H_{20}O_2$	$C_{12}H_{24}O_2$
Structure	$CH_3-(CH_2)_4-CH=CH-CH=CH-\overset{\overset{O}{\|\|}}{C}-O-CH_2-CH_3$	$CH_3-(CH_2)_8-\overset{\overset{O}{\|\|}}{C}-O-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless oil	Colorless liquid
Assay		98% min[2]
Molecular weight	196.28	200.31
Melting point		−20°C
Boiling point	70–72°C at 0.05 mm Hg	241–242°C; 118–121°C at 15 mm Hg
Specific gravity		0.863–0.868 at 25°/25°C;[2] 0.865 at 15.5°C
Refractive index		1.4240–1.4270[2] (1.4260) at 20°C
Acid value		Not more than 1.0[2]
Solubility		1:4 in 80% alcohol[2]
Organoleptic characteristics	Characteristic pear-like flavor	Fruity odor reminiscent of grape (cognac)
Synthesis	Synthetically via the lithium vinyl cuprates[6]	By esterification of decanoic acid and ethyl alcohol in the presence of HCl[9] or H_2SO_4[10]
Natural occurrence	Reported found as a volatile component in Bartlett pears[7,8]	Reported present in cognac
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 2.1 ppm Alcoholic beverages 3.0–10 ppm Ice cream, ices, etc. 4.5 ppm Candy 8.3 ppm Baked goods 23 ppm Gelatins and puddings 5.3 ppm
Regulatory status	FEMA No. 3148	FDA 121.1164; FEMA No. 2432

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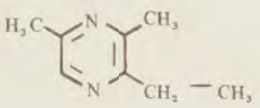
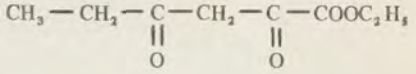
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	2-Ethyl-3,5 or 6-dimethylpyrazine
Other names	(1) 3,5-Dimethyl-2-ethylpyrazine (2) 2,5-Dimethyl-3-ethylpyrazine
Empirical formula	$C_8H_{12}N_2$
Structure	
Physical/chemical characteristics	
Appearance	C: 70.55%; H: 8.88%; N: 20.57%
Assay	136.20
Melting point	64-66°C at 8 mm Hg (2-ethyl-3,5-dimethylpyrazine)
Mass spectra[9]	39(72), 42(53), 53(18), 56(63), 65(8), 66(13), 80(7), 81(3), 94(6), 95(4), 108(11), 109(20), 119(2), 120(10), 135(100), 136(15)
NMR spectra[8]	(CCl_4) δ 8.05 (S, 1, ring – H); 270 (q, J = 8,2, CH_2 – CH_3) 2.42 (S, 3, ring – CH_3) 2.38 (S, 3, mg – CH_3) 1.24 (t, J = 8, 3, CH_2 – CH_3)
IR spectra[9]	8.80, 7.17, 3.37, 8.52, 7.33, 9.78, 7.83 μm
Organoleptic characteristics	(1) Odor threshold: 15,000 ppb in water[8] (2) Odor threshold: 43,000 ppb in water[8]
Synthesis	The 2-ethyl-3,5-dimethylpyrazine is obtained by alkylation of dimethyl-2,6-pyrazine;[6] the 2,5-dimethyl-3-ethylpyrazine is obtained by alkylation of 2,5-dimethylpyrazine with ethyllithium;[10] a mixture of the two can be obtained by condensation of 2,3-pentanedione with propylenediamine; a mixture of the two is obtained from the side chain alkylation of trimethylpyrazine[10]
Natural occurrence	Reported to be present in the following foods: roasted barley, cocoa products, coffee, meat, peanuts, filberts, pecans, popcorn, rum and whisky, soy products[7]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 2.0 ppm Condiments 2.0 ppm Meat, meat sauces 2.0 ppm Milk, dairy products 1.0 ppm Cereals 2.0 ppm
Regulatory status	FEMA No. 3149

REFERENCES

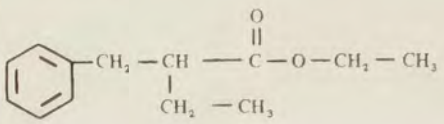
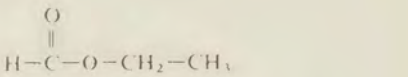
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7. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
8. Koehler et al., *J. Food Sci.*, 36, 816, 1971.
9. Friedel et al., *J. Agric. Food Chem.*, 19, 530, 1971.
10. Rizzi, *J. Org. Chem.*, 33(4), 1333, 1968.

	3-Ethyl-2,6-dimethylpyrazine	Ethyl-2,4-dioxo hexanoate
Other names	2,6-Dimethyl-3-ethylpyrazine 2-Ethyl-3,5-dimethylpyrazine 3,5-Dimethyl-2-ethylpyrazine	Ethyl-2,4-diketocaproate Ethyl propionyl pyruvate
Empirical formula	$C_8H_{12}N_2$	$C_8H_{12}O_4$
Structure		
Physical/chemical characteristics		
Assay	C: 70.55%; H: 8.88%; N: 20.57%	
Molecular weight	136.20	172.18
Boiling point		100 105°C at 6 mm Hg
Mass spectra[11]	39(72), 42(53), 53(18), 56(63), 65(8), 66(13), 80(7), 81(3), 94(6), 95(4), 108(11), 109(20), 119(2), 120(10), 135(100), 136(15)	
IR spectra[11]	6.20, 7.17, 3.37, 8.52, 7.33, 9.78, 7.83μm	
NMR spectra[12]	(CCl_4) δ 8.05 (S, 1, ring –H), 2.70 (q, J = 8, 2, CH_2 –CH_3), 2.42 (S, 3, ring –CH_3), 2.38 (S, 3, ring –CH_3), 1.24 (t, J = 8, 3, CH_2 –CH_3)	
Organoleptic characteristics	Odor threshold: 15,000 ppb in water[9]	
Synthesis	By alkylation of 2,6-dimethylpyrazine with ethyllithium[10]	From methyl ethyl ketone and ethyl oxalate[6]
Natural occurrence	Reported found in the basic fractions of whisky and rum,[6] in roasted peanuts,[7] in roasted barley,[8] in coffee, filberts, and potato and soy products[13]	
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	Non-alcoholic beverages 15.0 ppm Candy 20.0 ppm Baked goods 120.0 ppm Syrups 60.0 ppm Jellies 30.0 ppm Milk, dairy products 10.0 ppm Hard candy 120.0 ppm
Regulatory status	FEMA No. 3150	FEMA No. 3278

REFERENCES

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

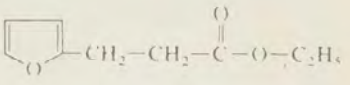
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11. Friedel et al., *J. Agric. Food Chem.*, 19, 530, 1971.
12. Rizzi, *J. Agric Food Chem.*, 20, 1081, 1972.
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	Ethyl 2-ethyl-3-phenyl propanoate	Ethyl formate
Other names	Ethyl 2-ethyl dihydrocinnamate	Formic ether
Empirical formula	$C_{13}H_{18}O_2$	$C_3H_6O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless, mobile, flammable liquid
Assay		95% min[2]
Molecular weight	206.27	74.08
Melting point		−80.5 C
Boiling point		64.3 C
Flash point		−20 C
Specific gravity		0.918–0.921 at 25 /25 C;[2] 0.9250–0.9315 at 15 C
Refractive index		1.3590–1.3630[2] (1.3600–1.3615) at 20 C
Free acid content		0.1% max[2] (0.9%) (as formic acid)
Solubility		1:0.5 and more in 50% alcohol;[2] soluble in most organic solvents; slightly soluble in water
Organoleptic characteristics		Characteristic pungent odor similar to ethyl acetate and reminiscent of pineapple; slightly bitter taste
Synthesis		Usually prepared by esterification of ethyl alcohol and formic acid or by distillation of ethyl acetate and formic acid in the presence of concentrated H_2SO_4.[6]
Natural occurrence	Reported not found in nature	Reported in the oil of *Boronia denti-geroides*.[7] It has been identified in Florida orange juice,[8] several varieties of honey,[9] apple and pear,[10] and distilled liquors, such as rum.[11–13]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Alcoholic beverages 25.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 50.0 ppm Preserves and spreads 50.0 ppm	Non-alcoholic beverages 9.4 ppm Alcoholic beverages 10 ppm Ice cream, ices, etc. 21 ppm Candy 50 ppm Baked goods 98 ppm Gelatins and puddings 0.35–11 ppm Chewing gum 430 ppm
Regulatory status	FEMA No. 3341	FDA 121.1164 and 121.1096; FEMA No. 2434

REFERENCES

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

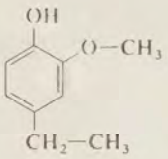
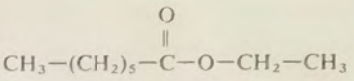
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	2-Ethylfuran	Ethyl 2-furanpropionate
Other names		Ethyl furfurylacetate Ethyl-3-(2-furyl)-propanoate Ethyl furylpropionate
Empirical formula	C_6H_8O	$C_9H_{12}O_3$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid	Low-melting solid; turns yellow on exposure to air
Molecular weight	96.13	168.19
Melting point		24.5 C
Boiling point	93 C	260 C; 120–121 C at 17 mm Hg
Refractive index		1.54876 at 20 C
Solubility	Almost insoluble in water; soluble in alcohol.	
Organoleptic characteristics	Powerful, sweet, burnt odor; when dilute, warm, sweet odor; coffee-like flavor (aroma)	Fruity odor reminiscent of camomile
Synthesis	By dehydration of furyl methyl carbinol followed by reduction	By direct esterification of the acid, which in turn is prepared by condensation of furfural with acetic anhydride and sodium acetate, followed by hydrogenation of the furacrylic acid[6,7]
Natural occurrence	In tomato, coffee, and *Mentha piperita* L.	Not reported found in nature
Reported uses[3]		Non-alcoholic beverages 1.6 ppm Ice cream, ices, etc. 1.6 ppm Candy 5.6 ppm Baked goods 7.5 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2435

REFERENCES

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

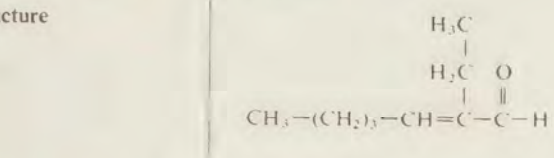
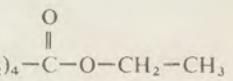
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	4-Ethylguaiacol	Ethyl heptanoate
Other names	4-Ethyl-2-methoxyphenol	Ethyl heptoate Ethyl heptylate
Empirical formula	$C_9H_{12}O_2$	$C_9H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	Colorless liquid
Assay		98% min[2] (97.5%)
Molecular weight	152.19	158.24
Melting point	229–230°C	−66.3 C
Boiling point		188.6°C (192 C)
Flash point		65 C
Specific gravity		0.867–0.872 at 25/25 C;[2] 0.8725–0.8755 at 15 C
Refractive index		1.4110–1.4150[2] (1.4120–1.4140) at 20°C
Acid value		1.0 max[2] (0.2 max)
Solubility		1:3 in 70% alcohol;[2] also soluble in most organic solvents
Organoleptic characteristics		Fruity odor reminiscent of cognac with a corresponding taste
Synthesis	Reported found in several distillates of plant origin. It was identified in camphor oil,[9] and it had been reported previously in Tolu and Peru balsam, as well as in various wood distillates.	By esterification of heptoic acid; by reacting the silver salt of the acid with ethyliodide[6] or with ethyl alcohol in the presence of mineral acids[7,8]
Natural occurrence		Reported found in several natural products.
Reported uses[3]	Non-alcoholic beverages 0.05 ppm Ice cream, ices, etc. 1.1 ppm Gelatins and puddings 0.23 ppm	Non-alcoholic beverages 6.8 ppm Alcoholic beverages 8.5–20 ppm Ice cream, ices, etc. 7.5 ppm Candy 17 ppm Baked goods 24 ppm Gelatins and puddings 0.06–350 ppm Chewing gum 340 ppm
Regulatory status	FDA 121.1164; FEMA No. 2436	FDA 121.1164; FEMA No. 2437

REFERENCES

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

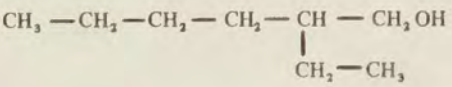
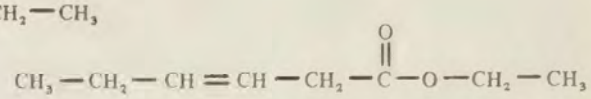
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	2-Ethyl-2-heptenal	Ethyl hexanoate
Other names	2-Ethyl-3-butylacrolein	Ethyl caproate Ethyl capronate Ethyl hexylate
Empirical formula	$C_9H_{16}O$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless to yellowish liquid
Assay		98% min[2]
Molecular weight	140.23	144.21
Melting point		−67 to −68°C
Boiling point		168°C (166°C)
Specific gravity		0.867–0.871 at 25°/25°C;[2] 0.8712 at 20°C
Refractive index		1.4060–1.4090[2] (1.4071) at 20°C
Acid value		Not more than 1[2]
Solubility		1:2 and more in 70% alcohol;[2] insoluble in water; soluble in most organic solvents
Organoleptic characteristics		Powerful, fruity odor with a pineapple-banana note
Synthesis		By esterification of caproic acid with ethyl alcohol in the presence of concentrated H_2SO_4 or HCl[6,7]
Natural occurrence	Not reported found in nature	Reported found in the fruits of *Ananas sativus*[8]
Reported uses[3]	Non-alcoholic beverages 0.40 ppm Candy 0.03–2.0 ppm	Non-alcoholic beverages 7.0 ppm Ice cream, ices, etc. 18 ppm Candy 12 ppm Baked goods 12 ppm Gelatins and puddings 10 ppm Chewing gum 32 ppm Jellies 1.3 ppm
Regulatory status	FDA 121.1164; FEMA No. 2438	FDA 121.1164; FEMA No. 2439

REFERENCES

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

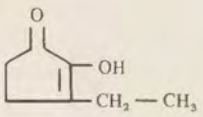
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	2-Ethyl-1-hexanol		Ethyl 3-hexenoate	
Other names	2-Ethyl hexyl alcohol		Hydrosorbic acid, ethyl ester	
Empirical formula	$C_8H_{18}O$		$C_8H_{14}O_2$	
Structure				
Physical/chemical characteristics[5]				
Appearance	Colorless oily liquid			
Molecular weight	130.22		142.19	
Boiling point	184–185°C		63–64°C at 12 mm Hg 63–65°C at 11 mm Hg	
Flash point	81°C			
Specific gravity	0.8344 at 20°C			
Refractive index	1.4300 at 20°C		1.4233 at 24°C	
Solubility	Insoluble in water; soluble in alcohol and oils			
Organoleptic characteristics	Mild, oily, sweet, slightly floral odor reminiscent of rose; sweet, fatty-floral taste with a fruital note		Green, fruity aroma	
Synthesis	By hydrogenation of aldehydes obtained by the oxo process;[6] also synthesized from propylene;[7,8] by catalytic reduction of 2-ethyl-2-hexenal[9] and other similar patented processes		From 3-hexenoic acid and dicyclohexylcarbodiimide;[13] by fungal fermentation (20°C) of 3-hexenoic acid using *Saccharomyces cerevisiae*;[10] from trialkylboranes and ethyl-4-bromocrotonate in the presence of 2,6-di-*tert*-butylphenoxide;[11] by pyrolysis of acetates[12]	
Natural occurrence			Reported found in pineapple;[13] a volatile flavor component in pineapple;[14] the *cis*-form has been reported found as a flavor component of passion fruit *(Passiflora edulis* f. *flavicarpa)*[15]	
Reported uses[3]	Non-alcoholic beverages	10.0 ppm	Non-alcoholic beverages	2.0 ppm
	Ice cream, ices, etc.	10.0 ppm	Ice cream, ices, etc.	2.0 ppm
	Candy	10.0 ppm	Candy	4.0 ppm
	Chewing gum	10.0 ppm	Baked goods	4.0 ppm
			Gelatins and puddings	2.0 ppm
			Preserves and spreads	2.0 ppm
Regulatory status	FEMA No. 3151		FEMA No. 3342	

REFERENCES

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

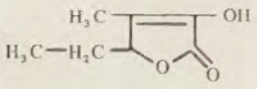
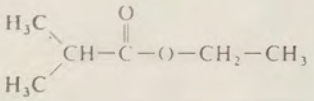
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8. Orlicek, German Patent 1,913,198, 1970.
9. Boettger et al., German Patent 1,949,296; *Chem. Abstr.*, 74, 140943n, 1971.
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15. Winter and Kloti, *Helv. Chim. Acta*, 55(6), 1916, 1972.

	Ethyl-3-hydroxybutyrate	3-Ethyl-2-hydroxy-2-cyclopenten-1-one
Other names	Ethyl-3-hydroxybutanoate	3-Ethyl-2-cyclopenten-2-ol-1-one
Empirical formula	$C_6H_{12}O_3$	$C_7H_{10}O_2$
Structure	$CH_3-CH(OH)-CH_2-COOC_2H_5$	
Physical/chemical characteristics		
Molecular weight	132.16	126.13
Melting point		38–40°C
Boiling point	81°C at 18 mm Hg	78–80°C at 4 mm Hg
Specific gravity	1.0052 at 25°C	65–68°C at 1 mm Hg
Refractive index	1.4200 at 25°C	
Organoleptic characteristics		Caramel-like flavor, often employed to impart a caramel flavor or coconut notes in food; a threshold value of 5 ppm, similar to the 3-methyl analog, has been determined by comparative sensory evaluation; the compound exhibits flavor-enhancing characteristics[21]
Synthesis	By catalytic hydrogenation of acetoacetate[6–8]	From 5-methyl-3,5-dicarbethoxy-2-cyclopenten-2-ol-1-one and phosphoric acid;[17] by a patented process;[18] also from dimethyl adipate[19]
Natural occurrence	In passion fruit,[9] rum,[10] sherry,[11] and wine[12–16]	Reported found in coffee[20]
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 50.0 ppm Milk, dairy products 3.0 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 10.0 ppm Condiments 10.0 ppm Meat, meat sauces, soups 10.0 ppm Milk, dairy products 10.0 ppm Cereals 10.0 ppm
Regulatory status	FEMA No. 3428	FEMA No. 3152

REFERENCES

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

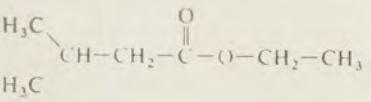
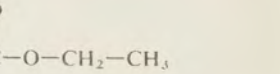
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9. Winter et al., *Helv. Chim. Acta*, 55, 1916, 1972.
10. Maarse et al., *J. Food Sci.*, 31, 951, 1966.
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16. Kahn, *J. Assoc. Off. Agric. Chem.*, 52, 1166, 1969.
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	5-Ethyl-3-hydroxy-4-methyl-2(5H)-furanone	Ethyl isobutyrate
Other names	2,4-Dihydroxy-3-methyl-2-hexenoic acid, γ-lactone 2-Ethyl-3-methyl-4-hydroxydihydro-2,5-furan-5-one 2-Hydroxy-3-methyl-γ-2-hexenolactone	
Empirical formula	$C_7H_{10}O_3$	$C_6H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Molecular weight	142.15	116.16
Melting point		−88°C
Boiling point		112–113°C
Specific gravity		0.8693 at 20 C
Refractive index		1.3903 at 20 C
Solubility		Slightly soluble in water; completely miscible in most organic solvents
Organoleptic characteristics		Apple-like odor
Natural occurrence		Reported in the phlegma oils from molasses[6] and in some varieties of Russian champagne.[7] It is one of the volatile constituents of strawberry juice,[8] honey, and beer.
Reported uses[3]	Candy 1.0 ppm Baked goods 1.0 ppm Gelatins and puddings 1.0 ppm	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 25 ppm Candy 73 ppm Baked goods 200 ppm Gelatins and puddings 6.0 ppm Toppings 1.5 ppm
Regulatory status	FEMA No. 3153	FDA 121.1164; FEMA No. 2428

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	Ethyl isovalerate	Ethyl lactate
Other names	Ethyl β-methylbutyrate	Ethyl α-hydroxy propionate
Empirical formula	$C_7H_{14}O_2$	$C_5H_{10}O_3$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid	
Assay	97% min[2] (98%)	
Molecular weight	130.18	119.12
Boiling point	134 C	154 C; *d*-, 58–59 C at 18 mm Hg; *l*-, 58 C at 20 mm Hg
Flash point	35 C	
Specific gravity	0.860–0.865 at 25 /25 C;[2] 0.8695–0.8725 at 15 C	1.0302 (*l*-, 1.033; *d*-, 1.0315) at 20 C
Refractive index	1.3950–1.3990[2] (1.3960–1.3970) at 20 C	1.4124 at 20 C (*l*-, 1.4125; *d*-, 1.4150 at 16°C)
Acid value	Not more than 1.0[2] (0.06)	
Optical rotation		At 16 C: *l*-, −5.7 ; *d*-, +11.4 (undiluted)
Solubility	1:4 in 60% alcohol[2]	
Organoleptic characteristics	Fruity odor reminiscent of apple with a corresponding sweet taste	
Synthesis	By esterification of isovaleric acid with ethyl alcohol in the presence of concentrated H_2SO_4[6]	*d*-Ethyl lactate is obtained from *d*-lactic acid by azeotropic distillation with ethyl alcohol or benzene in the presence of concentrated H_2So_4.[9] The *l*-form is prepared in a similar fashion starting from *l*-lactic acid. The racemic product is prepared by boiling for 24 hours optically inactive lactic acid with ethyl alcohol in carbon tetrachloride,[10] or with an excess of ethyl alcohol in the presence of chlorosulfonic acid,[11] or in the presence of benzenesulfonic acid in benzene solution.[12]
Natural occurrence	Reported in pineapple fruits;[7] also in some varieties of Russian champagne	Both the optically active and the racemic forms are reported found in nature.
Reported uses[3]	Non-alcoholic beverages 4.9 ppm Ice cream, ices, etc. 7.5 ppm Candy 29 ppm Baked goods 27 ppm Gelatins and puddings 5.0 ppm Chewing gum 80–430 ppm Condiments 1.0 ppm	Non-alcoholic beverages 5.4 ppm Alcoholic beverages 1,000 ppm Ice cream, ices, etc. 17 ppm Candy 28 ppm Baked goods 71 ppm Gelatins and puddings 8.3 ppm Chewing gum 580–3,100 ppm Syrups 35 ppm
Regulatory status	FDA 121.1164; FEMA No. 2463	FDA 121.1164; FEMA No. 2440

REFERENCES

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

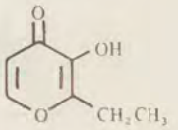
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9. Gerrard, Kenyon and Phillips, *J. Chem. Soc.*, p. 155, 1937.
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	Ethyl laurate	Ethyl levulinate
Other names	Ethyl dodecanoate Ethyl dodecylate	Ethyl γ-ketovalerate Ethyl-4-oxopentanoate
Empirical formula	$C_{14}H_{28}O_2$	$C_7H_{12}O_3$
Structure	$CH_3-(CH_2)_{10}-\overset{O}{\overset{\|}{C}}-O-CH_2-CH_3$	$CH_3-\overset{O}{\overset{\|}{C}}-CH_2-CH_2-\overset{O}{\overset{\|}{C}}-O-C_2H_5$
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Liquid
Assay	98% min	
Molecular weight	228.37	144.17
Boiling point	272–273°C; 141–142°C at 8 mm Hg	206°C; 103–105°C at 24 mm Hg
Flash point	>100°C	
Specific gravity	0.858–0.862 at 25°C	1.0135 at 20°C
Refractive index	1.4300–1.4340 at 20°C	1.4218 at 20°C
Acid value	1 max	
Solubility	1:9 in 80% alcohol; 1:1 in 90% alcohol	Rather soluble in water; soluble in alcohol and most organic solvents
Organoleptic characteristics	Floral, fruity odor	
Synthesis	From lauroyl chloride and ethyl alcohol in the presence of Mg in ether solution,[6] or by transesterification of coconut oil with ethyl alcohol in the presence of HCl[7]	Usually obtained by direct esterification of levulinic acid with ethanol and H_2SO_4 in benzene[8] or in toluene;[9] also in the presence of HCl in ethanol.[10–12] Other methods starting from glucose, fructose, and others are of less importance.
Natural occurrence	Reported found in nature	Reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.7 ppm Alcoholic beverages 3.0 ppm Ice cream, ices, etc. 3.7 ppm Candy 17 ppm Baked goods 17 ppm Gelatins and puddings 4.4 ppm Chewing gum 39 ppm	Non-alcoholic beverages 5.8 ppm Ice cream, ices, etc. 11 ppm Candy 12 ppm Baked goods 12 ppm
Regulatory status	FDA 121.1164; FEMA No. 2441	FDA 121.1164; FEMA No. 2442

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11. Cox and Dodds, *J. Am. Chem. Soc.*, 55, 3392, 1933.
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	Ethyl maltol		Ethyl-2-mercapto propionate	
Other names	3-Hydroxy-2-ethyl-4-pyrone 2-Ethyl pyromeconic acid 3-Ethyl-2-hydroxy-4H-pyran-4-one 2-Ethyl-3-ol-4H-pyran-4-one		2-Mercapto propionic acid, ethyl ester	
Empirical formula	$C_7H_8O_3$		$C_5H_{10}O_2S$	
Structure			$CH_3-CH(SH)COOCH_2-CH_3$	
Physical/chemical characteristics				
Appearance	White crystalline powder			
Assay	99% minimum			
Assay procedure	See References 6–8			
Molecular weight	140.14		134.19	
Melting point	89–93°C			
Boiling point	Considerable volatility at room temperature			
Solubility	In water: 1 g/65 ml at 15°C, 1 g/55 ml at 25°C; 12% in alcohol, 5% in phenylethyl alcohol, 5.5% in propylene glycol; slowly soluble in glycerine (1 g in 500 ml); 1 g/5 ml in chloroform; 1 g in 10 ml benzyl alcohol			
Organoleptic characteristics	Very sweet, caramel-like odor of immense tenacity; sweet, fruity taste with initial bitter-tart flavor; rapid loss of flavor *per se*; four to six times more potent than maltol			
Synthesis	From kojic acid[9-11]		By a patented process[12]	
Natural occurrence	Not reported found in nature			
Reported uses[3]	Non-alcoholic beverages	1.5–6 ppm	Non-alcoholic beverages	0.1 ppm
	Ice cream, ices, etc.	5–15 ppm	Ice cream, ices, etc.	0.1 ppm
	Candy	5–50 ppm	Candy	1.2 ppm
	Gelatins and puddings	5–50 ppm	Baked goods	1.5 ppm
	Chewing gum	5–50 ppm	Jellies	0.2 ppm
	Condiments (e.g., catsup)	5–15 ppm	Mint oils	10.0 ppm
	Toppings	5–50 ppm	Other	0.01 ppm
	Jellies	5–15 ppm		
	Soups (e.g., tomato)	5–15 ppm		
	Desserts	5–50 ppm		
Regulatory status	FDA 121.1164		FEMA No. 3279	

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

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7. **Pazdera et al.,** *Anal. Chem.*, 29, 1649, 1957.
8. **Pfizer,** Chemical Division Data Sheet No. 635, 1970.
9. **Pfizer,** Belgian Patent 651,427, 1965.
10. **Pfizer,** U.S. Patent 3,468,916.
11. **Pfizer,** U.S. Patent 3,594,195.
12. **Dumesnil,** U.S. Patent 3,061,511, 1958.

2-Ethyl (3 or 5 or 6)-methoxypyrazine (85%) plus 2-methyl (3 or 5 or 6)-methoxypyrazine (13%)

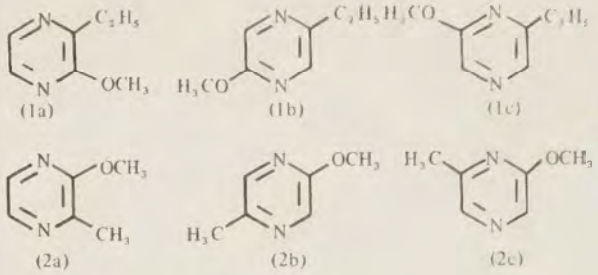
Other names

(1a) 2-Ethyl-3-methoxypyrazine
(1b) 2-Ethyl-5-methoxypyrazine
(1c) 2-Ethyl-6-methoxypyrazine
(2a) 2-Methoxy-3-methylpyrazine
(2b) 2-Methoxy-5-methylpyrazine
(2c) 2-Methoxy-6-methylpyrazine

Empirical formula

$C_7H_{10}N_2O$ (ethyl substituent)
$C_6H_8N_2O$ (methyl substituent)

Structure



Physical/chemical characteristics

Assay

(1) C: 60.85%; H: 7.30%; N: 20.27%; O: 11.58%
(2) C: 58.05%; H: 6.50%; N: 22.57%; O: 12.89%

Molecular weight

138.17 (ethyl substituent)
124.14 (methyl substituent)

Mass spectra[8]

(1a): 41(27), 42(18), 52(23), 53(19), 54(20), 56(23), 68(25), 107(22), 123(65), 137(35), 138(100)

IR spectra[8]

(1a): 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, 11.2, 13.7) VW (5.3, 5.6, 10.5, 10.8, 12.5)

Synthesis

2-methylchloropyrazine in methanol is added to a solution of sodium in methanol, and the mixture is refluxed to give a fraction (b.p. = 48–50°C at 15 mm) containing ~75% 2-methyl-3-methoxypyrazine and ~25% mixture of 2-methyl-5-methoxypyrazine and 2-methyl-6-methoxypyrazine; the ethyl substituent can be obtained in a similar manner[6]

Natural occurrence

The 2-ethyl-3-methoxypyrazine occurs in some brands of dehydrated and mashed potatoes[7]

Reported uses[3]

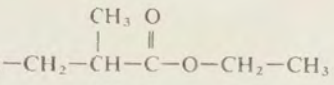
Non-alcoholic beverages	5.0 ppm
Ice cream, ices, etc.	5.0 ppm
Candy	5.0 ppm
Baked goods	5.0 ppm
Gelatins and puddings	5.0 ppm
Meat, meat sauces, soups	5.0 ppm
Milk, dairy products	5.0 ppm
Cereals	5.0 ppm

Regulatory status

FEMA No. 3280

REFERENCES

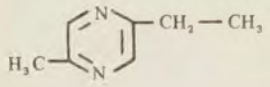
For References 1–5, see end of Part III.
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7. Guadagni et al., *J. Food Sci.*, 36, 373, 1971.
8. Seifert et al., *J. Agric. Food Chem.*, 20(1), 137, 1972.

	Ethyl 2-methylbutyrate
Empirical formula	$C_7H_{14}O_2$
Structure	
Physical/chemical characteristics[4]	
Molecular weight	130.18
Boiling point	132–133 C
Specific gravity	0.8695 at 22 C; 0.8687 at 20 C
Refractive index	1.3970 at 20 C
Synthesis	The racemic form can be prepared catalytically by several methods: from butene and $Ni(CO)_4$ under nitrogen in ethyl alcohol/acetic acid solution,[6,7] or from ethylene and CO under pressure using HBF_4 and HF as catalysts[8,9]
Natural occurrence	Reported found in nature; the ethyl *l*-methylbutyrate has been identified in strawberry juice;[10] because of the presence of the asymmetric carbon, the compound should exhibit optically active forms as well as the racemic form; however, only the *d*-form and the racemic form are known
Reported uses[3]	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 3.0 ppm Candy 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2443

REFERENCES

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

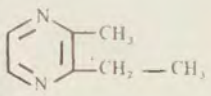
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	2-Ethyl-5-methylpyrazine
Other names	2-Methyl-5-ethylpyrazine
Empirical formula	$C_7H_{10}N_2$
Structure	
Physical/chemical characteristics	
Assay	C: 68.82%; H: 8.25%; N: 22.93
Molecular weight	122.17
Boiling point	79–80°C at 50 mm Hg
Refractive index	1.4925 at 25°C
Mass spectra[8]	39(24), 42(10), 54(8), 56(16), 66(2), 67(2), 79(1), 80(3), 93(2), 94(13), 107(4), 121(100), 122(68)
IR spectra[8]	S (3.4, 6.7, 8.6, 9.6) M (3.2, 3.5, 6.8, 7.2, 7.4, 7.4, 8.4, 9.3, 11.2)
UV spectra[8]	W (5.5, 8.0, 8.2, 11.4, 11.7, 12.1) (272.0, 276.7)
NMR spectra[9]	(CCl_4) δ 8.18 (S,2, ring–H), 2.74 (g,2,–CH_2 –CH_3) 2.45(S,3, ring–CH_3), 1.28 (t,J = 8,3, CH_2 –CH_3)
Organoleptic characteristics	Odor threshold: 100 ppb in water[10]
Synthesis	By alkylation of dimethyl-2,5-pyrazine[6]
Natural occurrence	Reported found as a constituent in coffee aroma,[7] in roasted barley, cocoa, meats, dairy products, peanuts, pecans, filberts, popcorn, and potato and soy products;[11] a volatile flavor component in potato chips[12]
Reported uses[3]	Non-alcoholic beverages 5.0 ppm Candy 5.0 ppm Baked goods 5.0 ppm Gelatins and puddings 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	FEMA No. 3154

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

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	3-Ethyl-2-methylpyrazine	Ethyl-3-methylthiopropionate
Other names	2-Ethyl-3-methylpyrazine	Ethyl-β-methylthiopropionate
Empirical formula	$C_7H_{10}N_2$	$C_6H_{12}O_2S$
Structure		$CH_3-S-CH_2-CH_2-\underset{\underset{O}{\|}}{C}-O-CH_2-CH_3$
Physical/chemical characteristics		
Assay	C: 68.82%; H: 8.25%; N: 22.93%	
Molecular weight	122.17	148.23
Boiling point	57°C at 10 mm Hg 69–70°C at 16 mm Hg	
Refractive index	1.5023 at 22°C	
Mass spectra[8]	39 (18), 43 (16), 52 (7), 53 (13), 65 (6), 67 (30), 80 (14), 81 (16), 93 (9), 94 (19), 107 (7), 121 (100), 122 (92)	
NMR spectra[10]	δ 1.88 (m, ring protons, 2H), 7.57, (S, ring–CH_3, 3H), 7.28 (8, CH_2, 2H), 8.77 (t, chain – CH_3, 3H)	
IR spectra[8]	S (3.4, 6.8, 7.1, 8.6, 8.8, 9.7, 11.7) M (3.3, 3.5, 7.3, 7.5, 9.4, 10.2) W (5.2, 5.5, 6.5, 8.1, 9.2, 11.5, 12.1)	
UV spectra[8]	(273.0, 269.2 nm)	
Organoleptic characteristics	Odor threshold: 130 ppb in water[9]	
Synthesis	By condensation of ethylenediamine with 2,3-pentanedione[6]	
Natural occurrence	Reported to be present in the following foods: bakery products, roasted barley, coffee, peanuts, filberts, potato products, soy products[7]	Flavor constituent in pineapple[11-13]
Reported uses[3]	Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Gelatins and puddings 3.0 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 1.0 ppm Preserves and spreads 1.0 ppm
Regulatory status	FEMA No. 3155	FEMA No. 3343

REFERENCES

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

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7. Maga and Sizer, *Crit. Rev. Food Technol.*, 4(1), 39, 1973.
8. Bondarovich et al., *J. Agric. Food Chem.*, 15, 1093, 1967.
9. Guadagni et al., *J. Sci. Food Agric.*, 23, 1435, 1972.
10. Rizzi, *J. Org. Chem.*, 33(4), 1336, 1968.
11. Connell, *Aust. J. Chem.*, 17(1), 130, 1964; *Chem. Abstr.*, 56, 13308f, 1962.
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	Ethyl myristate	Ethyl nitrite
Other names	Ethyl tetradecanoate	Nitrous ether Sweet spirit of nitre
Empirical formula	$C_{16}H_{32}O_2$	$C_2H_5O_2N$
Structure	$CH_3-(CH_2)_{12}-\overset{\overset{O}{\|}}{C}-O-CH_2-CH_3$	$CH_3-CH_2-O-N=O$
Physical/chemical characteristics[5]		
Appearance	Colorless crystals	Very mobile, colorless liquid
Molecular weight	256.44	75.04
Melting point	10.5°C	
Boiling point	295°C	17.4°
Specific gravity	0.860 at 15.5°C	0.9009 at 15.5°C
Refractive index	1.4400 at 20°C	
Solubility	Very slightly soluble in alcohol and ether; slightly soluble in ligroin	Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Odor reminiscent of orris	Characteristic ether-like odor
Synthesis	By esterification of the acid with ethyl alcohol in the presence of gaseous HCl	From sodium nitrite in aqueous solution by displacing the acid with H_2SO_4 in the presence of ethyl alcohol. It forms azeotropic mixtures with isopentane (85%), amyl bromide (40%), and carbon disulfide (96%).
Natural occurrence	Reported found in the residue of fusel oil from molasses	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 6.7 ppm Alcoholic beverages 30 ppm Ice cream, ices, etc. 8.0 ppm Candy 10 ppm Baked goods 14 ppm	Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 4.5 ppm Candy 0.10–8.0 ppm Baked goods 0.10 ppm Chewing gum 3.9 ppm Syrups 52 ppm Icings 13 ppm
Regulatory status	FDA 121.1164; FEMA No. 2445	FDA 121.1164; FEMA No. 2446

REFERENCES

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

	Ethyl nonanoate	Ethyl 2-nonynoate
Other names	Ethyl nonylate Ethyl pelargonate	Ethyl octyne carbonate
Empirical formula	$C_{11}H_{22}O_2$	$C_{11}H_{18}O_2$
Structure	$CH_3(CH_2)_7-\overset{\overset{O}{\|}}{C}-O-C_2H_5$	$CH_3-(CH_2)_5-C\equiv C-\overset{\overset{O}{\|}}{C}-O-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Oily liquid
Assay	99% min	
Molecular weight	186.30	182.26
Melting point	−44.5°C (−36.7°C)	
Boiling point	228°C (220°C)	227°C (121–122°C at 13 mm Hg)
Flash point	85°C	
Specific gravity	0.8700–0.8725 at 15°C	0.9032 at 25°C; 0.935 at 15.5°C
Refractive index	1.4215–1.4230 at 20°C	1.4464 at 25°C; 1.4527 at 20°C
Acid value	0.9 max	
Solubility	Insoluble in water; soluble in water-ether mixtures; 1:1.5–2 in 80% alcohol	
Organoleptic characteristics	Odor reminiscent of cognac with a rosy-fruity note	Characteristic green, violet-like odor
Synthesis	By distillation of pelargonic acid and ethyl alcohol in toluene in the presence of small amounts of muriatic acid (HCl); also by hydrogenation of oenanthylidene acetate in the presence of Ni at 180°C	
Natural occurrence	In pineapple, banana, and apple	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 3.9 ppm Alcoholic beverages 20 ppm Ice cream, ices, etc. 4.0 ppm Candy 14 ppm Baked goods 15 ppm Gelatins and puddings 15 ppm Chewing gum 580 ppm Icings 39 ppm	Non-alcoholic beverages 0.56 ppm Ice cream, ices, etc. 0.55 ppm Candy 0.52 ppm Baked goods 1.2 ppm
Regulatory status	FDA 121.1164; FEMA No. 2447	FDA 121.1164; FEMA No. 2448

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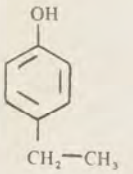
For References 1–5, see end of Part III.

	Ethyl octanoate	Ethyl *cis*-4-octenoate
Other names	Ethyl caprylate Ethyl octylate	
Empirical formula	$C_{10}H_{20}O_2$	$C_{10}H_{18}O_2$
Structure	$CH_3-(CH_2)_6-\overset{\overset{O}{\|}}{C}-O-CH_2-CH_3$	$CH_3-CH_2-CH_2-CH=CH-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-O-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Assay	98% min[2] (97.5%)	
Molecular weight	172.27	170.24
Melting point	−43°C	
Boiling point	208°C	105°C at 11 mm Hg
Flash point	85°C	
Specific gravity	0.865–0.869 at 25°/25°C;[2] 0.8710–0.8750 at 15°C	
Refractive index	1.4170–1.4190[2] at 20°C	
Acid value	Not more than 1[2] (1.9)	
Solubility	1:4 and more in 70% alcohol;[2] 1:1–2 in 90% alcohol; insoluble in water; soluble in most organic solvents	
Organoleptic characteristics	Pleasant, fruity, floral odor (wine-apricot note)	
Synthesis	Usually prepared by esterification of caprylic acid with ethyl alcohol and sulfuric acid as catalyst;[6] also by alcoholysis of coconut oil in the presence of HCl[7]	From *cis*-1-pentenyl bromide via the lithium vinyl cuprates[8]
Natural occurrence	Reported found in nature	Reported found as a volatile flavor component apple;[9] also reported found among the aroma components of yellow passion fruit[10]
Reported uses[3]	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 2.4 ppm Candy 9.0 ppm Baked goods 11 ppm Gelatins and puddings 0.10–2.7 ppm Chewing gum 4.0–60 ppm	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 Preserves and spreads 3.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2449	FEMA No. 3344

REFERENCES

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

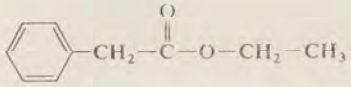
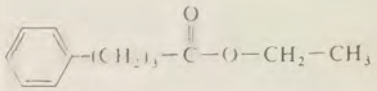
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	Ethyl oleate	*p*-Ethylphenol
Other names	Ethyl 9-octadecenoate	1-Ethyl-4-hydroxybenzene 4-Ethylphenol
Empirical formula	$C_{20}H_{38}O_2$	$C_8H_{10}O$
Structure	$CH_3-(CH_2)_7-CH=CH-(CH_2)_7-\overset{\overset{O}{\|\|}}{C}-O-CH_2-CH_3$	
Physical/chemical characteristics[5]		
Appearance	Oily, slightly yellowish liquid	Colorless or white needles; tend to yellow on exposure to light
Assay	99% min	
Molecular weight	310.52	122.17
Melting point		47–48°C
Boiling point	207 C at 13 mm Hg; 205–208 C for commercial product	218–219°C 99.5°C at 10 mm Hg
Flash point	175 C	
Specific gravity	0.87196 at 20 C	1.011 at 20°C
Refractive index	1.4515 at 20 C	1.5239 at 25°C
Solubility	Insoluble in water; soluble in alcohol and ether	Slightly soluble in water; soluble in alcohol, ether, benzene, carbon disulfide, and acetone
Organoleptic characteristics	Faint, floral note	Powerful woody-phenolic, yet somewhat sweet odor
Synthesis	By direct esterification of oleic acid with ethyl alcohol in the presence of HCl at the boil;[6] in the presence of Twitchell reagent[7] or chlorosulfonic acid[8]	By catalytic reaction between phenol and ethylene or ethanol;[9] by heating 8-chloro-3-ethylbenzene with NaOH in the presence of copper powder[10]
Natural occurrence	Reported found in nature	Reported found in coal tar; also reported found in yellow passion fruit[11]
Reported uses[3]	Non-alcoholic beverages 0.10 ppm Ice cream, ices, etc. 0.10 ppm Candy 0.10–40 ppm Baked goods 0.10–55 ppm Gelatins and puddings 0.10 ppm	Baked goods 0.20 ppm Margarine 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2450	FEMA No. 3156

REFERENCES

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

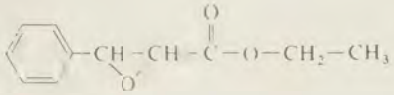
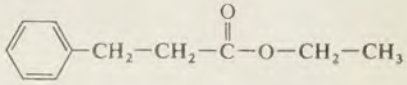
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11. Winter and Kloti, *Helv. Chim. Acta*, 55(6), 1916, 1972.

	Ethyl phenylacetate	Ethyl-4-phenylbutyrate
Other names	Ethyl α-toluate	Ethyl phenylbutyrate Ethyl-γ-phenylbutyrate
Empirical formula	$C_{10}H_{12}O_2$	$C_{12}H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless or nearly colorless liquid	Colorless, somewhat oily liquid
Assay	98% min[2]	
Molecular weight	164.21	192.26
Boiling point	229°C (100°C at 10 mm Hg)	
Flash point	>100°C	
Specific gravity	1.027–1.032 at 25°/25°C[2]	
Refractive index	1.4960–1.5000[2] (1.4960–1.4980) at 20°C	
Acid value	1 max[2]	
Solubility	1:3 in 70% alcohol;[2] 1:10 in 60% alcohol; insoluble in water	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Pleasant, strong, sweet odor suggestive of honey; bittersweet flavor	Sweet, fruity, plum-like odor and cooked plum-prune taste
Synthesis	By heating to the boil phenylacetonitrile and sulfuric acid in alcohol solution;[6,7] by esterification of the acid catalyzed by HCl[8,9] or H_2SO_4[10]	By esterification of ethanol with γ-phenylbutyric acid obtained by Grignard reaction from γ-bromopropylbenzene
Natural occurrence	Reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.4 ppm Ice cream, ices, etc. 5.2 ppm Candy 8.1 ppm Baked goods 6.0 ppm Syrups 24 ppm	Non-alcoholic beverages 0.06 1.0 ppm Ice cream, ices, etc. 0.06 ppm
Regulatory status	FDA 121.1164; FEMA No. 2452	FDA 121.1164; FEMA No. 2453

REFERENCES

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

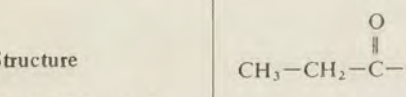
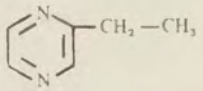
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10. Senderens and Aboulenc, *Compt. Rend.*, 152, 1856, 1911.

	Ethyl-3-phenylglycidate	Ethyl 3-phenylpropionate
Other names	Ethyl 3-phenyl-2,3-epoxypropionate	Ethyl hydrocinnamate
Empirical formula	$C_{11}H_{12}O_3$	$C_{11}H_{14}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to pale-yellow liquid	Colorless liquid
Assay	99% min[2] (98%)	
Molecular weight	192.22	178.23
Boiling point		249°C (123°C at 16 mm Hg)
Flash point	100 C	
Specific gravity	1.120–1.128[2] (1.120–1.125) at 25°/25°C	1.015 at 20°C
Refractive index	1.5190–1.5230[2] (1.516–1.521) at 20°C	1.4951 at 17.8°C
Acid value	Not more than 1.0[2]	
Solubility	1:6 in 70% alcohol;[2] 1:1 in 80% alcohol	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Strong, fruity odor suggestive of strawberry with a corresponding sweet flavor	Floral odor
Synthesis	Usually prepared by the reaction of benzaldehyde and the ethyl ester of monochloracetic acid in the presence of an alkaline condensing agent; by reacting the silver salt of phenyl glycidic acid with ethyl iodide[6]	By hydrogenation of the corresponding ethyl cinnamate in the presence of nickel in alcohol solution[7,8]
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 4.6 ppm Ice cream, ices, etc. 12 ppm Candy 18 ppm Baked goods 20 ppm Gelatins and puddings 10–70 ppm	Non-alcoholic beverages 1.8 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.5 ppm Baked goods 0.50–30 ppm
Regulatory status	FDA 121.1164; FEMA No. 2454	FDA 121.1164; FEMA No. 2455

REFERENCES

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

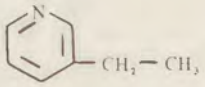
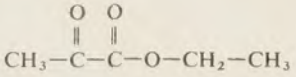
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	Ethyl propionate	2-Ethylpyrazine
Other names		2-Ethyl-1,4-diazine Ethylpyrazine
Empirical formula	$C_5H_{10}O_2$	$C_6H_8N_2$
Structure		
Physical/chemical characteristics		
Appearance	Colorless, mobile liquid	C: 66.64%; H: 7.46%; N: 25.90%
Assay	98% min	108.14
Molecular weight	102.14	
Melting point	99°C	155°C
Boiling point		122–124°C at 90 mm Hg
Flash point	12°C (approx 15°C)	
Specific gravity	0.8945–0.8985 at 15°C; 0.8917 at 20°C	
Refractive index	1.3830–1.3850 at 20°C	
Acid value	Not more than 0.2	
Mass spectra[8]		39 (16), 40 (4), 52 (18), 53 (18), 64 (1), 66 (3), 80 (23), 81 (14), 92 (1), 93 (2), 107 (100), 108 (82)
IR spectra[8]		S (3.4, 6.8, 7.1, 8.6, 9.4, 9.8, 11.8) M (3.3, 3.5, 6.3, 6.5, 6.9, 7.7, 8.1, 10.3) W (5.2, 5.4, 5.6, 5.7, 7.5, 10.7)
UV spectra[8]		(266.2, 272.2 nm)
Solubility	Completely miscible in 95% alcohol; readily soluble in most organic solvents; 1:1–2 in 60% alcohol	
Organoleptic characteristics	Odor reminiscent of rum and pineapple	Odor threshold: 22,000 ppb in water,[9] 6,000 ppb in water[10]
Synthesis	From propionic acid, ethyl alcohol, and concentrated H_2SO_4 in chloroform at the boil[11]	By alkylation of methylpyrazine with methyliodide[6]
Natural occurrence	Reported found in several type of wine,[12] in white grape var. *Sauvignon*,[13,14] and in cocoa	Reported to be present in the following foods: bakery products, cocoa products, coffee, meat, peanuts, filberts, potato products[7]
Reported uses[3]	Non-alcoholic beverages 7.7 ppm Ice cream, ices, etc. 29 ppm Candy 78 ppm Baked goods 110 ppm Gelatins and puddings 10–15 ppm Chewing gum 1,100 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 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
Regulatory status	FDA 121.1164; FEMA No. 2456	FEMA No. 3281

REFERENCES

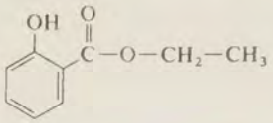
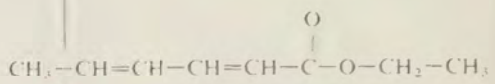
For References 1–5, see end of Part III.

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11. Henecka, *Houben-Weyl*, 8, 524, 1952.
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	3-Ethylpyridine	Ethyl pyruvate
Other names	β-Ethylpyridine β-Lutidine	Ethyl α-ketopropionate Ethyl-2-oxopropanoate
Empirical formula	C_7H_9N	$C_5H_8O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to brownish liquid	Colorless liquid
Molecular weight	107.15	116.12
Melting point		−50°C
Boiling point	162–165°C at 762 mm Hg	155–156°C (66°C at 18 mm Hg)
Specific gravity	0.940 at 23°C 0.9539 at 0°C	1.080 at 14°C
Refractive index	1.5021 at 22°C	1.408 at 15.4°C
Solubility	Slightly soluble in water; soluble in alcohol and ether	Slightly soluble in water; miscible with alcohol and ether
Organoleptic characteristics	Tobacco flavor[7]	
Synthesis		By direct esterification of pyruvic acid with absolute ethyl alcohol at the boil and subsequent vacuum distillation; by esterification via oxidation of vapors of ethyl lactate in the presence of V_2O_5 at 155°C
Natural occurrence	Reported found in coffee[6]	Reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.05 ppm Ice cream, ices, etc. 0.05 ppm Candy 0.06 ppm Baked goods 0.06 ppm Gelatins and puddings 0.05 ppm Meat, meat sauces, soups 0.05 ppm	Non-alcoholic beverages 50 ppm Ice cream, ices, etc. 20–150 ppm Candy 35 ppm Baked goods 40 ppm
Regulatory status	FEMA No. 3394	FDA 121.1164; FEMA No. 2457

REFERENCES

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7. *Chem. Abstr.*, 74, 1083353j, 1971.

	Ethyl salicylate	Ethyl sorbate
Other names	Ethyl *o*-hydroxy benzoate	Ethyl-2,4-hexadienoate
Empirical formula	$C_9H_{10}O_3$	$C_8H_{12}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Assay	99% min[2]	
Molecular weight	166.18	140.18
Boiling point	232–235°C (107–108°C at 12 mm Hg)	81°C at 15 mm Hg
Specific gravity	1.126–1.130 at 25/25°C;[2] 1.130–1.135 at 15°C	0.9560 at 20°C
Refractive index	1.520–1.523 at 20°C[2]	1.502 at 20°C
Acid value	Not more than 1[2]	
Solubility	1:4 in 80% alcohol;[2] slightly soluble in water	
Organoleptic characteristics	Characteristic aromatic odor similar to wintergreen; tends to darken on exposure to light and air	
Synthesis	By esterification of salicylic acid with ethyl alcohol and concentrated H_2SO_4 at 100°C in the presence of aluminum sulfate;[6] by heating to the boil an alkaline solution of salicylic acid and ethyl *p*-toluenesulfonate[7]	By reacting gaseous HCl with a solution of sorbic acid in ethyl alcohol,[8] or by direct esterification by reaction of sorbyl chloride with absolute ethyl alcohol
Natural occurrence	Reported found in nature (e.g., currant and strawberry)	Reported found in nature
Reported uses[4]	Non-alcoholic beverages 2.8 ppm Ice cream, ices, etc. 11 ppm Candy 10 ppm Baked goods 16 ppm Gelatins and puddings 0.04 ppm Chewing gum 16 ppm	Non-alcoholic beverages 5.5 ppm Ice cream, ices, etc. 14 ppm Candy 15 ppm Baked goods 18 ppm
Regulatory status	FDA 121.1164; FEMA No. 2458	FDA 121.1164; FEMA No. 2459

REFERENCES

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

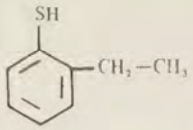
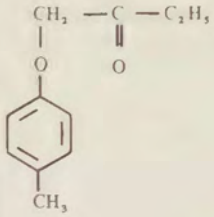
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8. Hoffmann, *Annalen*, 110, 137, 1859.

	Ethyl thioacetate	Ethyl tiglate
Other names	Thioacetic acid, ethyl ester	Ethyl *trans*-2,3-dimethyl acrylate Ethyl *trans*-2-methyl-2-butenoate
Empirical formula	C_4H_8OS	$C_7H_{12}O_2$
Structure	$CH_3-\overset{\overset{O}{\|\|}}{C}-S-CH_2-CH_3$	$CH_3-CH=\overset{\overset{H_3C}{\|}}{C}-\overset{\overset{O}{\|\|}}{C}-O-CH_2-CH_3$
Physical/chemical characteristics		
Appearance		Liquid
Molecular weight	104.18	128.17
Boiling point	116.4°C	156 C (55-57 C at 15 mm Hg)
Specific gravity	0.9792 at 20°C	0.9239 at 16.8 C
Refractive index	1.4583 at 21°C	1.4347 at 16.8 C
Solubility	Insoluble in water; very soluble in alcohol and ether	Soluble in most organic solvents
Synthesis	From acetyl chloride and ethyl mercaptan[6]	By direct esterification of tiglic acid with ethyl alcohol in the presence of concentrated H_2SO_4[7] or by reaction of bromomethylethyl acetic acid ethyl ester with dimethylaniline[8]
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 Baked goods 1.0 ppm Gelatins and puddings 1.0 ppm Chewing gum 1.0 ppm Condiments, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm Milk, dairy products 1.0 ppm Cereals 1.0 ppm	Non-alcoholic beverages 5.3 ppm Ice cream, ices, etc. 6.0 ppm Candy 20 ppm Baked goods 6.5 ppm
Regulatory status	FEMA No. 3282	FDA 121.1164; FEMA No. 2460

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

6. **Schaefgen,** *J. Am. Chem. Soc.*, 70, 1308, 1948.
7. **Auwers,** *Ann. Chem.*, 432, 71, 1923.
8. **Gardner and Rydon,** *J. Chem. Soc.*, p. 53, 1938.

	2-Ethylthiophenol		Ethyl (*p*-tolyloxy) acetate	
Other names	2-Ethylphenyl mercaptan-2-ethylbenzene-thiol		Ethyl *p*-cresoxy acetate	
Empirical formula	$C_8H_{10}S$		$C_{11}H_{14}O_2$	
Structure				
Physical/chemical characteristics				
Molecular weight	138.23		178.22	
Natural occurrence			Not reported found in nature.	
Reported uses[3]	Non-alcoholic beverages	0.2 ppm	Non-alcoholic beverages	8.0 ppm
	Ice cream, ices, etc.	0.2 ppm	Candy	40.0 ppm
	Candy	0.3 ppm		
	Baked goods	0.3 ppm		
	Gelatins and puddings	0.2 ppm		
	Meat, meat sauces, soups	0.2 ppm		
Regulatory status	FEMA No. 3345		FEMA No. 3157	

REFERENCES

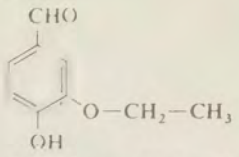
For References 1–5, see end of Part III.

	Ethyl undecanoate	Ethyl 10-undecenoate
Other names	Ethyl hendecanoate Ethyl undecylate	Ethyl 10-hendecenoate Ethyl undecylenoate
Empirical formula	$C_{13}H_{26}O_2$	$C_{13}H_{24}O_2$
Structure	$CH_3-(CH_2)_9-C(=O)-O-CH_2-CH_3$	$CH_2=CH-(CH_2)_8-C(=O)-O-CH_2-CH_3$
Physical chemical characteristics[2]		
Appearance	Liquid	Liquid
Molecular weight	214.35	212.33
Boiling point	255 C (102–107 C at 1 mm Hg)	258–259 C (131.5 C at 14.5 mm Hg)
Specific gravity	0.870 at 15.5 C	0.8788 at 20 C
Refractive index	1.9325 at 20 C	1.4382 at 20 C
Solubility	Insoluble in water	
Organoleptic characteristics	Odor similar to the corresponding ethyl heptanoate and coconut-like aroma	Wine-like odor
Synthesis	By reduction of the *l*-undecen-11-oic acid ethyl ester with hydrogen in the presence of Ni at 180 C,[6] or by direct esterification of *n*-undecanoic acid with ethyl alcohol under reflux	By heating the corresponding acid together with HCl in ethyl alcohol solution at 70 C[7] or with H_2SO_4 in alcoholic solution[8]
Natural occurrence	In rum, whisky, and wine	Not reported found in nature
Reported uses[3]		Non-alcoholic beverages 1.7 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 8.7 ppm Candy 10 ppm Baked goods 11 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2461

REFERENCES

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

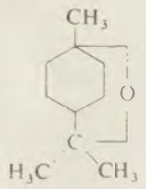
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7. Sörensen and Sorensen, *Acta Chem. Scand.*, 2, 173, 1948.
8. Jeffery and Vogel, *J. Chem. Soc.*, p. 562, 1948.

	Ethyl valerate	Ethyl vanillin
Other names		3-Ethoxy-4-hydroxybenzaldehyde
Empirical formula	$C_7H_{14}O_2$	$C_9H_{10}O_3$
Structure	$CH_3-(CH_2)_3-\overset{O}{\overset{\|}{C}}-O-CH_2-CH_3$	
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Crystalline, white powder
Molecular weight	130.18	166.17
Melting point		77–78 C
Boiling point	144 C at 734 mm Hg; 72–74 C at 65 mm Hg	285 C
Specific gravity	0.8736 at 20 C	
Refractive index	1.4004 at 20 C; 1.3980 at 24 C	
Solubility	Slightly soluble in water; soluble in alcohol and ether	Slightly soluble in water (1.3% at 50 C); soluble in alcohol, ether, glycerin, and chloroform; 1 gm in 3 cc of 95% alcohol or more
Organoleptic characteristics	Fruity odor suggestive of apple	Intense vanilla odor and sweet taste. Its flavoring power is 2–4 times stronger than vanillin. One must be careful not to exceed certain use levels, as this might cause an unpleasant flavor in the product. The product is not stable; in contact with iron or alkali, it exhibits a red color and loses its flavoring power.
Synthesis	By refluxing valeric acid and ethyl alcohol in the presence of concentrated H_2SO_4[6]	From safrole by isomerization to isosafrole and subsequent oxidation to piperonal. The methylene linkage is then broken by heating piperonal in an alcoholic solution of KOH; finally the resulting protocatechualdehyde is reacted with ethyl alcohol.[7] From guaethol by condensation with chloral to yield 3-ethoxy-4-hydroxyphenyl trichloromethyl carbinol. This is then boiled with an alcoholic solution of KOH or NaOH, acidified, and extracted with chloroform to yield ethyl vanillin.[7,8]
Natural occurrence	Reported found in the essential oil of rue	Not reported found in nature. It can be distinguished from vanillin because of the yellow color developed in the presence of concentrated H_2SO_4.
Reported uses[3]	Non-alcoholic beverages, 4.2 ppm; ice cream, ices, etc., 4.4 ppm; candy, 15 ppm; baked goods, 8.3 ppm; gelatins and puddings, 5.5 ppm; chewing gum, 260 ppm	Non-alcoholic beverages, 20 ppm; alcoholic beverages, 100 ppm; ice cream, ices, etc., 47 ppm; candy, 65 ppm; baked goods, 63 ppm; gelatins and puddings, 74 ppm; chewing gum, 110 ppm; icings and toppings, 140–200 ppm; chocolate, 250 ppm; imitation vanilla extracts, 28,000 ppm
Regulatory status	FDA 121.1164; FEMA No. 2462	FDA GRAS; FEMA No. 2464

REFERENCES

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

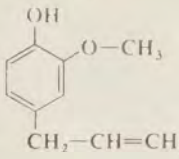
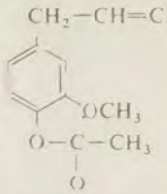
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7. Bedoukian, *Perfumery: Synthetics and Isolates*, D. Van Nostrand Co., 1951, 418.
8. Guglielmina, *Choc. Confiserie Fr.*, 24, May 1965.

	Eucalyptol
Other names	Cajeputol Cineole (1,8-cineole) 1,8-Epoxy-*p*-menthane
Empirical formula	$C_{10}H_{18}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless, mobile liquid
Molecular weight	154.24
Boiling point	176–177°C
Congealing point	0 to +1°C
Flash point	47–48°C
Specific gravity	0.9245 (0.928–0.930) at 20°C
Refractive index	1.4574 (1.454) at 20°C
Solubility	Almost insoluble in water; 1:2 in 70% alcohol; soluble in alcohol, ether, and most organic solvents
Organoleptic characteristics	Characteristic camphoraceous odor and fresh, pungent taste
Synthesis	By fractional distillation (170–180°C) from those essential oils containing high levels of eucalyptol, such as *Eucalyptus globulus* (approx 60%), and subsequent separation of the product by congealing the distillate
Natural occurrence	Its name is derived from its presence in the essential oils of *Eucalyptus globulus* and *Melaleuca leucadendron* L. (essential oil of cajeput). It was originally identified in the essential oil of *Artemisia maritima*[6] and subsequently in a large number (approx 270) of other essential oils: rosemary, laurel leaves, clary sage, myrrh, cardamom, star anise, camphor, lavender, peppermint, *Litsea guatemalensis*, *Luvunga scudens* Roxb., *Achillea micrantha*, and *Salvia triloba*. The essential oil of *Eucalyptus polibractea* has been reported to contain up to 91% eucalyptol.[7]
Reported uses[3]	Non-alcoholic beverages 0.13 ppm Ice cream, ices, etc. 0.50 ppm Candy 15 ppm Baked goods 0.50–4.0 ppm Chewing gum 190 ppm
Regulatory status	FDA 121.1164; FEMA No. 2465

REFERENCES

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

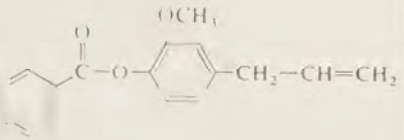
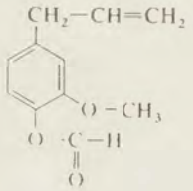
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	Eugenol	Eugenyl acetate
Other names	4-Allylguaiacol 4-Allyl-2-methoxyphenol 1-Hydroxy-2-methoxy-4-allyl benzene	Acetyl eugenol Eugenol acetate
Empirical formula	$C_{10}H_{12}O_2$	$C_{12}H_{14}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to slightly yellow liquid; tends to darken on exposure to air	Semisolid mass at room temperature; yellowish liquid when heated
Assay	95–100%	98% min
Molecular weight	164.21	206.24
Melting point	10.3 C	29–30 C
Boiling point	253 C (121 C at 10 mm Hg)	281–282 C at 752 mm Hg
Congealing point		25 C
Flash point	Approx 104 C	
Specific gravity	1.053–1.064 at 25 C; 1.0664 at 20 C	1.077–1.082 at 25 C; solid—1.0842 at 15 C
Refractive index	1.5380–1.5420 at 20 C; 1.5416 at 19.5 C	1.52069 at 20 C
Optical rotation	−1 30′	
Solubility	1:2 in 60% alcohol; almost insoluble in water; soluble in most organic solvents	1:5 in 70% alcohol; soluble in essential oils and most organic solvents
Organoleptic characteristics	Strong, clove-like odor and spicy, pungent taste	Characteristic odor reminiscent of clove oil, with burning, aromatic flavor
Synthesis	The oil containing eugenol is treated with a 3% aqueous solution of NaOH; the nonacid components are extracted with ether. The alkaline solution is acidified to isolate the phenols and subsequently is fractionally distilled under reduced pressure. To avoid the formation of emulsions, a pretreatment of the oil with tartaric acid is preferred.[6] Eugenol is the starting material in one of the syntheses for the preparation of vanillin.	By direct acetylation of eugenol using acetic anhydride
Natural occurrence	Reported found as a constituent in several volatile oils: clove oil, laurel, and cinnamon leaf oil. Smaller amounts of eugenol also are present in the oil of camphor, Java citronella, California laurel, and acacia flowers. Remarkable amounts of eugenol are found in *Ocimum sanctum* (70%) and *Ocimum gratissimum* (60%). Eugenol is also found in the oil from violet flowers (21%).[7] In some plants eugenol probably occurs as glucoside.[8]	Reported found in the essential oils of *Laurus nobilis* and clove buds and in clove leaves[6]
Reported uses[3]	Non-alcoholic beverages 1.4 ppm Ice cream, ices, etc. 3.1 ppm Candy 32 ppm Baked goods 33 ppm Gelatins and puddings 0.60 ppm Chewing gum 500 ppm Condiments 9.6–100 ppm Meats 40–2,000 ppm	Non-alcoholic beverages 0.43 ppm Ice cream, ices, etc. 3.3 ppm Candy 20 ppm Baked goods 10 ppm Chewing gum 25–100 ppm Condiments 2.0 ppm
Regulatory status	FDA GRAS; FEMA No. 2467	FDA 121.1164; FEMA No. 2469

REFERENCES

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

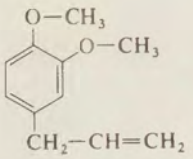
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7. Sabetay and Trabaud, *Compt. Rend.*, 209, 843, 1939.
8. Bourguelot and Herissey, *Compt. Rend.*, 140, 870, 1905.
9. Smith, *Perfum. Essent. Oil Rec.*, 37, 143, 1946.

	Eugenyl benzoate	Eugenyl formate
Other names	4-Allyl-2-methoxyphenyl benzoate Benzoyl eugenol Eugenol benzoate	4-Allyl-2-methoxyphenyl formate Eugenol formate
Empirical formula	$C_{17}H_{16}O_3$	$C_{11}H_{12}O_3$
Structure		
Physical/chemical characteristics[1]		
Appearance	Colorless, crystalline solid	
Assay		94% min
Molecular weight	268.32	192.22
Melting point	69–70 C	
Boiling point	360 C	270°C
Flash point		102 C
Specific gravity		1.1050–1.1090 at 15 C; 1.120 at 15.5 C
Refractive index		1.5240–1.5265 at 20 C
Acid value		0.9 max
Solubility	Insoluble in water; soluble in alcohol and ether	1:2–3.5 in 80% alcohol
Organoleptic characteristics	Balsamic odor with an undertone reminiscent of clove	Odor reminiscent of orris; often used in combination with methylionones to yield orris-like notes
Synthesis		
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.03–0.13 ppm Ice cream, ices, etc. 0.25–2.0 ppm Candy 0.25–10 ppm Baked goods 0.13–10 ppm	Condiments 0.20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2471	FDA 121.1164; FEMA No. 2473

REFERENCES

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

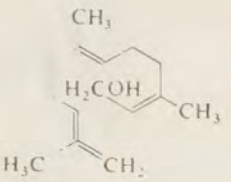
Eugenyl methyl ether

Other names	4-Allylveratrole 1,2-Dimethoxy-4-allylbenzene Methyl eugenol Methyl eugenyl ether
Empirical formula	$C_{11}H_{14}O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless to pale-yellow liquid
Molecular weight	178.23
Boiling point	244–245°C
Specific gravity	1.032–1.036 at 25°/25°C;[2] 1.055 at 15°C
Refractive index	1.5320–1.5360 at 20°C[2]
Eugenol content	Not more than 1%[2]
Solubility	1:4 in 60% alcohol;[2] 1:2 in 70% alcohol; almost insoluble in water. Forms azeotropic mixtures with ethylene glycol (31.5%), eugenol (55%), benzoic acid (11%), and others.
Organoleptic characteristics	Delicate clove-carnation odor with a bitter, burning taste
Synthesis	Usually prepared by methylation of eugenol
Natural occurrence	Reported in the essential oils of *Myrtaceae* and *Lauraceae*. It was identified originally in the essential oil from roots of *Asarum europaeum* L. and *Asarum canadense* L.;[6] subsequently it was identified as the main constituent of the oil from wood of *Dacrydium franklinii* Hook (97.5%), in *Melaleuca bracteata* F.v.M. (leaves, 90–95%), in *Cinnamomum oliveri* Bail. (leaves, 90–95%), and as a minor constituent in the oils of: betel,[7] citronella,[8] Japanese calamus,[9] pimenta, hyacinth, rose, basil, bay, cajeput, and others.
Reported uses[3]	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 4.8 ppm Candy 11 ppm Baked goods 13 ppm Jellies 52 ppm
Regulatory status	FDA 121.1164; FEMA No. 2475

REFERENCES

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

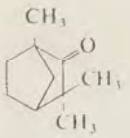
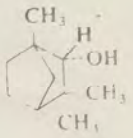
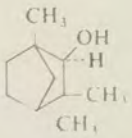
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7. *Schimmel Ber.*, p. 15, 1907.
8. Schimmel and Co., *Chem. Zentralbl.*, 2, 879, 1889.
9. Asahina, *Apoth. Ztg.*, 21, 987, 1906.

	Farnesol
Other names	2,6,10-Trimethyl-2,6,10-dodecatrien-12-ol 3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol
Empirical formula	$C_{15}H_{26}O$
Structure	
Physical/chemical characteristics[5]	The physical constants vary slightly, depending on the source and the method of preparation.
Appearance	Colorless liquid
Assay	97% min
Molecular weight	222.36
Boiling point	131–132°C at 3 mm Hg (from petitgrain) 124–125°C at 2.2 mm Hg (from Tolu balsam) 118–120°C at 2 mm Hg (from cabreuva) 118–120°C at 2 mm Hg (from geranyl acetone)
Specific gravity	0.887–0.889 at 25°C (0.8880 from petitgrain) (0.8883 at 20°C from Tolu balsam) (0.8886 from cabreuva) (0.8886 from geranyl acetone)
Refractive index	1.4890–1.4910 at 20°C (1.4891 from petitgrain) (1.4892 at 20°C from Tolu balsam) (1.4894 from cabreuva) (1.48906 from geranyl acetone)
Solubility	1:3 in 70% alcohol; almost insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Characteristic flowery odor
Synthesis	One method uses cabreuva as the starting material (Swiss Patent 261,120—Givaudan & Co.), while a second method starts from ambrette seeds (German Patent 149,603—Haarmann & Reimer).
Natural occurrence	For structure see references 6, 7, and 8. The presence of this terpene alcohol in nature has been reported in more than 30 essential oils. The levels are generally low (0.5—1.0%) with the exception of cabreuva, which contains up to 2.5% farnesol,[9] and the distillate from flowers of *Oxystigma buccholtzii* Harms., which contains up to 18% farnesol.[10] Among the essential oils containing farnesol are lemon grass, Ceylon citronella, cananga, ambrette seeds, ylang-ylang, *Acacia farnesiana*, Peru balsam, palmarosa, tuberose, and others.
Reported uses[3]	Non-alcoholic beverages 0.76 ppm Ice cream, ices, etc. 0.40 ppm Candy 1.4 ppm Baked goods 1.7 ppm Gelatins and puddings 0.10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2478

REFERENCES

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

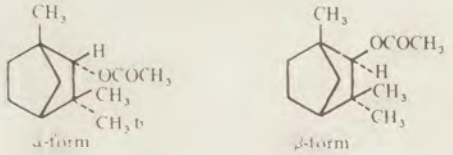
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	d-Fenchone	Fenchyl alcohol
Other names	*d*-2-Fenchanone Fenchone 1,3,3,-Trimethylbicyclo-1,2,2-heptanone-2 *d*-1,3,3-Trimethyl-2-norbornanone	2-Fenchanol Fenchol 1,3,3-Trimethyl-2-norbornanol
Empirical formula	$C_{10}H_{16}O$	$C_{10}H_{18}O$
Structure		 α-form  β-form
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid; solidifies when cold	Colorless to straw-yellow crystals for the α-form; β-forms are liquids at room temperature
Molecular weight	152.23	154.24
Melting point	*dl*, − 0°C; *d,l*, 5–6°C	*d*, 48°C; *l*, 49°C
Boiling point	193°C	
Specific gravity	*d*, 0.948 at 18°C; *l*, 0.948 at 20°C; 0.9501 at 15°C	
Refractive index	*d*, 1.46355 at 18°C; *l*, 1.4636 at 20°C; 1.4702 at 20°C	
Optical rotation	*d*, + 66 9′ at 20°C; *l*, − 66 9′ (+ 58 57′) at 23°C from ethanol	
Solubility	Very soluble in alcohol and ether; insoluble in water	Very slightly soluble in water; soluble in alcohol
Organoleptic characteristics	Camphor-like odor, powerful and sweet; warm, somewhat bitter, burning taste	Camphor-like odor with citrus notes; bitter, lime-like flavor
Synthesis	Isolated from cedarleaf oil (thuja oil)	By reduction of fenchone or from pine terpenes
Natural occurrence	Reported found in several essential oils: *Thuja plicata*, *Thuja occidentalis*, *Thuja standishii*, Russian anise, fennel, a few *Artemisia* varieties (*A. frigida*, *A. verlotorum*, *A. santolinaefolia*), *Lavanda stoechas*, *Lavanda burmannii*, and others. The highest levels are found in fennel oil (12–19%). Two optically active forms have been isolated.[6] For structural studies see reference 7.	Both the α- and the β-fenchyl alcohols are reported found in nature. In mixture they are present in the essential oils of: *Picea alba*, *Pinus silvestris*, pine oil, *Artemisia santolinaefolia*, and others. For structural studies and additional information, see references 8 and 9. The isofenchyl alcohol (1,5,5-trimethyl-2-norbornanol) is not found in nature.
Reported uses[3]	Non-alcoholic beverages 0.13–0.80 ppm Alcoholic beverages 5.0 ppm Ice cream, ices, etc. 0.25 ppm Candy 0.25–30 ppm Baked goods 0.25 ppm	Non-alcoholic beverages 1.8 ppm Ice cream, ices, etc. 0.25 ppm Candy 4.7 ppm Baked goods 0.25 ppm
Regulatory status	FDA 121.1164; FEMA No. 2479	FDA 121.1164; FEMA No. 2480

REFERENCES

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

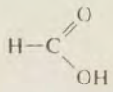
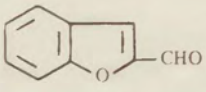
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7. Jacob, Owisson and Rassat, *Bull. Soc. Chim. Fr.*, p. 1374, 1959.
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	Fenchyl acetate
Other names	1,3,3-Trimethyl-2-norbornanyl acetate
Empirical formula	$C_{12}H_{20}O_2$
Structure	 α-form β-form
Physical/chemical characteristics	
Appearance	Colorless, mobile liquid
Molecular weight	196.29
Boiling point	*d*-α, 87°C at 10 mm Hg *dl*-α, 79°C at 5 mm Hg
Specific gravity	*dl*-α, 09744 at 15°C *dl*-β, 0.9073 at 15°C
Refractive index	*dl*-α, 1.4560 at 20°C *dl*-β, 1.3577 at 20°C
Optical rotation	*d*-α, +69.5° at 20°C (undiluted) *l*-α, -68.7°C at 20°C *l*-β, +39.6° at 20°C
Solubility	Insoluble in water; soluble in alcohol and oils; slightly soluble in propylene glycol
Organoleptic characteristics	Mild, sweet odor reminiscent of fir needles oil
Synthesis	By esterification of fenchyl alcohol with acetic anhydride in pyridine[6-10]
Natural occurrence	Reported found in the oil from leaves and terminal branches of *Juniperus rigida*;[11] in *Seseli sihiricum*;[12,13] in rosemary oil;[14] in fennel oil;[15] in the oil of hinoki leaves[16]
Reported uses[3]	Non-alcoholic beverages 0.2 ppm Ice cream, ices, etc. 0.2 ppm Candy 0.3 ppm Baked goods 0.3 ppm Gelatins and puddings 0.2 ppm Preserves and spreads 0.2 ppm
Regulatory status	FEMA No. 3390

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

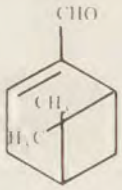
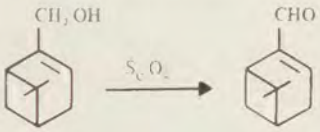
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	Formic acid	2-Formyl benzofuran
Other names		2-Benzofuran carboxaldehyde
Empirical formula	CH_2O_2	$C_9H_6O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, fuming liquid	
Molecular weight	46	146.15
Melting point	8.3 C	
Boiling point	100–101 C	130–131°C at 13 mm Hg
Specific gravity	1.2196 at 20°C	
Refractive index	1.3714	
Solubility	Completely miscible with water, alcohol, ether, and glycerol	
Organoleptic characteristics	Pungent, penetrating odor	
Synthesis	From anhydrous sodium formate and concentrated H_2SO_4 at low temperature followed by distillation	By the Gattermann process;[12] also from coumaryloyl cyanide[13]
Natural occurrence	Widespread in a large variety of plants. Reported identified in *Cistus labdanum*[6] and the oil of *Artemisia transiliensis*;[7] also found among the constituents of petitgrain lemon[8] and bitter orange essential oil;[9] reported found in strawberry aroma.[10]	
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 5.0 ppm Candy 5.0–18 ppm Baked goods 5.0–6.1 ppm	Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 20.0 ppm Gelatins and puddings 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2487	FEMA No. 3128

REFERENCES

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

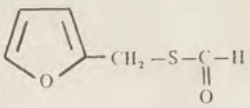
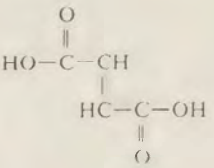
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	2-Formyl-6,6-dimethyl bicyclo [3.1.1] hept-2-ene
Other names	Myrtenal Benihinal 2-Formyl-6,6-dimethyl-2-norpinene 6,6-Dimethyl-2-norpinene-2-aldehyde
Empirical formula	$C_{10}H_{14}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless liquid; readily polymerizes in the presence of air
Molecular weight	150.22
Boiling point	199°C 99–100°C at 15 mm Hg
Specific gravity	0.9872 at 20°C
Refractive index	1.5030 at 20°C
Optical rotation	+14.75° at 20°C
Solubility	Insoluble in water; soluble in alcohol and in oils
Organoleptic characteristics	Refreshing, spicy-herbaceous odor of bay leaf, reminiscent of cinnamon[14,15]
Synthesis	From myrtenol by oxidation with chromic acid; by isolation from higher-than-cineole boiling fractions in the distillation of eucalyptus oil[13] 
Natural occurrence	Reported found in the oils from leaves of *Eucalyptus globulus*[6] and *Callytrix tetragona*;[7] in the oils of *Herrandia peltata*[8] and *Perovskia abrotanoides*;[9] in the oils from wood of *Chamaecyparis formonensis*[10] and *Chamaecyparis obtusa*;[11] also in cumin seeds and in mint[12]
Reported uses[3]	Non-alcoholic beverages 0.5 ppm Candy 2.0 ppm
Regulatory status	FEMA No. 3395

REFERENCES

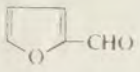
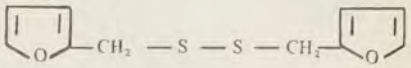
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	2-Furanmethanethiol formate		Fumaric acid	
Other names			Allomalenic acid Boletic acid *trans*-Butenedioic acid *trans*-1,2-Ethylenedicarboxylic acid	
Empirical formula	$C_6H_6O_2S$		$C_4H_4O_4$	
Structure				
Physical/chemical characteristics				
Appearance			Colorless, crystalline solid; sublimes at 200 C	
Molecular weight	142.17		116.07	
Melting point			300–302°C[11] (287°C)	
Specific gravity			1.625	
Solubility			Slightly soluble in water and most organic solvents	
Organoleptic characteristics			Used as a replacement for tartaric acid; odorless, tart, acidic-sour flavor	
Synthesis			By the action of certain fungi (*Rhizopus nigricans*) on glucose; by oxidation of furfural with sodium chlorate in the presence of vanadium pentoxide	
Natural occurrence			Reported found in several plants: *Fumaria officinalis* L., *Boletus scaber* Boll., and others	
Reported uses[3]	Non-alcoholic beverages	1.0 ppm	Non-alcoholic beverages	50 ppm
	Ice cream, ices, etc.	1.0 ppm	Baked goods	1,300 ppm
	Candy	1.0 ppm	Gelatins and puddings	3,600 ppm
Regulatory status	FEMA No. 3158		FDA 121.1130; FEMA No. 2488	

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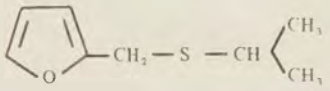
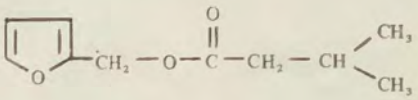
For References 1–5, see end of Part III.

	Furfural	2-Furfuryl disulfide
Other names	2-Furaldehyde 2-Furfuraldehyde Pyromucic aldehyde	2,2′-(Dithiodimethylene)difuran
Empirical formula	$C_5H_4O_2$	$C_{10}H_{10}O_2S_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Colorless liquid when freshly prepared; tends to darken on aging	Pale-yellow, oily liquid
Molecular weight	96.08	226.32
Melting point	36.5 C	10°C
Boiling point	161.7 C (72 C at 25 mm Hg)	112–113°C at 0.5 mm Hg
Flash point	65 C	
Specific gravity	1.1544 at 25 C; 1.1598 at 10 C	
Refractive index	1.52345 at 25 C; 1.5260 at 20 C	
Solubility	Rather soluble (1:1) in water; soluble in alcohol, ether, and most common organic solvents	Slightly soluble in water; very soluble in alcohol and in organic solvents
Organoleptic characteristics	Characteristic penetrating odor	Repulsive mercaptan-like odor; "roasted" at high dilution
Synthesis	Industrially prepared from pentosans that are contained in cereal straws and brans. These materials are previously digested with diluted H_2SO_4, and the formed furfural steam is distilled.	From furfural and hydrogen sulfide[13]
Natural occurrence	Reported found in several essential oils from plants of the *Pinaceae* family, in the essential oil from Cajenne linaloe,[6] in the oil from leaves of *Trifolium pratense*[7] and *Trifolium incarnatum*,[8] in the distillation waters of several essential oils, such as ambrette[9] and angelica seeds[10], in Ceylon cinnamon essential oil,[11] in petitgrain oil,[12] ylang-ylang, lavender, lemongrass, calamus, eucalyptus, neroli, sandalwood, tobacco leaves, and others. Also reported found in rum and toasted coffee.	
Reported uses[3]	Non-alcoholic beverages, 4.0 ppm; alcoholic beverages, 10 ppm; ice cream, ices, etc., 13 ppm; candy, 12 ppm; baked goods, 17 ppm; gelatins and puddings, 0.80 ppm; chewing gum, 45 ppm; syrups, 30 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 Milk, dairy products 1.0 ppm
Regulatory status	FDA status not fully defined; FEMA No. 2489	FEMA No. 3146

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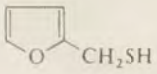
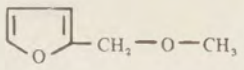
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	Furfuryl isopropyl sulfide		Furfuryl isovalerate	
Other names			Furfuryl-2-methylbutanoate	
Empirical formula	$C_8H_{12}OS$		$C_{10}H_{14}O_3$	
Structure				
Physical/chemical characteristics				
Molecular weight	156.25		182.21	
Boiling point	84°C at 16 mm Hg		97–98°C at 11 mm Hg	
Synthesis			By esterification of furfuryl alcohol with isovaleric chloride[6]	
Natural occurrence			Reported found as a constituent in coffee aroma[6]	
Reported uses[3]	Non-alcoholic beverages	0.5 ppm	Non-alcoholic beverages	5.0 ppm
	Ice cream, ices, etc.	0.5 ppm	Ice cream, ices, etc.	5.0 ppm
	Candy	0.5 ppm	Candy	10.0 ppm
	Baked goods	0.5 ppm	Gelatins and puddings	5.0 ppm
Regulatory status	FEMA No. 3161		FEMA No. 3283	

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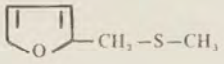
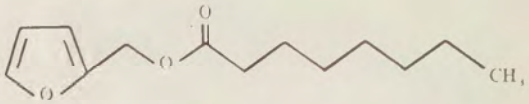
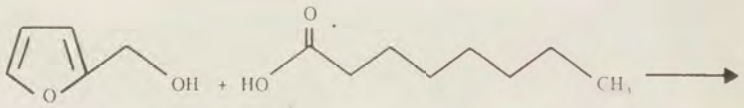
For References 1–5, see end of Part III.
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	Furfuryl mercaptan	Furfuryl methyl ether
Other names	2-Furanmethanethiol 2-Furyl methanethiol	
Empirical formula	C_5H_6OS	$C_6H_8O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Oily liquid	
Molecular weight	130.17	112.14
Boiling point	155 C (47 C at 12 mm Hg)	134–135°C 108–109° at 750 mm Hg
Specific gravity	1.1319 at 20 C	1.0163 at 20°C 1.046 at 25°C
Refractive index	1.5329 at 20 C	1.4570 at 20°C
Solubility	Insoluble in water; soluble in most organic solvents and diluted alkali solutions	Insoluble in water; soluble in alcohol; very soluble in ether
Organoleptic characteristics	Characteristic unpleasant odor	
Synthesis	Prepared by reacting thiourea and furfuryl chloride with subsequent hydrolysis of the reaction product;[6] also by reduction of difurfuryl disulfide in alcoholic solution using zinc dust and a small amount of acetic acid or using activated alumina[7]	From furfuryl chloride and potassium methoxide in ether solution[8]
Natural occurrence	Reported found in nature. Tends to polymerize when heated in the presence of mineral acids	Reported found as a constituent in the aroma of roasted coffee[9]
Reported uses[3]	Non-alcoholic beverages, 0.52 ppm; ice cream, ices, etc., 0.78 ppm; candy, 2.0 ppm; baked goods, 2.1 ppm; gelatins and puddings, 0.10 ppm; icings, 0.50 ppm	Non-alcoholic beverages 2.0 ppm Candy 2.0 ppm Gelatins and puddings 2.0 ppm Sauces 2.0 ppm
Regulatory status	FDA status not fully defined; FEMA No. 2493	FEMA No. 3159

REFERENCES

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

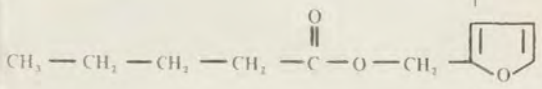
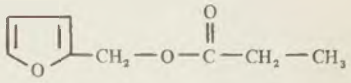
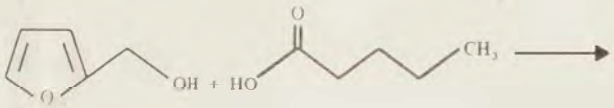
6. **Kirner and Richter,** *J. Am. Chem. Soc.*, 51, 3134, 1929.
7. German Patent 484,244.
8. **Kirner,** *J. Am. Chem. Soc.*, 50, 1960, 1928.
9. **Stoll, Winter, Gautschi, Flament and Willhalm,** *Helv. Chim. Acta,* 50, 628, 1967.

	Furfuryl methyl sulfide	α-Furfuryl octanoate
Other names		α-Furfuryl caprylate
Empirical formula	C_6H_8OS	$C_{13}H_{20}O_3$
Structure		
Physical/chemical characteristics		
Molecular weight	128.11	224.29
Boiling point	62–63°C at 28 mm Hg	
Refractive index	1.5210 at 22.5°C	
Synthesis	From 2-furfuryl mercaptan and dimethyl sulfate[6]	
Natural occurrence	Reported found as a minor constituent in coffee aroma	
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	Baked goods 4.0 ppm Gelatins and puddings 2.0 ppm Meat, meat sauces, soups 2.0 ppm Margarine 2.0 ppm Snacks 10.0 ppm
Regulatory status	FEMA No. 3160	FEMA No. 3396

REFERENCES

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

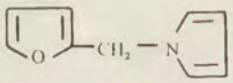
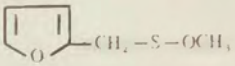
6. Gianturco et al., *Tetrahedron Lett.*, 20, 2951,1964.

	α-Furfuryl pentanoate	Furfuryl propionate
Other names	α-Furfuryl valerate	
Empirical formula	$C_{10}H_{14}O_3$	$C_8H_{10}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance		Oily liquid; darkens on exposure to light
Molecular weight	182.22	154.16
Boiling point	228–229°C at 764 mm Hg 82–83°C at 1 mm Hg	195–196°C 59–60°C at 1 mm Hg
Specific gravity	1.0284 at 20°C	1.1085 at 20°C
Synthesis		By heating propionic anhydride with furfuryl alcohol[7]
Natural occurrence	Reported found in milk[6]	Reported found as a constituent in coffee aroma[8]
Reported uses[3]	Non-alcoholic beverages 1.5 ppm Candy 3.0 ppm	Non-alcoholic beverages 0.5 ppm Ice cream, ices, etc. 0.5 ppm Candy 1.0 ppm Baked goods 1.0 ppm Gelatins and puddings 1.0 ppm Chewing gum 1.0 ppm Meat, meat sauces, soups 1.0 ppm Cereals 1.0 ppm
Regulatory status	FEMA No. 3397	FEMA No. 3346

REFERENCES

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

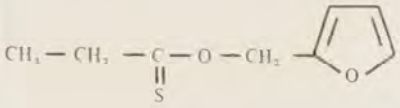
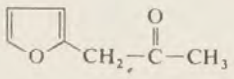
6. Kinlin et al., *J. Agric. Food Chem.*, 20, 1021, 1972.
7. Zanetti, *J. Am. Chem. Soc.*, 47, 535, 1925.
8. Stoll et al., *Helv. Chim. Acta*, 50, 628, 1967.

	N-Furfuryl pyrrole		Furfuryl thioacetate	
Other names	1-(2-furfuryl)pyrrole		Furfuryl thiol acetate	
Empirical formula	C_9H_9ON		$C_7H_8O_2S$	
Structure				
Physical/chemical characteristics[5]				
Molecular weight	147.08		156.20	
Boiling point	76–78°C at 1 mm Hg		90–92°C at 12 mm Hg	
Refractive index	1.5317 at 21°C			
Solubility	Soluble in most common organic solvents			
Synthesis	From furfuryl amino mucate[6]			
Natural occurrence	Reported found as a constituent in coffee aroma;[7] a volatile flavor component in roasted filberts[8]		Reported found as a constituent in coffee[9]	
Reported uses[3]	Non-alcoholic beverages	2.0 ppm	Non-alcoholic beverages	0.20 ppm
	Ice cream, ices, etc.	2.0 ppm	Ice cream, ices, etc.	1.0 ppm
	Candy	2.0 ppm	Candy	1.5 ppm
	Baked goods	2.0 ppm	Gelatins and puddings	1.0 ppm
	Gelatins and puddings	2.0 ppm		
	Milk, dairy products	2.0 ppm		
	Cereals	2.0 ppm		
Regulatory status	FEMA No. 3284		FEMA No. 3162	

REFERENCES

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

6. **Reichstein,** *Helv. Chim. Acta*, 13, 349, 1930.
7. **Reichstein and Standinger,** *Angew. Chem.*, 62, 212, 1950.
8. **Sheldon et al.,** *J. Food Sci.*, 37(2), 313, 1972.
9. **Stoll et al.,** *Helv. Chim. Acta*, 50(2), 628, 1967.

	Furfuryl thiopropionate		(2-Furyl)-2-propanone	
Other names			Furfuryl methyl ketone Furyl acetone Methyl furfuryl ketone	
Empirical formula	$C_8H_{10}O_2S$		$C_7H_8O_2$	
Structure				
Physical/chemical characteristics				
Appearance			Liquid	
Molecular weight	170.23		124.14	
Boiling point	95–97°C at 10 mm Hg		179–180°C	
Solubility			Soluble in diluted HCl and most organic solvents	
Organoleptic characteristics			Odor and taste suggestive of radish	
Synthesis			By heating the α-methyl-β-(α-furyl) glycidic acid ethyl ester in aqueous NaOH[6]	
Natural occurrence			Reported found in roasted coffee	
Reported uses[3]	Non-alcoholic beverages	1.0 ppm	Ice cream, ices, etc.	5.0 ppm
	Ice cream, ices, etc.	1.0 ppm	Candy	3.8–20 ppm
	Candy	1.0 ppm	Baked goods	2.0–20 ppm
	Baked goods	1.0 ppm		
Regulatory status	FEMA No. 3347		FDA 121.1164; FEMA No. 2496	

REFERENCES

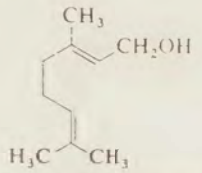
For References 1–5, see end of Part III.

6. Darzens, *Compt. Rend.*, 142, 215, 1906.

	Fusel oil, refined
Other names	Amyl alcohol, commercial (Not well defined)
Structure	A volatile, oily mixture consisting largely of amyl alcohols. Isoamyl alcohol and active amyl alcohol (2-methyl-1-butanol) are the chief constituents. Acids, esters, and aldehydes are also present.
Physical/chemical characteristics[5]	This specification refers to the rectified material.
Appearance	Water-white liquid
Molecular weight	
Boiling point	Distillation range: <110°C—none <120°C—>15% <130°C—>60% >135°C—none
Flash point	123°F
Specific gravity	0.811–0.815 at 20°/20°C
Solubility	Soluble in water, alcohol, and ether
Organoleptic characteristics	Disagreeable odor. An appreciable percentage of fusel oil in a liquor has an adverse effect, while trace amounts are necessary for the characteristic flavor.
Synthesis	As a by-product in the fermentation of starch- or sugar-containing materials (potatoes, grapes, beetroots, grain); purified by rectification
Reported uses[3]	Non-alcoholic beverages 21 ppm Alcoholic beverages 2.5 ppm Ice cream, ices, etc. 4.1 ppm Candy 30 ppm Baked goods 34 ppm Gelatins and puddings 4.0 ppm Chewing gum 270 ppm
Regulatory status	FDA 121.1164; FEMA No. 2497

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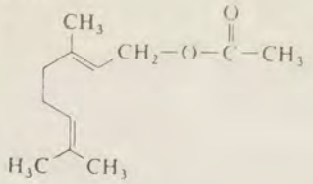
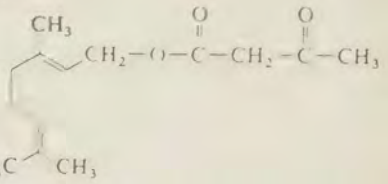
For References 1–5, see end of Part III.

	Geraniol
Other names	2-*trans*-3,7-Dimethyl-2,6-octadien-1-ol
Empirical formula	$C_{10}H_{18}O$
Structure	
Physical/chemical characteristics[5]	The physical constants vary for the various commercial products, depending on the total geraniol content. Specific gravity and refractive index may be indicative of the purity of the product.
Appearance	Colorless liquid
Assay	88% min.[2]
Molecular weight	154.24
Boiling point	110–111 C at 10 mm Hg
Flash point	101 C
Specific gravity	0.870–0.885 at 25/25 C;[2] 0.8793 at 20 C
Refractive index	1.4690–1.4780 at 20 C;[2] 1.47773 at 20 C
Optical rotation	−2 to +2[2] (0)
Ester content	Not more than 1%[2] (as geranyl acetate)
Aldehyde content	Not more than 1%[2] (as citronellol)
Solubility	1:2 in 70% alcohol;[2] almost insoluble in water; soluble in most common organic solvents
Organoleptic characteristics	Characteristic rose-like odor
Synthesis	By fractional distillation from those essential oils rich in geraniol, or synthetically from myrcene. Commercial geraniol cannot be classified according to its alcohol content, as most of the recurring impurities are alcoholic in nature (nerol, citronellol, tetrahydrogeraniol). Gas-chromatography techniques may be usefully employed to determine the geraniol content in a product.
Natural occurrence	The presence of geraniol in nature has been reported in more than 160 essential oils: ginger grass, lemongrass, Ceylon and Java citronella, tuberose, oak musk, orris, champaca, ylang-ylang, mace, nutmeg, sassafras, Cajenne bois-de-rose, rose, *Acacia farnesiana*, geranium, clary sage, spike, lavandin, lavender, jasmine, coriander, carrot, myrrh, eucalyptus, linaloe, lime, mandarin petitgrain, bergamot petitgrain, bergamot, lemon, orange, and others. The essential oils of palmarosa and *Cymbopogon winterianus* contain the highest levels of geraniol (approx 80–95%).[6]
Reported uses[3]	Non-alcoholic beverages 2.1 ppm Ice cream, ices, etc. 3.3 ppm Candy 10 ppm Baked goods 11 ppm Gelatins and puddings 2.0 ppm Chewing gum 0.80–2.9 ppm Toppings 1.0 ppm
Regulatory status	FDA GRAS; FEMA No. 2507

REFERENCES

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

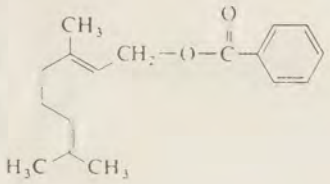
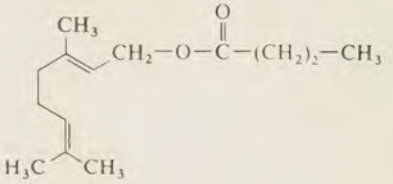
6. **Pietramellara,** *Riv. Ital. EPPOS,* 39, 60, 1957.

	Geranyl acetate	Geranyl acetoacetate
Other names	2,6-Dimethyl-2,6-octadiene-8-yl acetate Geraniol acetate	*trans*-3,7-Dimethyl-2,6-octadien-l-yl acetoacetate Geranyl β-ketobutyrate Geranyl 3-oxobutanoate
Empirical formula	$C_{12}H_{20}O_2$	$C_{14}H_{22}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Liquid
Assay	90% min;[2] 92% (85% tech.)	
Molecular weight	196.29	238.33
Boiling point	127–129 C (245°C) at 22 mm Hg	
Flash point	104 C	
Specific gravity	0.900–0.914 at 25 /25°C;[2] 0.900–0.910; 0.896–0.913 tech.	0.9625 at 25 C
Refractive index	1.4580–1.4640 at 20 C;[2] 1.4570–1.4620	1.4670 at 25 C
Optical rotation	−2.0° to +3.0 °[2] (±1°)	
Solubility	1:8 in 70% alcohol;[2] 1:25–30 in 60% alcohol; soluble in most organic solvents	
Organoleptic characteristics	Pleasant, flowery odor reminiscent of rose lavender; burning taste, initially somewhat bitter and then sweet	
Synthesis	From geraniol by acetylation or by fractional distillation of essential oils in which it is present	From diketene and geraniol in the presence of the sodium salt of geraniol
Natural occurrence	Reported found in a large number of essential oils: Ceylon citronella, palmarosa, lemongrass, petitgrain, neroli bigarade, geranium, coriander, lavender, carrot, sassafras, in various *Callitris* species (*C. verrucosa*, *C. robusta*, and others) and *Eucalyptus* species (*E. acervula*, *E. urnigera*, etc.). A 60% level has been reported in the essential oil of *Eucalyptus macarthuri*[6] and up to 50% in the essential oil of *Orthodon citraliferum*.[7] Also identified in bitter orange essential oil.[8]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 1.6 ppm Ice cream, ices, etc. 6.5 ppm Candy 15 ppm Baked goods 17 ppm Gelatins and puddings 6.8–7.5 ppm Chewing gum 0.30–1.2 ppm Syrups 1.0 ppm	Non-alcoholic beverages 0.50 ppm Ice cream, ices, etc. 1.0 ppm Candy 1.0–3.0 ppm Baked goods 1.0–10 ppm
Regulatory status	FDA GRAS; FEMA No. 2509	FDA 121.1164; FEMA No. 2510

REFERENCES

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

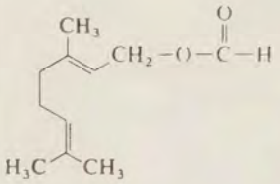
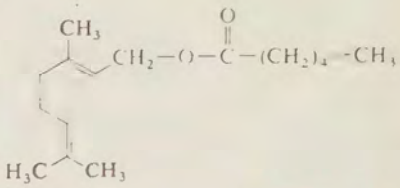
6. Arctander, *Parfuem. Kosmet.*, 39, 7, 1958.
7. Fujita and Minamino, *Nippon Kagaku Zasshi*, 79, 1017, 1958.
8. Mehlitz and Minas, *Ind. Obst Gemueseverwert.*, 50, 861, 1965.

	Geranyl benzoate	Geranyl butyrate
Other names		
Empirical formula	$C_{17}H_{22}O_2$	$C_{14}H_{24}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Yellowish, oily liquid	Colorless liquid
Assay	92% min	92% min
Molecular weight	258.37	224.34
Boiling point	198–200 C at 15 mm Hg	151–153 C at 18 mm Hg; 142–143 C at 13 mm Hg
Flash point	100 C	93 C
Specific gravity	0.978–0.984 at 25 /25 C	0.891–0.896 at 25 /25 C; 0.9008 at 17 C
Refractive index	1.513–1.518 at 20 C	1.456–1.462 at 20 C
Optical rotation	−1	±1
Acid value	1 max	1 max
Solubility	1:4 in 90% alcohol	1:7 in 80% alcohol; 1:1 in 90% alcohol; almost insoluble in water
Organoleptic characteristics	Sweet, light odor reminiscent of ylang-ylang	Characteristic fresh, fruity, rose-like odor and sweet apricot-like taste
Synthesis	From geraniol and benzoyl chloride in anhydrous pyridine;[6] also from geraniol and benzoyl chloride using the Schotten-Bauman reaction[7]	By heating geraniol and butyryl chloride in the presence of pyridine,[8] or from geraniol and butyric anhydride in the presence of camphor sulfonic acid[9]
Natural occurrence	Not reported found in nature	Reported found in the essential oil of *Darwinia grandiflora*. It has been identified in lavender oil[10] and in other essential oils.
Reported uses[3]	Non-alcoholic beverages 0.10–0.13 ppm Ice cream, ices, etc. 0.16–0.25 ppm Baked goods 0.50 ppm Gelatins and puddings 0.50 ppm	Non-alcoholic beverages 1.6 ppm Ice cream, ices, etc. 2.8 ppm Candy 10 ppm Baked goods 10 ppm Gelatins and puddings 5.3 ppm Chewing gum 0.30–1.5 ppm
Regulatory status	FDA 121.1164; FEMA No. 2511	FDA 121.1164; FEMA No. 2512

REFERENCES

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

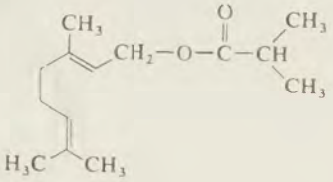
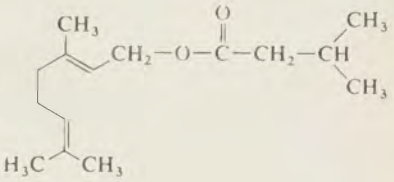
6. **Erdmann and Huth,** *J. Prakt. Chem.*, 2(56), 14, 1897.
7. **Bacon,** *Chem. Zentralbl.*, 2, 947, 1908.
8. **Erdmann,** *Ber. Dtsch. Chem. Ges.*, 31, 356, 1898.
9. **Reycher,** *Chem. Zentralbl.*, 1, 1042, 1908.
10. **Sfiras,** *Riv. Ital. EPPOS*, 7, 450, 1966.

	Geranyl formate	Geranyl hexanoate
Other names		Geranyl caproate Geranyl hexylate
Empirical formula	$C_{11}H_{18}O_2$	$C_{16}H_{28}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless to pale yellow liquid	
Assay	85% min[2]	
Molecular weight	182.26	252.40
Boiling point	113–114°C at 15 mm Hg; 92°C at 11 mm Hg	240°C
Specific gravity	0.906–0.920[2] (0.9886) at 25°/25°C	0.890 at 15.5°C
Refractive index	1.4580–1.4660 at 20°C[2]	1.4500 at 20°C
Optical rotation	±1°	
Acid value	Not more than 3.0[2]	
Solubility	1:3 in 80% alcohol;[2] insoluble in water	
Organoleptic characteristics	Fresh, green, leafy, rose odor with a bitter taste	Rose-geranium odor with a strong undertone reminiscent of pineapple and banana
Synthesis	Prepared by direct esterification of geraniol with formic acid	
Natural occurrence	Reported found in geranium oil and in the oil of *Ledum palustre*[6]	Reported found in the essential oil of palmarosa and in the leaves of *Phebalium dentatum*
Reported uses[3]	Non-alcoholic beverages 1.9 ppm Ice cream, ices, etc. 1.6 ppm Candy 7.5 ppm Baked goods 4.1 ppm Gelatins and puddings 3.4 ppm Chewing gum 0.80 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 0.90 ppm Candy 3.2 ppm Baked goods 2.0 ppm
Regulatory status		FDA 121.1164; FEMA No. 2515

REFERENCES

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

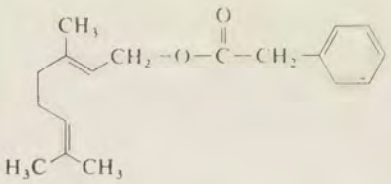
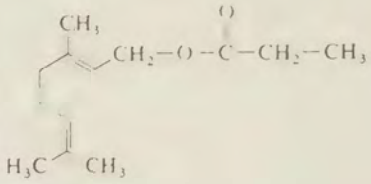
6. Hasebe, *J. Chem. Soc. Jap.*, 64, 1041, 1943.

	Geranyl isobutyrate	Geranyl isovalerate
Other names		
Empirical formula	$C_{14}H_{24}O_2$	$C_{15}H_{26}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	224.34	238.37
Specific gravity	0.8997 at 15 C	
Refractive index	1.4576 at 20 C	1.4538 at 20 C
Solubility	Insoluble in water; soluble in most organic solvents	
Organoleptic characteristics	Light rose odor and sweet, apricot-like taste	Rose odor with an apple-pineapple undertone and sweet apple taste
Synthesis	By heating geraniol and acetic isobutyric aldehyde in the presence of sodium acetate in toluene and then distilling the formed acetic acid as an azeotrope[6]	
Natural occurrence	Reported found in the essential oils of Japanese hops[7] and valerian	In *Eucalyptus citriodora* Hook.
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 0.80 ppm Candy 5.0 ppm Baked goods 4.9 ppm Gelatins and puddings 0.60 ppm Chewing gum 15 ppm	Non-alcoholic beverages 4.2 ppm Ice cream, ices, etc. 11 ppm Candy 10 ppm Baked goods 6.8 ppm
Regulatory status	FDA 121.1164; FEMA No. 2513	FDA 121.1164; FEMA No. 2518

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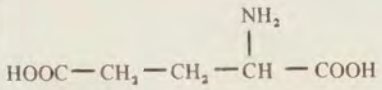
For References 1–5, see end of Part III.

6. Norda Essential Oil and Co., U.S. Patent 2,423,545, 1944.
7. Shigematzu and Kitazawa, *Chem. Abstr.*, 60, 8343d, 1964.

	Geranyl phenylacetate	Geranyl propionate
Other names	Geranyl *o*-toluate	2,6-Dimethyl octadien-6-yl-8-*n*-propionate
Empirical formula	$C_{18}H_{24}O_2$	$C_{13}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellowish liquid	Colorless liquid
Assay	97% min	92% min[2]
Molecular weight	272.39	210.31
Boiling point		253°C (128°C at 15 mm Hg)
Flash point	99°C	99°C
Specific gravity	0.971–0.978 at 25°/25°C	0.896–0.913 at 25°/25°C[2]
Refractive index	1.5070–1.5110 at 20°C	1.4570–1.4650 at 20°C[2]
Optical rotation	±1°	=1°
Acid value	2 max	Not more than 2; not more than 1[2]
Solubility	1:4 in 90% alcohol	1:4 or more in 80% alcohol[2]
Organoleptic characteristics	Honey- and rose-like odor	Fruity, somewhat flowery odor and bitter taste
Synthesis		By esterification of geraniol with propionic acid in the presence of a catalyst
Natural occurrence	Not reported found in nature	Reported found in *Fortunella margarita*
Reported uses[3]	Non-alcoholic beverages 1.1 ppm Ice cream, ices, etc. 3.1 ppm Candy 6.7 ppm Baked goods 4.7 ppm Chewing gum 11 ppm	Non-alcoholic beverages 1.5 ppm Ice cream, ices, etc. 1.3 ppm Candy 3.7 ppm Baked goods 4.9 ppm Gelatins and puddings 3.0 ppm Chewing gum 30–70 ppm
Regulatory status	FDA 121.1164; FEMA No. 2516	FDA 121.1164; FEMA No. 2517

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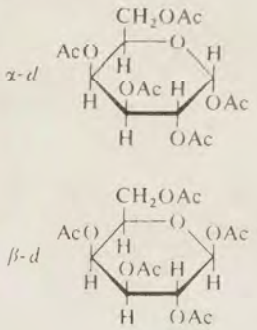
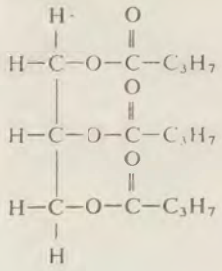
For References 1–5, see end of Part III.

	L-Glutamic acid
Other names	Aminoglutaric acid 2-Aminopentanedioic acid 1-Aminopropane-1,3-dicarboxylic acid
Empirical formula	$C_5H_9NO_4$
Structure	
Physical/chemical characteristics[5]	
Appearance	White or colorless platelets
Molecular weight	147.13
Melting point	247–249°C (decomposes)
Boiling point	175°C at 10 mm Hg (sublimes)
Specific gravity	1.538 at 20°C (*in vacuo*)
Optical rotation	+31.4° at 22°C (c = 1 in 6*N* HCl)
Solubility	Slightly soluble in water and ether; insoluble in alcohol, acetone, benzene, methanol, and acetic acid
Organoleptic characteristics	Very faint odor reminiscent of yeast or freshly baked bread; mild, somewhat sweet, meat-like taste
Synthesis	By hydrolysis of gluten (wheat, corn, or other vegetable sources);[6] by fermentation from glucose-containing raw materials;[7] the racemic acid may be resolved into the *d*- and *l*-isomer by fractional crystallization;[8] from 2-cyclopentenylamine;[9] by microbial conversion of α-ketoglutaric acid;[10] or by an alternative method, using *Bacillus megatherium-cereus*;[11,12] from fumaric acid, using *B. pumilus*;[13] from starch[14]
Natural occurrence	Reported as occurring in many vegetable proteins,[15,16] in beef fibrin, in the chrysalis of silkworm, in the hydrolysate of crystalline insulin;[17] also present in other important peptides, such as glutathione, tyrocidin, folic acid, β-lactoglobulin, secretin, and bacitracin, and in a growth hormone[18,19]
Reported uses[3]	Non-alcoholic beverages 400.0 ppm Baked goods 400.0 ppm Condiments, pickles 400.0 ppm Meat, meat sauces, soups 400.0 ppm Milk, dairy products 400.0 ppm Cereals 400.0 ppm
Regulatory status	FEMA No. 3285

REFERENCES

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

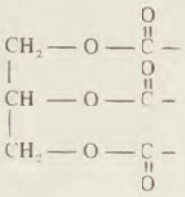
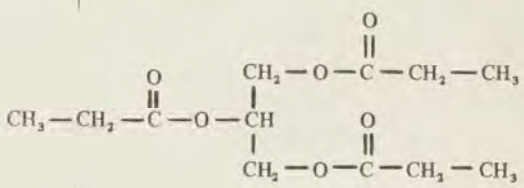
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	Glucose pentaacetate	Glycerol tributyrate
Other names	Pentaacetyl glucose 1,2,3,4,6-Pentaacetyl-α-*d*-glucose 1,2,3,4,6-Pentaacetyl-β-*d*-glucose *Not* 2,3,4,5,6-Pentaacetyl-*d*-glucose	Butyrin Glyceryl tributyrate Tributyrin
Empirical formula	$C_{16}H_{22}O_{11}$	$C_{15}H_{26}O_6$
Structure		
Physical/chemical characteristics[5]		
Appearance	White, crystalline powder	Colorless, somewhat oily liquid
Assay	Commercial product probably a mixture of 90% β-*d* and 10% α-*d*	Not less than 99% of $C_{15}H_{26}O_6$
Molecular weight	390.34	302.37
Melting point	Pure α-*d*, 114°C; pure β-*d*, 135°C	−75°C
Boiling point		287–288°C; 190°C at 15 mm Hg; distills between 305–310 C
Specific gravity		1.034–1.037 at 20°C
Refractive index		1.4359 at 20°C
Optical rotation	At 20°C: α-d, + 101.6°; β-*d*, + 3.8°	
Solubility	Insoluble in water and pet ether; soluble in alcohol, benzene, and ether; α-*d*, 5 gm/100 ml $CHCl_3$; β-*d*, 7 gm/100 ml $CHCl_3$	Insoluble in water; soluble in benzene, acetone, and alcohol; very soluble in ether
Organoleptic characteristics	Odorless; bitter flavor	Characteristic odor and bitter taste
Synthesis	By acetylation of glucose using any number of techniques, including: $ZnCl_2$ and pyridine, sodium acetate, and acetic anhydride and pyridine. For an extensive review including methods of preparation, see reference 6.	See Reference 7.
Natural occurrence	Not reported found in nature	
Reported uses[3]	Non-alcoholic beverages 100 ppm Baked goods 1,500 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2524	FDA GRAS

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

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	Glyceryl tribenzoate	Glyceryl tripropanoate
Other names	1,2,3-Propanetriol tribenzoate Tribenzoin	Propionic acid, triglyceride Tripropionin
Empirical formula	$C_{24}H_{20}O_6$	$C_{12}H_{20}O_6$
Structure		
Physical/chemical characteristics		
Appearance		
Assay		
Molecular weight	404.43	260.29
Melting point	76°C	175–176°C at 20 mm Hg
Boiling point		130–132°C at 3 mm Hg
Congealing point		
Flash point		
Specific gravity	1.228 at 12°C	1.100 at 20°C/18°C
Refractive index		1.4318 at 19°C
Solubility	Very soluble in ether, ethyl acetate, benzene, and chloroform; soluble in hot	Insoluble in water; soluble in alcohol and chloroform; very soluble in ether
Reported uses[3]	Non-alcoholic beverages 190 ppm	Non-alcoholic beverages 20.0 ppm Baked goods 50.0 ppm Desserts 20.0 ppm
Regulatory status	FEMA No. 3398	FEMA No. 3286

REFERENCES

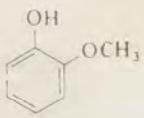
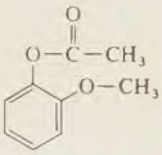
For References 1–5, see end of Part III.

	Glycine	
Other names	Glycocoll Aminoacetic acid Aminoethanoic acid	
Empirical formula	$C_2H_5O_2N$	
Structure	H_2N-CH_2-COOH	
Physical/chemical characteristics[5]		
Appearance	Monoclinic or trigonal prisms (from diluted alcohol); exists in three different polymorphic forms (α, β, γ)[6]	
Assay		
Molecular weight	75.07	
Melting point	262°C (decomposes; turns brown at 228°C and is completely sintered at 290°C)	
Refractive index	0.828 at 17° C	
Solubility	Very soluble in water; insoluble in alcohol and ether; slightly soluble in acetone and pyridine	
Organoleptic characteristics	Sweet taste	
Synthesis	From chloroacetic acid and ammonia;[7] from protein sources, such as gelatin and silk fibroin;[8] from ammonium bicarbonate and sodium cyanide;[9] by catalytic cleavage of serine;[10] from hydrobromic acid and methyleneaminoacetonitrile[11]	
Natural occurrence	Gelatin and silk fibroin are reportedly the best natural sources of this amino acid	
Reported uses[3]	Non-alcoholic beverages	150.0 ppm
	Candy	150.0 ppm
	Baked goods	150.0 ppm
	Condiments, pickles	150.0 ppm
	Meat, meat sauces, soups	150.0 ppm
	Preserves and spreads	150.0 ppm
Regulatory status	FEMA No. 3287	

REFERENCES

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

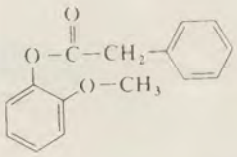
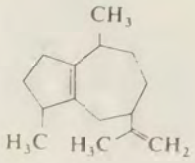
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	Guaiacol	Guaiacyl acetate
Other names	*o*-Hydroxyanisole *o*-Methoxyphenol Methylcatechol Pyrocatechol monomethyl ether	Acetyl guaiacol *o*-Methoxyphenyl acetate
Empirical formula	$C_7H_8O_2$	$C_9H_{10}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellowish, low-melting crystals or liquid; tends to darken on exposure to light	Colorless liquid
Molecular weight	124.14	166.18
Melting point	27.9°C	
Boiling point	205°C; 107°C at 24 mm Hg	235–240°C; 123–124°C at 13 mm Hg
Specific gravity	1.1395 (1.112 liquid)	1.156 at 0°C
Refractive index	1.5341 at 34.8°C	
Solubility	Slightly soluble in water; soluble in alcohol, ether, and chloroform	Almost insoluble in water; miscible with alcohol and ether
Organoleptic characteristics	Characteristic sweet odor; slightly phenolic	Odor similar to that of guaiacol
Synthesis	Obtained from hardwood tar or synthetically from *o*-nitrophenol via *o*-anisidine[6]	From guaiacol and excess acetic anhydride in the presence of trace amounts of H_2SO_4
Natural occurrence	Discovered in the distillation product from guaiac resin. Guaiacol is found in castoreum oil,[7] in the essential oil from flowers of *Pandanus odoratissimus* L.,[8] in the distillation waters of orange leaves,[9] in the essential oil of *Ruta montana* L.,[10] in the essential oil from celery seeds,[11] and in the oil from tobacco leaves[12]	
Reported uses[3]	Non-alcoholic beverages 0.95 ppm Ice cream, ices, etc. 0.52 ppm Candy 0.96 ppm Baked goods 0.75 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2532	FDA 121.1164

REFERENCES

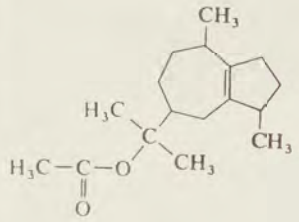
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	Guaiacyl phenylacetate	Guaiene
Other names	Guaiacol phenylacetate *o*-Methoxyphenyl phenylacetate	1,4-Dimethyl-7-isopropenyl-Δ-9,10-octahydroazulene
Empirical formula	$C_{15}H_{14}O_3$	$C_{15}H_{24}$
Structure		
Physical/chemical characteristics[5]		
Appearance	Amber, viscous liquid	Mobile, greenish-yellow liquid
Molecular weight	242.28	
Boiling point		123°–124°C at 9 mm Hg; 128°–130°C at 12 mm Hg
Specific gravity		0.9115 at 19°C; 0.9085 at 20°C
Refractive index		1.5022 at 19°C; 1.5049 at 20°C
Optical rotation		−40°21′ (−16°48′) at 20°C
Solubility	Insoluble in water; soluble in alcohol	Soluble in alcohol
Organoleptic characteristics	Heavy, dry, woody, herbaceous odor; woody, spicy, smoky flavor	Very little odor; delicate, woody flavor
Synthesis	From phenylacetyl chloride and guaiacol in aqueous alkaline solutions or using pyridine	Usually prepared by dehydrating guaiol with $KHSO_4$
Natural occurrence	Not reported found in nature	Guaiene is a bicyclic sesquiterpene found naturally in patchouli oil and other essential oils in small quantities.
Reported uses[3]	Non-alcoholic beverages 0.38 ppm Ice cream, ices, etc. 1.0 ppm Candy 2.2 ppm Baked goods 3.2 ppm Toppings 1.0 ppm	
Regulatory status	FDA 121.1164; FEMA No. 2535	FDA 121.1164

REFERENCES

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

	Guaiol acetate
Other names	1,4-Dimethyl-7-(α-hydroxy-isopropyl)-Δ-9,10-octahydroazulene acetate
Empirical formula	$C_{17}H_{28}O_2$
Structure	
Physical/chemical characteristics[5]	
Appearance	Yellowish liquid
Assay	83% min (70% min)
Molecular weight	264.41
Flash point	>100°C
Specific gravity	0.975–0.985 (0.975–0.990) at 25°C
Refractive index	1.487–1.495 (1.4880–1.4980) at 20°C
Acid value	1 max
Solubility	1:6 in 80% alcohol; 1:1 in 90% alcohol
Organoleptic characteristics	Faint but lasting rose odor; sweet taste suggestive of currant; not very stable
Synthesis	By acetylation of guaiol, which is one of the constituents of the essential oil from guaiac wood
Natural occurrence	Not reported found in nature
Regulatory status	FDA 121.1164

REFERENCES

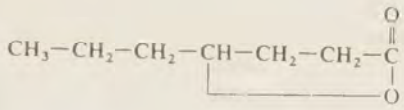
For References 1–5, see end of Part III.

	2,4-Heptadienal
Empirical formula	$C_7H_{10}O$
Structure	$CH_3-CH=CH-CH=CH-CH_2-CHO$
Physical/chemical characteristics[5]	
Molecular weight	110.15
Boiling point	84.0–84.5°C at 20 mm Hg 58–60°C at 5 mm Hg
Specific gravity	0.881 at 25°C
Refractive index	1.5313 at 27°C
Solubility	
Organoleptic characteristics	In autooxidizing fats and oils, it retards or prevents the development of "off-flavors"[6]
Synthesis	By reduction with $LiAlH_4$ of the dienoic acid prepared by the Doebner synthesis, followed by oxidation with MnO_2 of the resulting dienol to the corresponding dienol;[7] by the method of Marshall and Whiting[8]
Natural occurrence	Reported found as a volatile component in boiled chicken,[9] in peas by enzymatic formation from lipids,[10] as the odorous component in *Vaccinium macrocarpon*;[11] additional products in which 2,4-heptadienal has been reportedly identified include soy bean oil,[12-14] fishy butterfat,[15] the oxidized flavor of skim milk,[16] homogenized milk,[17] salmon oil,[18] black-tea aroma (*trans*- and *cis*-form);[19] bilberry aroma (*Vaccinium myrtillus*);[20] frozen peas,[21] sunflower oil,[22] autooxidized lard,[23] salted salmon, sturgeon caviar, and salmon roe;[24] the *trans,trans*-form has been reported found among the volatile flavor components of potato chips[25] and tomato[6]
Reported uses[3]	Candy 1.0 ppm Baked goods 1.0 ppm Condiments 1.0 ppm Meat, meat sauces, soups 1.0 ppm
Regulatory status	FEMA No. 3164

REFERENCES

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

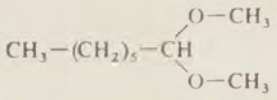
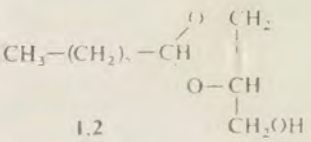
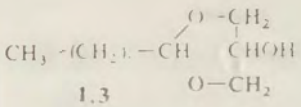
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	γ-Heptalactone	Heptanal
Other names	Heptanolide-(4,1) 4-Hydroxyheptanoic acid, γ-lactone γ-*n*-Propyl-γ-butyrolactone	Aldehyde C-7 Enanthaldehyde *n*-Heptaldehyde *n*-Heptyl aldehyde
Empirical formula	$C_7H_{12}O_2$	$C_7H_{14}O$
Structure		$CH_3-(CH_2)_5-CHO$
Physical/chemical characteristics[5]		
Appearance	Colorless, slightly oil liquid	Colorless liquid
Molecular weight	128.17	114.18
Melting point		43.71°C
Boiling point		152.6 C
Specific gravity		0.8219 at 20 C
Refractive index		1.4133 at 20 C
Solubility	Almost insoluble in water; soluble in alcohol	Insoluble in water; 1:12 in 50% alcohol; 1:4 in 60% alcohol; 1:2 in 70% alcohol; soluble in most organic solvents
Organoleptic characteristics	Sweet, nut-like, caramel odor; malty, caramel, sweet, herbaceous taste	Very strong, fatty, harsh, pungent odor; unpleasant, fatty taste
Synthesis	Obtained in low yields by hydrogenation of ethyl β-furylacrylate;[6] by lactonization of heptenoic acid; also by condensation of methylacrylate butyl alcohol using a catalyst	Obtained by distilling castor oil, preferably under reduced pressure
Natural occurrence	Reported found in *Prunus persica*	Heptanal is a constituent of the essential oils of ylang-ylang, clary sage, California lemon, bitter orange,[7] rose, and hyacinth.
Reported uses[3]	Non-alcoholic beverages 18 ppm Ice cream, ices, etc. 40 ppm Candy 28 ppm Baked goods 26 ppm	Non-alcoholic beverages 4.9 ppm Alcoholic beverages 4.0 ppm Ice cream, ices, etc. 1.2 ppm Candy 2.0 ppm Baked goods 2.6 ppm
Regulatory status	FDA 121.1164; FEMA No. 2539	FDA 121.1164

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

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	Heptanal dimethyl acetal	Heptanal 1,2- and 1,3-glyceryl acetal
Other names	1,1-Dimethoxy heptane	A mixture of acetals in the 1,2 and 1,3 positions: A. 2-Hexyl-4-hydroxymethyl-1,3-dioxolan B. 2-Hexyl-4-hydroxy-1,3-dioxan
Empirical formula	$C_9H_{20}O_2$	$C_{10}H_{20}O_3$
Structure		 1,2  1,3
Physical/chemical characteristics[5]		
Appearance	Oily liquid	Colorless, viscous liquid
Molecular weight	160.26	188.27
Commercial product		Mixture of 1,2 and 1,3 acetals
Boiling point	164–165 C; 59–61 C at 1 mm Hg	
Specific gravity	0.849 at 20 /20 C	
Refractive index	1.4130 at 20 C; 1.4089 at 26 C	
Solubility		Very soluble in water; soluble in alcohol
Organoleptic characteristics	Pleasant odor reminiscent of walnut and cognac	Weak, fungus-like, sweet odor; mushroom (champignon) taste
Synthesis	From heptyl aldehyde and HCl in methanol solution;[6,7] from heptyl aldehyde and methanol in the presence of Twitchell reagent[8]	By condensing heptaldehyde with glycerin
Natural occurrence		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.10–0.13 ppm Ice cream, ices, etc. 0.25 ppm Candy 0.25 ppm Baked goods 0.25 ppm Condiments 1.0 ppm	Non-alcoholic beverages 5.0 ppm Ice cream, ices, etc. 10 ppm Candy 10 ppm Baked goods 10 ppm Condiments 100 ppm
Regulatory status	FDA 121.1164; FEMA No. 2541	FDA 121.1164; FEMA No. 2542

REFERENCES

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

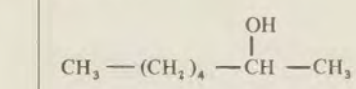
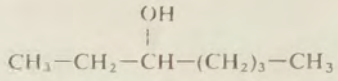
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7. Kirrmann, *Ann. Chim.*, 10(11), 261, 1929.
8. Zaganiaris, *Ber. Dtsch. Chem. Ges.*, 71, 2004, 1938.

	2,3-Heptanedione	Heptanoic acid
Other names	Acetyl pentanoyl Acetyl valeryl Valeryl acetyl	Oenanthic acid Heptoic acid Oenanthylic acid Enanthic acid
Empirical formula	$C_7H_{12}O_2$	$C_7H_{14}O_2$
Structure	$CH_3-C(=O)-C(=O)-(CH_2)_3-CH_3$	$CH_3-(CH_2)_5-COOH$
Physical/chemical characteristics[5]		
Appearance	Yellowish liquid	Colorless oily liquid; tends to solidify in cold weather
Molecular weight	128.17	130.19
Melting point		-7.5°C
Boiling point		223°C 115–116°C at 11 mm Hg
Congealing point		-6.26°C
Specific gravity		0.9214 at 15°C 0.9200 at 20°C
Refractive index		1.4289 at 15°C 1.4216 at 20°C
Solubility	Slightly soluble in water; soluble in alcohol	Slightly soluble in water; soluble in alcohol, ether, acetone, and nitric acid; also soluble in dimethylformamide and dimethyl sulfoxide (DMSO)
Organoleptic characteristics	Powerful, cheesy, pungent odor with a sweet, oily character; sweet, buttery taste	Disagreeable rancid odor; the spectroscopically pure acid exhibits a faint tallow-like odor
Synthesis	From butyl acetoacetate, ethyl butyl ketone, or methyl-*n*-amyl ketone	By oxidation of heptaldehyde with potassium permanganate in diluted sulfuric acid[6]
Natural occurrence	Not reported found in nature	Reported as occurring naturally in calamus, hops, *Acacia dealbata*, and Japanese peppermint and violet leaves; its presence in rancid oils has been observed; also reported found in yellow passion fruit[7]
Reported uses[3]	Non-alcoholic beverages 0.96 ppm Ice cream, ices, etc. 3.1 ppm Candy 8.2 ppm Baked goods 7.9 ppm Chewing gum 1.7 ppm	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 2.0 ppm Candy 6.0 ppm Baked goods 8.0 ppm Gelatins and puddings 6.0 ppm Preserves and spreads 2.0 ppm Margarine 5.0 ppm
Regulatory uses	FDA 121.1164; FEMA No. 2543	FEMA No. 3348

REFERENCES

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

6. **Ruhoff,** in *Organic Syntheses,* Coll. Vol. 2, Blatt, A. H., Ed., Wiley & Sons, New York, 1943, 315.
7. **Winter and Klöt,** *Helv. Chim. Acta,* 55(6), 1916, 1972.

	2-Heptanol	3-Heptanol
Other names	2-Hydroxyheptane *n*-Amyl methyl carbinol *sec*-Heptyl alcohol	Butyl ethyl carbinol Ethyl butyl carbinol
Empirical formula	$C_7H_{16}O$	$C_7H_{16}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless, oily liquid
Molecular weight	116.20	116.20
Boiling point	157–160°C *d*-, 73.5°C at 20 mm Hg *l*-, 74.5°C at 23 mm Hg	157°C at 750 mm Hg
Specific gravity	0.8344 at 0°C; 0.8193 at 20°C *d*-, 0.8190 at 20°C *l*-, 0.8184 at 20°C	
Refractive index	1.4213	
Optical rotation	+11.45 at 20°C (in ethanol) −10.48 at 20°C	
Solubility	Soluble in alcohol, ether, and benzene; slightly soluble in water	Insoluble in water; soluble in alcohol
Organoleptic characteristics	Brassy, herbaceous odor reminiscent of lemon; fruity, green, somewhat bitter taste	Powerful, herbaceous odor; pungent, slightly bitter taste
Synthesis	From amyl magnesium bromide and acetaldehyde;[6] by reduction of amyl methyl ketone with sodium metal in alcohol;[7] by the action of *Penicillium palitans* on peanut oil[8]	By catalytic hydrogenation of ethyl-*n*-butyl ketone
Natural occurrence	Reported found in bud oil[9] and, in small amounts, in rank coconut	In strawberry, mint, and banana
Reported uses[3]	Non-alcoholic beverages 0.5 ppm Ice cream, ices, etc. 0.5 ppm Candy 1.0 ppm Baked goods 15.0 ppm Gelatins and puddings 5.0 ppm Chewing gum 10.0 ppm Dips, spreads 12.0 ppm Salad dressing 80.0 ppm	
Regulatory status	FEMA No. 3288	FDA 121.1164

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

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7. Whitemore and Ottenbacher, *Org. Synth.*, 10, 60, 1930.
8. Stokoe, *Biochem. J.*, 22, 82, 1928.
9. Masson, *Compt. Rend.*, 149, 630, 1909.

	2-Heptanone	3-Heptanone
Other names	Amyl methyl ketone Ketone C-7 Methyl amyl ketone	Butyl ethyl ketone Ethyl butyl ketone Ethyl-*n*-butyl ketone
Empirical formula	$C_7H_{14}O$	$C_7H_{14}O$
Structure	$CH_3-(CH_2)_4-\overset{\overset{O}{\|}}{C}-CH_3$	$CH_3-(CH_2)_3-\overset{\overset{O}{\|}}{C}-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Assay		95% min
Molecular weight	114.18	114.18
Melting point	−26.9°C	
Boiling point	150.6 C; 20 C at 2.6 mm Hg	148.5 C (143–148 C)
Flash point	Approx 49 C	
Specific gravity	0.8166 (0.8243) at 20°C	0.8191 (0.8183) at 20°/20°C
Refractive index	1.4043 at 30 C; 1.4110 at 20 C	1.4115 at 20 C
Acid value		0.034% (as acetic acid)
Solubility	Very slightly soluble in water; soluble in most organic solvents	Insoluble in water; completely miscible in most organic solvents
Organoleptic characteristics	Characteristic banana, slightly spicy odor	Powerful, green, fatty, fruity odor; melon, banana flavor
Synthesis	By oxidation of methyl *n*-amyl carbinol;[6] also from *n*-amyl propionic acid or from ethyl butyl acetate	From *n*-hept-2-one by hydration
Natural occurrence	Reported found in clove essential oil,[7] Ceylon cinnamon,[8] and rancid coconut oil; also identified in *Ruta montana*:[9] meat,[10] and cheese	Reported found in bread
Reported uses[2]	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 6.0 ppm Candy 6.4 ppm Baked goods 13 ppm Condiments 10–25 ppm	Non-alcoholic beverages 0.13–2.0 ppm Ice cream, ices, etc. 0.25–170 ppm Candy 67 ppm Baked goods 0.25–130 ppm
Regulatory status	FDA 121.1164; FEMA No. 2544	FDA 121.1164; FEMA No. 2545

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6. Schorlemmer, *Annalen*, 161, 263, 1872.
7. Schimmel and Co., *Chem. Zentralbl.*, 1, 1059, 1902.
8. Schimmel and Co., *Chem. Zentralbl.*, 2, 1486, 1902.
9. St. Pfau, *Helv. Chim. Acta*, 22, 382, 1939.
10. Anonymous, *Flavour Ind.*, 2, 212, 1971; *Z. Naturforsch. Teil B*, 24, 781, 1969; *J. Agric. Food Chem.*, 19, 772, 1971.

	4-Heptanone	2-Heptenal
Other names	Butyrone Dipropyl ketone	β-Butylacrolein 2-Heptenic aldehyde 4-Propylcrotonaldehyde α,β-Heptenoic aldehyde
Empirical formula	$C_7H_{14}O$	$C_7H_{12}O$
Structure	$CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-CH_2-CH_2-CH_3$	$CH_3-CH_2-CH_2-CH_2-CH=CH-CHO$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless mobile liquid
Molecular weight	114.18	112.17
Boiling point	144°C	165–167°C 80–85°C at 14 mm Hg
Specific gravity	0.8145 at 20°C	0.864 at 17°C
Refractive index	1.4069 at 20°C	1.4314 at 20°C
Solubility	Insoluble in water; soluble in alcohol and ether	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Penetrating odor and burning taste	Pungent green somewhat fatty odor, pleasant only on extreme dilution
Synthesis	By passing butyric acid over wood coal at 425°C and then over cerium oxide at 500°C or over thorium oxide;[6–8] also over manganese oxide at 400–425°C[9,10]	By oxidation of butylallyl alcohol[12,13]
Natural occurrence	Reported found in tobacco smoke[11]	Reported found in soybean oil; a volatile flavor component in potato chips[14]
Reported uses[3]	Non-alcoholic beverages 7.8 ppm Ice cream, ices, etc. 11 ppm Candy 19 ppm Baked goods 27 ppm Gelatins and puddings 0.60–8.0 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. 2546	FEMA No. 3165

REFERENCES

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

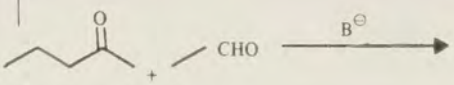
6. Maison Camus Duchemin S. A., German Patent 630,909, 1930.
7. Fischer, *Kraftstoff*, 15, 5, 1939.
8. Fischer, *Chem Zentralbl.*, 2, 4413, 1939.
9. Slobodin, *Zh. Obshch. Khim.*, 8, 250, 1938.
10. Cowan, Jeffery and Vogel, *J. Chem. Soc.*, p. 173, 1940.
11. Neuberg and Burkard, *Biochem. Z.*, 243, 480, 1931.
12. Delaby and Guillot-Allégre, *Compt. Rend.*, 192, 1467, 1931.
13. Martin, Schepartz and Daubert, *J. Am. Chem. Soc.*, 70, 2601, 1948.
14. Deck, Pokorny and Chang, *J. Food Sci.*, 38(2), 345, 1973.

	4-Heptenal (*cis*- and *trans*-)	4-Heptenal diethyl acetal
Other names	4-Hepten-1-al *n*-Propylidene butyraldehyde	1,1-Diethoxy-4-heptene
Empirical formula	$C_7H_{12}O$	$C_{11}H_{22}O_2$
Structure	$CH_3-CH_2-CH=CH-CH_2-CH_2-CHO$	$CH_3-CH_2-CH=CH-CH_2-CH_2-CH(OC_2H_5)(OC_2H_5)$
Physical/chemical characteristics[5]		
Appearance	Colorless oily liquid	Colorless liquid
Molecular weight	112.17	186.30
Boiling point	*trans*-, 112–113°C	
Solubility	Insoluble in water; soluble in alcohol and oils	Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics	Odor reminiscent of heptaldehyde; suggestive of fried fats on dilution; used to impart fried, buttery flavor	Imparts cream or butter-like flavor to food products[10]
Synthesis	From *Hemiptera* bugs (*trans*-form);[7] from penten-1-en-3-ol converted to the corresponding vinyl ether, which undergoes a Claisen rearrangement to 4-heptenal (*trans*-form)[8,9]	
Natural occurrences	Reported found as a constituent in butter fat[6] and in black *Hemiptera* bugs[7]	
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm Meat, meat sauces, soups 1.0 ppm Milk, dairy products 1.0 ppm Cereals 1.0 ppm	Non-alcoholic beverages 1.0 ppm Candy 1.0 ppm Baked goods 1.0 ppm Meat, meat sauces, soups 1.0 ppm Milk, dairy products 1.0 ppm Cereals 1.0 ppm
Regulatory status	FEMA No. 3289	FEMA No. 3349

REFERENCES

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

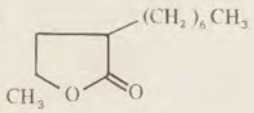
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7. Mukerji and Sharma, *Tetrahedron Lett.*, p. 2479, 1966.
8. Vig, Matta and Ray, *J. Indian Chem. Soc.*, 41, 752, 1964.
9. Burgstahler, *J. Am. Chem. Soc.*, 82, 4681, 1960.
10. Unilever Ltd., British Patent 1,068,712.

	2-Hepten-4-one	3-Hepten-2-one
Other names	Propenyl propyl ketone Ethyl ethylidene acetone 1-Butyryl propylene	1-Acetyl-1-pentene Butylidene acetone Methyl pentenyl ketone
Empirical formula	$C_7H_{12}O$	$C_7H_{12}O$
Structure	$CH_3-CH_2-CH_2-\overset{\overset{O}{\|\|}}{C}-CH=CH-CH_3$	$CH_3-CH_2-CH_2-CH=CH-\overset{\overset{O}{\|\|}}{C}-CH_3$
Physical/chemical characteristics[5]		
Appearance		Colorless oily liquid
Molecular weight	112.17	112.17
Boiling point	156–157°C 80.2°C at 51 mm Hg 74–75°C at 12 mm Hg	162°C *cis*-, 34–39°C at 11 mm Hg *trans*-, 51–52°C at 11 mm Hg
Specific gravity		*cis*-, 0.8840 at 20°C *trans*-, 0.8496 at 20°C
Refractive index	1.4430 at 20°C	*cis*-, 1.4325 at 20°C *trans*-, 1.4436 at 20°C
Solubility		Almost insoluble in water; soluble in alcohol and oils
Organoleptic characteristics		Powerful green-grassy, pungent odor[12]
Synthesis	From 4-heptanone by a catalytic process[6,7]; also 	By reacting 1-pentyne with acetic anhydride to yield 3-heptyn-2-one, which is then converted to *cis*-3-hepten-2-one by partial catalytic hydrogenation;[9] the *trans*-form is probably obtained from *trans*-2-hexenic acid treated with methyl lithium;[10] also 
Natural occurrence	Reported found in roasted filberts[8]	Reported found in roasted filberts[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 2.0 ppm Milk, dairy products 1.0 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 Milk, dairy products 0.7 ppm
Regulatory status	FEMA No. 3399	FEMA No. 3400

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

6. British Patent 1,152,817, assigned to Mobil Oil Corp.; *Chem. Abstr.*, 71, 112504q, 1969.
7. Baltz et al., German Patent 2,050,565; *Chem. Abstr.*, 75, 19800f, 1971.
8. Kinlin et al., *J. Agric. Food Chem.*, 20, 1021, 1972.
9. Theus et al., *Helv. Chim. Acta*, 38, 239, 1955.
10. Theus et al., *Helv. Chim. Acta*, 38, 239, 1955.
11. Kinlin et al., *J. Agric. Food Chem.*, 20, 1021, 1972.
12. Arctander, *Perfume and Flavor Chemicals*, Montclair, N.J., 1969, No. 472.

	3-Heptyl-5-methyl-2(3H)furanone	
Other names	The alternate name published by FEMA as α-*n*-heptyl-γ-valerolactone is incorrect	
Empirical formula	$C_{12}H_{22}O_2$	
Structure		
Physical/chemical characteristics		
Assay	99.0% by VPC	
Molecular weight	198.3	
Reported uses[3]	Baked goods	1.5 ppm
	Meat, meat sauces, soups	1.5 ppm
	Milk, dairy products	1.5 ppm
Regulatory status	FEMA No. 3350	

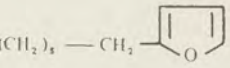
REFERENCES

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

	Heptyl acetate	Heptyl alcohol
Other names		Alcohol C-7 Enanthic alcohol 1-Heptanol Hydroxy heptane
Empirical formula	$C_9H_{18}O_2$	$C_7H_{16}O$
Structure	$CH_3-(CH_2)_5-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_3$	$CH_3-(CH_2)_5-CH_2OH$
Physical/chemical characteristics[2]		
Appearance	Colorless liquid	Colorless liquid
Assay		97% min
Molecular weight	150.18	116.20
Melting point	− 50°C	−34.6°C
Boiling point	46–47°C at 1 mm Hg; 192°C	175°C
Flash point		71°C
Specific gravity	0.87505 at 15°C	0.8219 at 20°C; 0.820–0.824 at 25°C
Refractive index	1.4150 (1.4200) at 20°C	1.42410 (1.4230–1.4270) at 20°C
Solubility	Insoluble in water; soluble in alcohol and ether	Insoluble in water; soluble in most organic solvents; 1:2.3 in 60% alcohol; 1:1 in 70% alcohol
Organoleptic characteristics	Pleasant odor suggestive of pear (rose); sweet, apricot-like taste	Faint, aromatic, fatty odor; pungent, spicy taste
Synthesis	From *n*-heptyl alcohol and acetyl chloride in ether solution in the presence of magnesium dust	By reduction of enanthic aldehyde, which is a distillation product of castor oil
Natural occurrence	Heptyl alcohol has been reported found in the essential oil of *Litsea zeylanica*; the corresponding ester has not yet been identified among the constituents of essential oils	Reported found in a few essential oils: hyacinth, violet leaves, *Litsea zeylanica*
Reported uses[3]	Non-alcoholic beverages 4.1 ppm Ice cream, ices, etc. 3.3 ppm Candy 4.9 ppm Baked goods 4.8 ppm	Non-alcoholic beverages 0.90 ppm Ice cream, ices, etc. 1.0–5.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2547	FDA 121.1164; FEMA No. 2548

REFERENCES

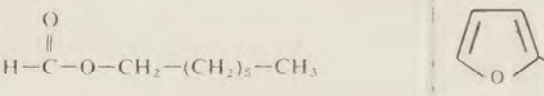
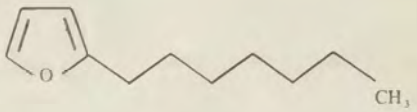
For References 1–5, see end of Part III.

	Heptyl butyrate	*n*-Heptyl cinnamate
Other names	*n*-Heptyl-*n*-butanoate *n*-Heptyl-*n*-butyrate	Heptyl-β-phenylacrylate Heptyl-3-phenyl propenoate
Empirical formula	$C_{11}H_{22}O_2$	$C_{16}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless to pale straw-yellow liquid; tends to polymerize
Molecular weight	186.30	246.36
Melting point	−57/−58 C	
Boiling point	105 C (226 C) at 10–12 mm Hg	
Specific gravity	0.8555 at 30 C	
Refractive index	1.4231 at 20 C	
Solubility	Almost insoluble in water; soluble in alcohol; soluble in propylene glycol	Insoluble in water; soluble in alcohol; almost insoluble in propylene glycol
Organoleptic characteristics	Fruity, camomile-like odor; sweet, green, tea-like taste suggestive of plum	Green, leafy odor with a secondary hyacinth note
Synthesis	From *n*-heptyl alcohol and butyric acid in the presence of HCl[6]	By esterification of *n*-heptanol with cinnamic acid
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 0.66 ppm Ice cream, ices, etc. 0.74 ppm Candy 2.7 ppm Baked goods 2.4 ppm	Non-alcoholic beverages 3.3 ppm Ice cream, ices, etc. 1.0–2.0 ppm Candy 1.0–6.0 ppm Baked goods 1.0 ppm Chewing gum 270 ppm
Regulatory status	FDA 121.1164; FEMA No. 2549	FDA 121.1164; FEMA No. 2551

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

6. Bilterys and Gisseleire, *Bull. Soc. Chim. Belg.*, 44, 569, 1935.

	Heptyl formate	2-Heptylfuran
Other names		1-(2-Furyl)-heptane
Empirical formula	$C_8H_{16}O_2$	$C_{11}H_{18}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Molecular weight	144.21	166.26
Boiling point	76–77 C at 25 mm Hg (176.7–178 C)	
Specific gravity	0.88277 at 15 C; 0.894 at 0 C	
Refractive index	1.4140 at 20 C	
Solubility	1:5 in 70% alcohol; insoluble in water; soluble in ether and most organic solvents	
Organoleptic characteristics	Fruity-floral odor with an orris-rose undertone; sweet taste reminiscent of plum	
Synthesis	From *n*-heptyl bromide and formamide at the boil[6]	
Natural occurrence	Not reported found in nature	Reported found in heated beef[7]
Reported uses[4]	Non-alcoholic beverages 1.7 ppm Ice cream, ices, etc. 0.87 ppm Candy 3.6 ppm Baked goods 3.3 ppm	Non-alcoholic beverages 0.02 ppm Ice cream, ices, etc. 0.02 ppm Baked goods 0.06 ppm Gelatins and puddings 0.05 ppm Chewing gum 0.06 ppm Milk, dairy products 0.02 ppm
Regulatory status	FDA 121.1164; FEMA No. 2552	FEMA No. 3401

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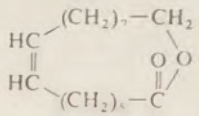
For References 1–5, see end of Part III.

6. **E. I. du Pont de Nemours & Co.**, U.S. Patent 2,375,301, 1942.
7. Volatile Compounds in Food, T.N.O. Report No. 4030, 3rd ed., Centraal Instituut vorr Voedingsonderzoek, Zeist, Netherlands.

	n-Heptyl octanoate	Heptyl isobutyrate
Other names	Heptyl caprylate Heptyl octylate	*n*-Heptyl dimethylacetate *n*-Heptyl isobutanoate *n*-Heptyl-2-methylpropanoate
Empirical formula	$C_{15}H_{30}O_2$	$C_{11}H_{22}O_2$
Structure	$CH_3-(CH_2)_6-\overset{O}{\overset{\|}{C}}-O-(CH_2)_6-CH_3$	$H_3C\diagdown\ \diagup CH-\overset{O}{\overset{\|}{C}}-O-CH_2-(CH_2)_5-CH_3$ $H_3C\diagup$
Physical/chemical characteristics[5]		
Appearance	Colorless, oily liquid	Colorless liquid
Molecular weight	242.41	186.30
Melting point	−10°C	
Boiling point	160°C at 14 mm Hg (291 C)	98 C at 10 mm Hg
Specific gravity	0.8520 at 30°C	0.8625 at 15°/15°C
Refractive index	1.4340 at 20°C	1.4190 at 20°C
Solubility	1:3 in 90%, alcohol; insoluble in water	Insoluble in water; soluble in most organic solvents
Organoleptic characteristics	Oily, green odor and flavor	Characteristic woody odor with distinctly herbaceous, sweet undernotes; sweet, herbaceous, fruity, and slightly warm, floral taste
Synthesis	By direct esterification of *n*-heptanol with *n*-octanoic acid	By esterification of *n*-heptanol with isobutyric acid
Natural occurrence	Not reported found in nature	Reported found in the essential oil of hops[6]
Reported uses[3]	Non-alcoholic beverages 1.0 ppm	Non-alcoholic beverages 1.2 ppm Ice cream, ices, etc. 0.82 ppm Candy 2.6 ppm Baked goods 3.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2553	FDA 121.1164; FEMA No. 2550

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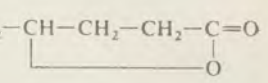
For References 1–5, see end of Part III.
6. **Buttery et al.,** *Nature,* 4933(202), 701, 1964.

	1-Hexadecanol	ω-6-Hexadecenlactone
Other names	Alcohol C-16 Cetyl alcohol	Ambrettolide Cyclohexadecen-7-olide 6-Hexadecenolide 16-Hydroxy-6-hexadecenoic acid, ω-lactone 16-Hydroxy-Δ7-hexadecenoic acid, lactone
Empirical formula	$C_{16}H_{34}O$	$C_{16}H_{28}O_2$
Structure	$CH_3-(CH_2)_{14}-CH_2OH$	
Physical/chemical characteristics[5]		
Appearance	White solid	Colorless liquid
Assay		98% min
Molecular weight	242.45	252.39
Melting point	47°C (49°C)	
Boiling point	344°C	185–190°C at 16 mm Hg
Congealing point	46°C	
Specific gravity	0.8152 at 55°C	0.955–0.957
Refractive index	1.4283 at 78.9°C	1.480–1.481
Solubility	Insoluble in water; soluble in ether; 1 gm in 3 ml of 90% alcohol	1:9 in 80% alcohol; 1:1 in 90% alcohol
Organoleptic characteristics	Odorless	Very strong, musk-like odor
Synthesis	See Reference 7.	Synthetically prepared by Baudart;[6] from bromohexadecenoic acid, dihydroxypalmitic acid, aleuritic acid, or juniperic acid
Natural occurrence	Reported as a major constituent of spermaceti oil, where it is present chiefly as cetyl palmitate	Reported found in ambrette seed oil (*Hibiscus abelmoschus* L.); identified by Kerschbaum (1927) and studied by Stoll and Gardner (1934)
Reported uses[3]	Ice cream, ices, etc. 2.0 ppm Candy 2.0 ppm	Non-alcoholic beverages 0.32 ppm Ice cream, ices, etc. 0.18 ppm Candy 0.16 ppm Baked goods 0.19 ppm Gelatins and puddings 0.007 ppm Chewing gum 0.70 ppm
Regulatory status	FDA 121.1164; FEMA No. 2554	FDA 121.1164; FEMA No. 2555

REFERENCES

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

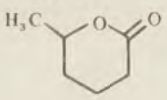
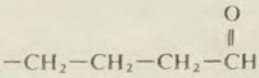
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	trans,trans-2,4-Hexadienol	γ-Hexalactone
Other names	Sorbic aldehyde	γ-Caprolactone Ethyl butyrolactone γ-Ethyl-*n*-butyrolactone Hexanolide-1,4 4-Hydroxy hexanoic acid γ-lactone Tonkalide
Empirical formula	C_6H_8O	$C_6H_{10}O_2$
Structure	$CH_3-CH=CH-CH=CH-CHO$	
Physical/chemical characteristics		
Appearance		Colorless liquid
Molecular weight	96.12	114.15
Melting point		−18°C
Boiling point	173–174°C at 754 mm Hg 76°C at 30 mm Hg 64–66°C at 11 mm Hg	220°C
Congealing point	−17.5 to −16.5°C	
Specific gravity	0.9087 at 22°C	
Refractive index	1.5372 at 22°C	
Solubility		Very slightly soluble in water; soluble in alcohol and propylene glycol
Organoleptic characteristics		Warm, powerful, herbaceous, sweet odor; sweet, coumarin-caramel taste
Synthesis	Can be obtained by slowly heating crotonaldehyde with acetaldehyde in the presence of pyridine at 85–90°C	By reduction of sorbic acid using Zn, Sn, or $SnCl_2$ and concentrated HCl in acetic acid solution at 85°C;[19] from ethylene oxide and sodio-malonic ester; also from propyl alcohol and methylacrylate in the presence of di-*tert*-butyl peroxide
Natural occurrence	In olive,[7] roasted peanuts,[8-11] tomato,[12-14] caviar and fish,[15] autooxidized salmon oil,[16] tea[17,18]	Identified among the volatile components of pineapple[21] and peach var. Red Globe[21,22]
Reported uses[3]	Non-alcoholic beverages 4.0 ppm Alcoholic beverages 1.0 ppm Ice cream, ices, etc. 4.0 ppm Candy 6.0 ppm Gelatins and puddings 4.0 ppm Condiments 4.0 ppm Jellies, preserves, spreads 2.0 ppm	Non-alcoholic beverages 7.0 ppm Ice cream, ices, etc. 0.07–84 ppm Candy 21 ppm Baked goods 21 ppm
Regulatory status	FEMA No. 3429	FDA 121.1164; FEMA No. 2556

REFERENCES

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

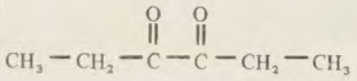
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13. **Buttery et al.**, *J. Agric. Food Chem.*, 19, 524, 1971.
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	Δ-Hexalactone	Hexanal
Other names	5-Hydroxyhexanoic acid, δ-lactone δ-Caprolactone Tetrahydro-6-methyl-2H-pyran-2-one	Aldehyde C-6 *n*-Caproaldehyde Caproic aldehyde Hexoic aldehyde
Empirical formula	$C_6H_{10}O_2$	$C_6H_{12}O$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless oily liquid	Liquid
Assay		96% min
Molecular weight	114.14	100.16
Melting point	31°C	
Boiling point	110–112°C at 15 mm Hg 59–60°C at 0.04 mm Hg	128–128.2 C
Flash point		25 C
Specific gravity	1.0162 at 20°C 1.037 at 21°C	0.8180–0.8210 at 15 C; 0.81392 at 20 C
Refractive index	1.4425 at 20°C 1.4564 at 25°C	1.4035–1.4050 at 20 C
Optical rotation	–47.2° at 24°C (as is) –39.1° (c = 4.1, in anhydrous ethanol)	
Acid value		7 max
Solubility	Soluble in ether	Very slightly soluble in water; soluble in alcohol and ether; 1:1.0–1.5 in 70% alcohol
Organoleptic characteristics		Characteristic fruity odor and taste (on dilution)
Synthesis	By oxidation of 1-substituted cycloalkanes[6]	Prepared from the calcium salt of caproic acid and formic acid[10]
Natural occurrence	Reported found as a volatile flavor component in coconut oil[7] and in heated milk fat;[8] reportedly isolated from high-quality Australian butter oil by degassation under high vacuum[9]	Reported found in some natural aromas of: apple,[11] strawberry,[12] camphor oil,[13] tea extracts,[14] tobacco leaves, *Eucalyptus globulus*, dwarf pine, and bitter orange;[15] also in coffee
Reported uses[3]	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 10.0 ppm Margarine 10.0 ppm Salad oil 10.0 ppm Shortening 10.0 ppm	Non-alcoholic beverages 1.3 ppm Ice cream, ices, etc. 2.8 ppm Candy 3.6 ppm Baked goods 4.2 ppm Gelatins and puddings 2.0–2.5 ppm Chewing gum 3.0 ppm
Regulatory status	FEMA No. 3167	FDA 121.1164; FEMA No. 2557

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	2,3-Hexanedione	3,4-Hexanedione
Other names	Acetyl butyryl Acetyl-*n*-butyryl Methyl propyl diketone	Dipropionyl 3,4-Dioxohexane Diethyl-α,β-diketone
Empirical formula	$C_6H_{10}O_2$	$C_6H_{10}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Yellow, oily liquid	Yellow oil
Molecular weight	114.15	114.04
Melting point		−10°C
Boiling point	128 C	130°C 49°C at 13 mm Hg
Specific gravity	0.93	0.941 at 21°C
Refractive index		1.4130 at 21°C
Solubility	Slightly soluble in water; soluble in propylene glycol, alcohol, and oils	Almost insoluble in water; soluble in alcohol and oils; very soluble in propylene glycol
Organoleptic characteristics	Powerful, creamy, sweet, and buttery odor (less than diacetyl); buttery, cheese taste	Pungent, unpleasant odor reminiscent of butter; taste similar to that of diacetyl
Synthesis	From propionyl aldehyde condensed over ethyl acetylacetate. The resulting product is then oxidized (H_2O_2 and sodium tungstate), hydrolyzed, and finally decarboxylated to 2,3-dexanedione;[7] from methyl butyl ketone or ethyl propyl ketone by way of the monoxime; also from acetoxy mesityl oxide	By condensation of ethyl propionate in the presence of sodium metal, followed by oxidation of the resulting propionin with copper acetate or ferric chloride[6]
Natural occurrence	Reported found in fermented soybean together with diacetyl and acetyl propionyl[8]	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 6.6 ppm Ice cream, ices, etc. 4.8 ppm Candy 7.3 ppm Baked goods 6.6 ppm	Non-alcoholic beverages 10.0 ppm Ice cream, ices, etc. 10.0 ppm Candy 10.0 ppm Gelatins and puddings 10.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2558	FEMA No. 3168

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	Hexanoic acid	3-Hexanol
Other names	*n*-Caproic acid Hexoic acid *n*-Hexylic acid Pentane-1-carboxylic acid	Ethyl propyl carbinol 3-Hydroxyhexane
Empirical formula	$C_6H_{12}O_2$	$C_6H_{14}O$
Structure	$CH_3-CH_2-CH_2-CH_2-CH_2-COOH$	$CH_3-CH_2-CH_2-\underset{\displaystyle OH}{\underset{\vert}{CH}}-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance	Oily, colorless liquid	
Molecular weight	116.16	102.18
Melting point	−3°C	
Boiling point	205.8°C	*l*-, 131–133°C *dl*- and *l*-, 135°C
Congealing point	−3.24°C	
Specific gravity	0.93136 at 15°C	*dl*- and *l*-, 0.8213 at 20°C *dl*-, 0.8182 at 20°C
Refractive index	1.41877 at 15°C; 1.4150 at 20°C	*d*-, 1.4150 at 20°C *l*-, 1.4140 at 22°C *dl*-, 1.4167 at 20°C
Optical rotation		*dl*-, +6.81 at 20° C (in chloroform) *l*-, 7.17 at 18°C
Solubility	Insoluble in water; slightly soluble in alcohol and ether	Slightly soluble in water; soluble in alcohol and acetone; soluble in ether in all proportions
Organoleptic characteristics	Unpleasant odor reminiscent of copra oil; exhibits an acrid taste	
Synthesis	By fractionation of the volatile fatty acids of coconut oil	By hydroboration of *cis*-3-hexene;[6,7] from 3-hexyne;[8] from 1-(and 2-) hexenes[9]
Natural occurrence	A secondary product of butyric fermentation. Reported found in the essential oils of: lavender, camphor, palmarosa, lemongrass, and *Juniperus phoenicea*; in a few fruital aromas: apple, currant, and strawberry.[13] Also identified among the constituents of petitgrain lime oil[14]	Reported found in lavender oil,[10] as a volatile flavor component in pineapple,[11] and in the odorous portion of *Vaccinium macrocarpon*[14]
Reported uses[3]	Non-alcoholic beverages 1.8 ppm Ice cream, ices, etc. 4.3 ppm Candy 28 ppm Baked goods 22 ppm Chewing gum 1.5 ppm Condiments 450 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 1.0 ppm Preserves and spreads 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2559	FEMA No. 3351

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3-Hexanone

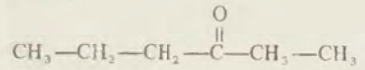
Other names

Ethyl propyl ketone
3-Oxohexane

Empirical formula

$C_6H_{12}O$

Structure



Physical/chemical characteristics[5]

Molecular weight	100.16
Boiling point	118°C at 745 mm Hg 123–124°C
Specific gravity	0.8118 at 20°C
Refractive index	1.4004 at 20°C

Solubility

Slightly soluble in water; soluble in acetone; soluble in alcohol and ether in all proportions

Synthesis

From organo-mercury compounds;[6] by dehydrogenation of 3-hexanol in the presence of Ni-zinc oxide-phosphate catalyst;[7] by hydrogenolysis of 2-ethylfuran;[8] by passing β-furylpropionic acid (or 2-furanpropionic acid) over 5% Pt-C catalyst to 250 to 300°C;[9] by two patented processes[10,11]

Natural occurrence

Reported found in coffee,[12] as a component in the volatile by-product developed during the catalytic hydrogenation of soybean oil using Ni catalysts;[13] in the scent of green-vegetable bug *Nezara viridula*;[14] a volatile flavor component in pineapple[15]

Reported uses[3]

Non-alcoholic beverages	20.0 ppm	Meat, meat sauces, soups	20.0 ppm
Candy	20.0 ppm	Milk, dairy products	20.0 ppm
Baked goods	20.0 ppm	Cereals	20.0 ppm
Gelatins and puddings	20.0 ppm		

Regulatory status

FEMA No. 3290

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	2-Hexenal	4-Hexene-3-one
Other names	α,β-Hexylenaldehyde β-Propyl acrolein	
Empirical formula	$C_6H_{10}O$	$C_6H_{10}O$
Structure	$CH_3-CH_2-CH_2-CH=CH-\overset{\overset{O}{\|}}{C}-H$	$CH_3-CH_2-\overset{\overset{O}{\|}}{C}-CH=CH-CH_3$
Physical/chemical characteristics[5]		
Appearance	Oily liquid	
Molecular weight	98.15	98.14
Boiling point	43°C at 12 mm Hg; 47–48°C at 17 mm Hg	136–137°C 76.2°C at 8.5 mm Hg
Specific gravity	0.8491 at 20°C; 0.8740 at 17.9°C	0.8537 at 20°C
Refractive index	1.4462 at 18°C; 1.44602 at 17.9°C	1.4385 at 20°C
Solubility	Soluble in most organic solvents	
Organoleptic characteristics	Characteristic green, leafy odor	
Synthesis	For the synthesis see reference 8.	By hydration of 4-hexen-2-yne with aqueous H_2SO_4-$HgSO_4$;[6] by hydrogenation of 2-hexen-5-yn-4-one over Pd-$CaCO_3$ catalyst in methanol[7]
Natural occurrence	Reported found in the distillation waters of several plants, such as *Carpinus betulus*;[9] also identified among the constituents of tea (leaves) oil[10] and in citronella[11]	
Reported uses[3]	Non-alcoholic beverages 3.1 ppm Ice cream, ices, etc. 0.70 ppm Candy 15 ppm Baked goods 16 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, pickles 1.0 ppm Meat, meat sauces, soups 1.0 ppm Milk, dairy products 1.0 ppm Cereals 1.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2560	FEMA No. 3352

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	trans-2-Hexenoic acid		3-Hexenoic acid	
Other names	Acrylic, β-propyl acid Hexen-2-oic acid α,β-Hexylenic acid α,β-Hexenoic acid		3-Hexenic acid Hydrosorbic acid β-Amylene-α-carboxylic acid 2-Pentene-1-carboxylic acid Propylidenepropionic acid	
Empirical formula	$C_6H_{10}O_2$		$C_6H_{10}O_2$	
Structure	$CH_3-(CH_2)_2-CH=CH-COOH$		$CH_3-CH_2-CH=CH-CH_2-COOH$	
Physical/chemical characteristics[5]				
Appearance	Colorless needle-like crystals			
Molecular weight	114.15		114.15	
Melting point	37°C		12°C	
Boiling point	217°C 118°C at 19 mm Hg		208°C 118–119°C at 22 mm Hg 103°C at 9–10 mm Hg 81–82°C at 2 mm Hg	
Specific gravity	0.965 at 20°C		0.964 at 23°C	
Refractive index	1.4467 at 40°C		1.4935 at 20°C	
Solubility	Slightly soluble in water; soluble in alcohol, propylene glycol, and oils; very soluble in ether			
Organoleptic characteristics	Pleasant fatty character, long-lasting			
Synthesis	By condensation of butryaldehyde with malonic acid[6]		By condensation of butyraldehyde and malonic acid;[8] also formed during the distillation of ethyl paraconic acid	
Natural occurrence	Reported found in Japanese peppermint oil[7]		The *cis*-form has been reported found in yellow passion fruit[9]	
Reported uses[3]	Non-alcoholic beverages	5.0 ppm	Non-alcoholic beverages	10.0 ppm
	Ice cream, ices, etc.	5.0 ppm	Ice cream, ices, etc.	10.0 ppm
	Candy	5.0 ppm	Candy	10.0 ppm
	Baked goods	5.0 ppm	Baked goods	10.0 ppm
	Gelatins and puddings	5.0 ppm	Gelatins and puddings	10.0 ppm
	Chewing gum	1.0 ppm	Chewing gum	10.0 ppm
	Salad dressings	50.0 ppm	Milk, dairy products	50.0 ppm
Regulatory status	FEMA No. 3169		FEMA No. 3170	

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2-Hexen-1-ol

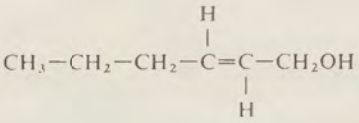
Other names

2-Hexenol
trans-2-Hexenol
α,β-Hexenol
Leaf alcohol
γ-Propyl allyl alcohol

Empirical formula

$C_6H_{12}O$

Structure



Physical/chemical characteristics[5]

Appearance	Colorless liquid
Molecular weight	100.16
Boiling point	61°C (155°C) at 12 mm Hg
Specific gravity	0.85
Refractive index	1.4410 at 20°C

Solubility

Very slightly soluble in water; soluble in alcohol and propylene glycol

Organoleptic characteristics

Powerful, fruity, green, wine-like, leafy odor; sweet, fruity flavor important to strawberry and orange juice

Synthesis

The *cis*-form can be prepared by hydrogenation of *cis*-2-hexenol, using an aqueous suspension of colloidal palladium;[6] from *cis*-4-chloro-2-butenol and magnesium ethyl bromide.[7,8] The commercial product is a mixture of the *cis*- and *trans*-isomers and can be prepared from propyl vinyl carbinol by heating with aluminum oxide.

Natural occurrence

Reported found as a constituent of fresh raspberry aroma;[9] also identified in Valencia orange juice[10] and apple aroma,[11] probably occurring as an ester.

Reported uses[3]

Non-alcoholic beverages	1.0 ppm
Ice cream, ices, etc.	0.63 ppm
Candy	3.8 ppm
Baked goods	4.1 ppm

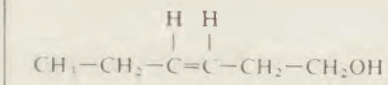
Regulatory status

FDA 121.1164; FEMA No. 2562

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	3-Hexen-1-ol
Other names	Blätter alcohol *cis*-3-Hexenol β,γ-Hexenol *m*-β-Hexenol Leaf alcohol (name also used for *trans*-2-Hexenol)
Empirical formula	$C_6H_{12}O$
Structure	
Physical/chemical characteristics[5]	
Appearance	Colorless, oily liquid
Molecular weight	100.16
Boiling point	156–157 C (55–56 C at 9 mm Hg)
Specific gravity	0.8508 at 15 C
Refractive index	1.4803 at 20 C
Solubility	Soluble in most organic solvents; slightly soluble in water
Organoleptic characteristics	Intense, green odor, not as strong as the corresponding aldehyde; characteristic herbaceous, leafy odor on dilution
Synthesis	Extracted from various essential oils and purified by reacting it to the corresponding phthalate or allophanate.[6] It was synthesized by Ruzička and Schinz,[7] who also clarified its chemical structure.[8] Stoll and Rouve reported on the most significant differences between the natural and the synthetic products.[9]
Natural occurrence	Main constituent of the oil distilled from the infusion of fermented tea leaves;[10] reported found as the corresponding ester of phenylacetic acid in the oil of Japanese mint (*Mentha arvensis*).[11] The volatile oil of *Thea chinensis* contains approximately 26–35% 3-hexen-1-ol, whereas larger amounts are reported in the oils of *Morus bombycis*, *Robinia pseudacacia*, and *Raphanus sativus*. Probably occurring also in several green leaves and herbs. Reported found in the fruit juices of raspberry,[12] grapefruit,[13] and others.
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 3.7 ppm Candy 5.0 ppm Baked goods 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2563

REFERENCES

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

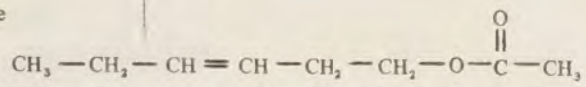
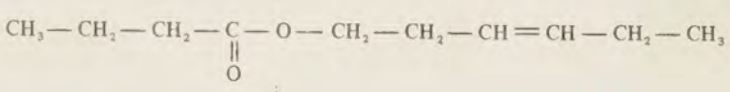
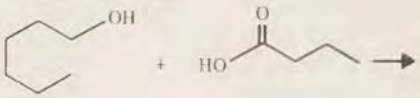
6. Ruzička, *Helv. Chim. Acta*, 27, 1561, 1944.
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9. Stoll and Rouve, *Helv. Chim. Acta*, 21, 1542, 1938; *Ber. Dtsch. Chem. Ges.*, 73, 1358, 1940.
10. Von Romburgh, *Versl. Plantentuin Buitenzorg*, p. 119, 1895.
11. Wahlbaum, *J. Prakt. Chem.*, 2(96), 245, 1917.
12. Bohnsack, *Ber. Dtsch. Chem. Ges.*, p. 75, 1942.
13. Kirchner and Miller, *Chem. Abstr.*, 47, 8924, 1953.

	4-Hexen-1-ol	2-Hexen-1-yl acetate
Other names	2-Hexen-ol-6 4-Hexenyl alcohol	
Empirical formula	$C_6H_{12}O_2$	$C_8H_{14}O_2$
Structure	$CH_3-CH=CH-CH_2-CH_2-CH_2-OH$	$CH_3-(CH_2)_2-CH=CH-CH_2-O-\overset{\overset{O}{\|}}{C}-CH_3$
Physical/chemical characteristics		
Appearance		Liquid
Molecular weight	100.16	142.19
Melting point	69.5°C at 17 mm Hg *cis*-, 158–159°C	
Boiling point	*trans*-, 159–159.4°C	67–68°C at 16 mm Hg
Specific gravity	0.8513 at 20°C	0.898 at 20°C
Refractive index	*cis*-, 1.4420 at 20°C *trans*-, 1.4402 at 20°C	1.42765 at 20°C
Organoleptic characteristics	Pungent oily odor	Pleasant, fruity odor and corresponding taste
Synthesis	By treating *cis*- or *trans*-3-chloro-2-methyltetrahydropyrone with sodium in ether[6,7]	By heating at the boil 1-bromohexen-2-ol with sodium acetate and acetic acid
Natural occurrence	The *cis*- and *trans*-forms occur in banana,[8-10] the *cis*-form in passion fruit;[11] in beans (isomer not specified)[12]	Reported found in *Fragaria vesca* and other fruits; only the *trans*-form is known
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 Vegetables 2.0 ppm	Non-alcoholic beverages 0.28 ppm Ice cream, ices, etc. 0.40 ppm Candy 1.7 ppm Baked goods 1.7 ppm
Regulatory status	FEMA No. 3430	FDA 121.1164; FEMA No. 2564

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9. Wick et al., *J. Agric. Food Chem.*, 17, 751, 1969.
10. Maroni et al., *Riv. Ital. EPPOS*, 55, 168, 1973.
11. Murray et al., *Aust. J. Chem.*, 25, 1921, 1972.
12. Stevens et al., *J. Am. Soc. Hort. Sci.*, 91, 833, 1967.

	cis-3-Hexen-1-yl acetate	*cis*-3-Hexenyl butyrate
Other names	Verdural®	β,γ-Hexenyl-*n*-butyrate *cis*-3-Hexenyl butanoate Leaf butyrate
Empirical formula	$C_8H_{14}O_2$	$C_{10}H_{18}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Colorless liquid
Molecular weight	142.19	170.25
Boiling point	66°C at 16 mm Hg	192°C at 760 mm Hg 103°C at 25 mm Hg
Specific gravity		0.899 at 25°C
Refractive index		1.4318 at 20°C
Solubility		Almost insoluble in water; soluble in alcohol and propylene glycol; miscible with oils
Organoleptic characteristics	Powerful green, floral note reminiscent of banana	Green, fruity, somewhat buttery aroma
Synthesis	By acetylation of the corresponding alcohol[6]	By esterification of *cis*-3-hexenol with *n*-butyric acid under azeotropic conditions[8]; also 
Natural occurrence	Reported found in apple, bilberry, guava, strawberry, and in black and green tea; a flavor componert of yellow passion fruit (*Passiflora edulis* f. *flavicarpa*)[7]	Reported found in passion fruit[9]
Reported uses[3]	Non-alcoholic beverages 0.40 ppm Ice cream, ices, etc. 0.40 ppm Candy 0.50 ppm Baked goods 0.50 ppm	Non-alcoholic beverages 0.5 ppm Ice cream, ices, etc. 5.0 ppm Candy 10.0 ppm Gelatins and puddings 5.0 ppm
Regulatory status	FEMA No. 3171	FEMA No. 3402

REFERENCES

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

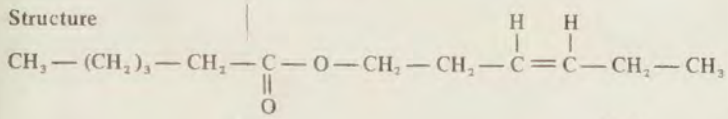
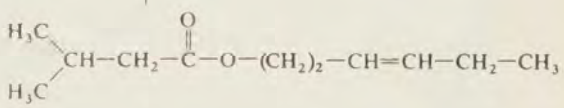
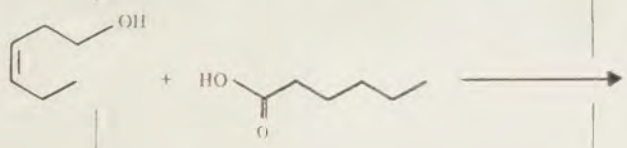
6. Bohnsack, *Chem. Ber.*, 75, 74, 1942.
7. Winter and Klöti, *Helv. Chim. Acta*, 55(6), 1916, 1972.
8. Arctander, *Perfume and Flavor Chemicals*, Montclair, N.J., 1969, No. 1613.
9. Eckert et al., *J. Agric. Food Chem.*, 20, 104, 1972.

	3-Hexenyl formate	*cis*-3-Hexenyl formate[6]
Other names	3-Hexenyl methanoate	
Empirical formula	$C_7H_{12}O_2$	$C_7H_{12}O_2$
Structure	$H_3C-CH_2-CH=CH-CH_2-CH_2-O-CHO$	$H-C(=O)-O-CH_2-CH_2-CH=CH-CH_2-CH_3$
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	
Molecular weight	128.17	128.17
Boiling point	155°C 85°C at 75 mm Hg	
Congealing point	53–55°C at 12 mm Hg	
Specific gravity	0.908 at 25°C/25°C	
Refractive index	1.4270 at 20°C	
Solubility	Almost insoluble in water; soluble in alcohol, propylene glycol, and oils	
Organoleptic characteristics	Green, vegetable-like odor	Light topnate; fruity fresh odor
Synthesis	From *cis*-3-hexenol and formic acid[6]	
Reported uses[3]	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 2.0 ppm Chewing gum 1.0 ppm Preserves and spreads 1.0 ppm	Non-alcoholic beverages 0.15 ppm Ice cream, ices, etc. 0.2 ppm Candy 0.5 ppm Baked goods 0.5 ppm Gelatins and puddings 0.2 ppm Milk, dairy products 0.2 ppm
Regulatory status	FEMA No. 3353	FEMA No. 3431

REFERENCES

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

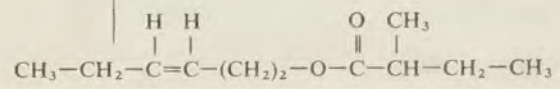
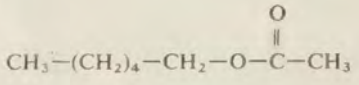
6. Bohnsack, *Chem. Ber.*, 75, 74, 1942.

	cis-3-Hexenyl hexanoate	*cis*-3-Hexenyl isovalerate
Other names	β,γ-Hexenyl hexoate *cis*-3-Hexenyl caproate Leaf caproate	β,γ-Hexenyl isopentanoate
Empirical formula	$C_{12}H_{22}O_2$	$C_{11}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	198.31	184.28
Boiling point		199°C
Specific gravity		0.89
Refractive index		
Solubility	Almost insoluble in water; soluble in alcohol, propylene glycol, and oils	Insoluble in water; soluble in alcohol and propylene glycol
Organoleptic characteristics	Powerful, diffusive fruity-green odor[9]; reminiscent of pear	Powerful, sweet, green odor of apple; buttery, apple-like taste
Synthesis	By azeotropic esterification of *cis*-3-hexanol with *n*-hexanoic acid; also	By esterification of *cis*-3-hexenol with isovaleric acid
		
Natural occurrence	Reported found among the high-boiling components in green tea;[6] also as a component in the volatile fraction of tabasco pepper (*Capsicum frutescens*);[7] in passion fruit, strawberry, and tea[8]	In mint; in tobasco pepper
Reported uses[2]	Non-alcoholic beverages 0.5 ppm Ice cream, ices, etc. 2.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm Gelatins and puddings 2.0 ppm Preserves and spreads 2.0 ppm	
Regulatory status	FEMA No. 3403	FDA 121.1164

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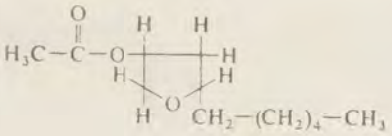
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9. **Arctander,** *Perfume and Flavor Chemicals*, Montclair, N.J., 1969, No. 1616.

	cis-3-Hexenyl-2-methylbutyrate	Hexyl acetate
Other names	*cis*-3-Hexenyl-α-methylbutyrate	
Empirical formula	$C_{11}H_{20}O_2$	$C_8H_{16}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Oily, colorless liquid
Molecular weight	184.28	144.21
Melting point		−81°C
Boiling point		171–172°C; 61–62°C at 12 mm Hg
Specific gravity		0.8718 at 20°C
Refractive index		1.4092 (1.4120) at 20°C
Solubility	Insoluble in water; soluble in alcohol	Insoluble in water; soluble in alcohol and ether
Organoleptic characteristics	Strong, warm, fruity odor of apple and pineapple; sweet, apple-like taste	Pleasant fruity odor and bittersweet taste suggestive of pear
Synthesis	From *cis*-3-hexenol via esterification with α-methylbutyric acid	From *n*-hexyl alcohol and excess acetic anhydride at the boil or with an excess of acetic acid in the presence of concentrated sulfuric acid
Natural occurrence	In mint	Reported found in fruital aromas (e.g., *Fragaria vesca*) and essential oils
Reported uses[3]		Non-alcoholic beverages 4.6 ppm Ice cream, ices, etc. 4.6 ppm Candy 26 ppm Baked goods 26 ppm Chewing gum 3.0 ppm
Regulatory status	FDA 121.1164	FDA 121.1164; FEMA No. 2565

REFERENCES

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

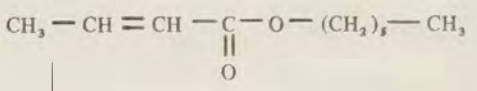
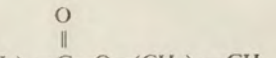
	2-Hexyl-4-acetoxytetrahydrofuran*	Hexyl alcohol
Other names	2-Hexyl-tetrahydrofuran-4-yl acetate	Alcohol C-6 1-Hexanol
Empirical formula	$C_{12}H_{22}O_3$	$C_6H_{14}O$
Structure		$CH_3-(CH_2)_4-CH_2OH$
Physical/chemical characteristics[4]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	214.31	102.17
Melting point		−51.6°C
Boiling point		157.2–157.8°C
Specific gravity		0.8186 at 20°C
Refractive index		1.4179 at 20°C
Solubility	Slightly soluble in water; soluble in alcohol	Rather soluble in water; soluble in most organic solvents
Organoleptic characteristics	Sweet, floral-fruity odor; sweet, powerful, fruity (peach-apricot) taste	Fruity odor and aromatic flavor
Synthesis		By reduction of *n*-caproic acid. The *n*-hexyl alcohol represents one of the 14 possible isomers of this alcohol.
Natural occurrence	Not reported found in nature	Reported found among the constituents of several essential oils and aromas: apple, strawberry, tea, violet (leaves and flowers), Java citronella, Bourbon geranium, lavender, lavandin, spike,[7] *Litsea zeylanica:*[8] also identified in bitter orange[9]
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm	Non-alcoholic beverages 6.6 ppm Ice cream, ices, etc. 26 ppm Candy 21 ppm Baked goods 18 ppm Gelatins and puddings 0.22–0.28 ppm
Regulatory status	FDA 121.1164; FEMA No. 2566	FDA 121.1164; FEMA No. 2567

* 2-Hexyl-4-acetoxytetrahydrofuran has been found not to have the identity indicated by this name, but instead to contain several non-isomeric components. In view of this and shifting considerations of technological value, it is being dropped from the GRAS list.[6]

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

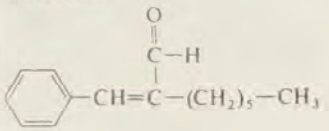
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7. **Girard,** *Chem. Abstr.*, 44, 4635, 1950.
8. **Sharma et al.,** *Chem. Abstr.*, 47, 11667, 1953.
9. **Mehlitz and Minas,** *Ind. Obst Gemueseverwert.*, 50, 861, 1965.

	n-Hexyl-2-butenoate	Hexyl butyrate
Other names	Hexyl crotonate	
Empirical formula	$C_{10}H_{20}O_2$	$C_{10}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance		Liquid
Molecular weight	172.27	172.27
Melting point		−78°C
Boiling point		208°C
Specific gravity		0.8567 at 30°C
Organoleptic characteristics		Characteristic fruity (apricot) odor and sweet taste suggestive of pineapple
Synthesis		From butyric acid and *n*-hexyl alcohol in the presence of HCl[6]
Natural occurrence	Reported as occurring naturally in banana, passion fruit, wine, cocoa, coffee and soybean	Reported found in the essential oils of lavender and lavandin[7] and in the oil from fruits of *Heracleum giganteum*[8]
Reported uses[3]	Non-alcoholic beverages 8.0 ppm Ice cream, ices, etc. 8.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 8.0 ppm Preserves 8.0 ppm	Non-alcoholic beverages 2.6 ppm Ice cream, ices, etc. 2.1 ppm Candy 7.8 ppm Baked goods 8.6 ppm
Regulatory status	FEMA No. 3354	FDA 121.1164; FEMA No. 2568

REFERENCES

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

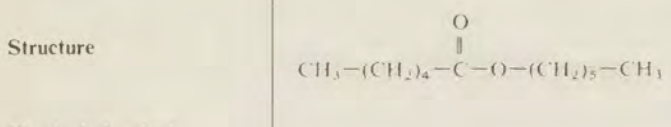
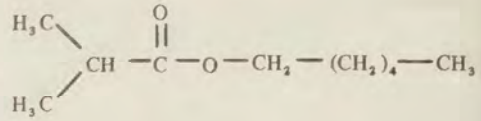
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7. Peyron and Benezet, *C. R. Séances Acad. Sci. Paris*, 262, 1105, 1966.
8. Franchimont and Zincke, *Ann. Chem.*, 163, 198, 1872.

	α-Hexyl cinnamaldehyde	Hexyl formate
Other names	2-Benzylidene-octanal α-*n*-Hexyl cinnamic aldehyde α-*n*-Hexyl-β-phenyl acrolein	
Empirical formula	$C_{15}H_{20}O$	$C_7H_{14}O_2$
Structure		$H-C(=O)-O-CH_2-(CH_2)_4-CH_3$
Physical/chemical characteristics[5]		
Appearance	Pale-yellow liquid	Colorless liquid
Assay	95% min[2]	
Molecular weight	216.33	130.18
Melting point	4 C	
Boiling point	174–176 C at 15 mm Hg	176.7 C
Specific gravity	0.953–0.959 at 25/25 C;[2] (0.95 at 24 C)	0.8789 at 20°C; (0.898 at 0°C)
Refractive index	1.5480–1.5520 at 20 C;[2] (1.5268 at 25 C)	1.4071 at 20 C
Acid value	Not more than 5.0[2]	
Solubility	1:1 and more in 90% alcohol[2]	Very slightly soluble in water; miscible with alcohol and ether
Organoleptic characteristics	Jasmine-like odor, particularly on dilution	Fruity, apple-like or unripe-plum odor; corresponding sweet taste
Synthesis	By condensation of octylaldehyde with benzaldehyde	By prolonged boiling of *n*-hexyl alcohol and formic acid,[6] or by azeotropic distillation of the alcohol and isopropyl formate[7]
Natural occurrence	Not reported found in nature	In peach, grape, and apple
Reported uses[3]	Non-alcoholic beverages 0.80 ppm Ice cream, ices, etc. 2.6 ppm Candy 6.5 ppm Baked goods 2.4 ppm Gelatins and puddings 0.05 ppm	Non-alcoholic beverages 12 ppm Ice cream, ices, etc. 45 ppm Candy 39 ppm Baked goods 52 ppm
Regulatory status	FDA 121.1164; FEMA No. 2569	FDA 121.1164; FEMA No. 2570

REFERENCES

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

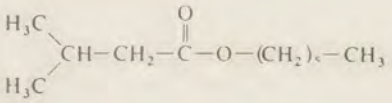
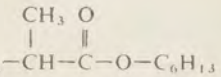
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7. **Cousort,** Electrochemical Industries, German Patent 721,300, 1939.

	Hexyl hexanoate	Hexyl isobutyrate
Other names	Hexyl caproate Hexyl capronate Hexyl hexylate	
Empirical formula	$C_{12}H_{24}O_2$	$C_{10}H_{20}O_2$
Structure		
Physical/chemical characteristics[4]		
Appearance	Oily liquid	Colorless liquid
Assay	97% min	
Molecular weight	200.32	172.27
Melting point	−55 C	
Boiling point	245 C; 84–86 C at 3 mm Hg	199°C
Flash point	68 C	
Specific gravity	0.8541 at 30 C; 0.8750–0.8780 at 15 C	0.87
Refractive index	1.4070–1.4090 at 20 C; 1.4140 at 20 C	
Acid value	0.2 max	
Solubility	1:2–2.5 in 70% alcohol	Almost insoluble in water; soluble in alcohol and propylene glycol; miscible with oils
Organoleptic characteristics	Herbaceous odor	Powerful, somewhat harsh fruity aroma
Synthesis	By passing *n*-hexyl alcohol over CuO · UO_3 catalyst at 220–310 C,[6] or by treating *n*-hexyl alcohol with $Ca(BrO_3)_2$ and diluted aqueous HBr at 30 C[7,8]	By direct esterification of *n*-hexanol with isobutyric acid
Natural occurrence	Reported found in several natural products	Reported found in lavender oil,[9] in hops oil[10–12] and in sherry[13]
Reported uses[3]	Non-alcoholic beverages 2.5–3.0 ppm Ice cream, ices, etc. 2.5 ppm Candy 3.6–10 ppm Baked goods 10 ppm	Non-alcoholic beverages 20.0 ppm Ice cream, ices, etc. 20.0 ppm Candy 20.0 ppm Gelatins and puddings 20.0 ppm Chewing gum 20.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2572	FEMA No. 3172

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11. Buttery, McFadden and Black, *Brew. Chem. Proc.*, p. 137, 1964.
12. Buttery, Black, Kealy and McFadden, *Nature*, 202(4933), 701, 1964.
13. Webb, Kepner and Galetto, *Am. J. Enol. Vitic.*, 15(1), 1, 1964.

	Hexyl isovalerate	Hexyl 2-methylbutyrate
Other names	*n*-Hexyl isopentanoate	2-Methylbutanoic acid, *n*-hexylester
Empirical formula	$C_{11}H_{22}O_2$	$C_{11}H_{22}O_2$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless liquid	Colorless liquid
Molecular weight	186.30	186.30
Boiling point	215 C	
Specific gravity	0.87	
Solubility	Insoluble in water; soluble in alcohol	Almost insoluble in water; soluble in alcohol
Organoleptic characteristics	Odor suggestive of unripe fruit; mainly employed in perfumery (earthy and tobacco notes)	Strong, green, fruity odor; sweet, fruity taste reminiscent of unripe strawberry
Synthesis	By esterification of *n*-hexanol with isovaleric acid	By esterification of *n*-hexanol with 2-methylbutanoic acid
Regulatory status	FDA 121.1164	FDA 121.1164

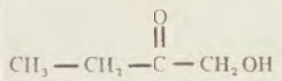
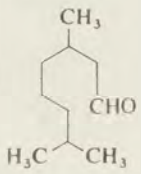
REFERENCES

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

	Hexyl octanoate	Hexyl propionate
Other names	Hexyl caprylate *n*-Hexyl-*n*-octanoate *n*-Hexyl-*n*-octoate *n*-Hexyl octylate	*n*-Hexyl propanoate
Empirical formula	$C_{14}H_{28}O_2$	$C_9H_{18}O_2$
Structure	$CH_3-(CH_2)_6-\overset{\overset{O}{\|}}{C}-O-(CH_2)_5-CH_3$	$CH_3-CH_2-\overset{\overset{O}{\|}}{C}-O-(CH_2)_5-CH_3$
Physical/chemical characteristics[5]		
Appearance	Liquid	Liquid
Molecular weight	228.37	158.24
Boiling point		180 C
Melting point	−31°C	
Specific gravity	277 C (260 C)	0.880 at 15.5 C
Refractive index	0.8527 (0.87) at 30°C	1.4105 at 20 C
Solubility	Insoluble in water; soluble in alcohol	Almost insoluble in water; soluble in alcohol and propylene glycol
Organoleptic characteristics	Fresh vegetable and slightly fruity odor; sweet, green, fruity taste	Earthy, acrid odor suggestive of rotting fruits; sweet, metallic-fruity taste
Synthesis	By esterification of *n*-hexanol with caproic acid	By esterification of *n*-hexanol with propionic acid
Natural occurrence	Reported found in several natural products (apple, strawberry, and banana)	Reported found in hops and apple
Reported uses[3]	Non-alcoholic beverages 1.0 ppm Gelatins and puddings 0.70 ppm	Non-alcoholic beverages 5.7 ppm Ice cream, ices, etc. 23 ppm Candy 21 ppm Baked goods 22 ppm
Regulatory status	FDA 121.1164; FEMA No. 2575	FDA 121.1164; FEMA No. 2576

REFERENCES

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

	1-Hydroxy-2-butanone	Hydroxycitronellal
Other names	2-Oxo-1-butanol Propionyl carbinol Ethyl hydroxymethyl ketone 1-Butanol-2-one	3,7-Dimethyl-7-hydroxy octanal 7-Hydroxy-3,7-dimethyl octan-1-al Laurine
Empirical formula	$C_4H_8O_2$	$C_{10}H_{20}O_2$
Structure		
Physical/chemical characteristics[5]		The physical constants for commercial products vary, depending on the source and the method of preparation.
Appearance	Colorless liquid	Colorless, viscous liquid
Assay		95% min[2] (97%) (94–96%)
Molecular weight	88.02	172.27
Boiling point	152–154°C	94–96°C at 1 mm Hg
Flash point	1.0186 at 20°C	132°C
Specific gravity	1.4200 at 20°C	0.917–0.921 at 25/25°C;[2] 0.920; 0.925–0.930 at 15°C
Refractive index		1.4470–1.4500 at 20°C;[2] 1.449; 1.448–1.450
Acid value		Not more than 5.0[2]
Optical rotation		+9 to +10.5 (Java citronella type) +0.5 to −0.5 (*Eucalyptus citriodora* type)
Solubility	Miscible with water, alcohol, and ether	1:1 and more in 50% alcohol;[2] slightly soluble in water and glycerol; soluble in essential oils
Organoleptic characteristics		Intense, sweet, floral, lily-type odor
Synthesis	From 1-chlorobutan-2-one by hydrolysis or by heating the chloro compound with potassium formate in methanol;[6] the ethyl ester may be prepared by bacterial oxidation of the corresponding glycol with *Aspergilus niger*[7]	By hydration of natural citronellal obtained from Java citronella or from *Eucalyptus citriodora*. β-Pinene is converted to myrcene, which on hydration may yield either linalool or a mixture of geraniol and nerol. The latter mixture can be hydrogenated to citronellol and subsequently converted to citronellal and hydroxycitronellal.[8] Also by hydrogenation of 3,7-dimethyl-7-hydroxy-2-octen-2-al over palladium carbon in ethyl acetate solution[9]
Natural occurrence		Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 80.0 ppm Ice cream, ices, etc. 80.0 ppm Candy 80.0 ppm Gelatins and puddings 80.0 ppm	Non-alcoholic beverages 3.5 ppm Ice cream, ices, etc. 13 ppm Candy 9.4 ppm Baked goods 10 ppm Gelatins and puddings 0.30 ppm Chewing gum 16 ppm
Regulatory status	FEMA No. 3173	FDA 121.1164; FEMA No. 2583

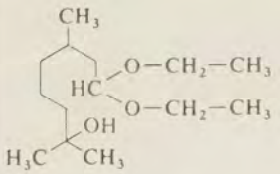
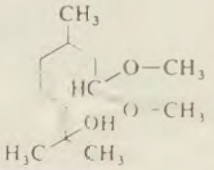
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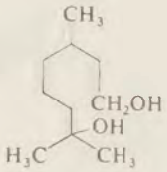
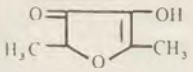
For further information on hydroxycitronellal see the following:

Webb (Glidden Co.), U.S. Patent 3,028,431, 1962; *Chem. Abstr.*, 61, 14727b, 1964.

	Hydroxycitronellal diethyl acetal	Hydroxycitronellal dimethyl acetal
Other names	8,8-Diethoxy-2,6-dimethyl-octanol-2	8,8-Dimethoxy-2,6-dimethyl-octanol-2
Empirical formula	$C_{14}H_{30}O_3$	$C_{12}H_{26}O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, slightly oily liquid	Colorless liquid
Assay		95% min[2]
Molecular weight	246.39	218.34
Boiling point	Approx 260°C	
Flash point		>100°C
Specific gravity		0.925–0.930 at 25/25°C[2]
Refractive index		1.4410–1.4440 at 20°C[2]
Acid value		Not more than 1[2]
Free aldehyde		Not more than 3% (as hydroxycitronellal)[2]
Solubility	Almost insoluble in water; soluble in alcohol	1:2 in 50% alcohol[2]
Organoleptic characteristics	Delicate, green-floral taste with almost no odor	Light, green, flowery odor similar to hydroxycitronellal
Synthesis	By condensation of hydroxycitronellal with ethanol using dry HCl	Usually prepared from hydroxycitronellal and methyl alcohol in the presence of a catalyst
Natural occurrence	Not reported found in nature	Not reported found in nature
Reported uses[3]	Non-alcoholic beverages 2.7 ppm Ice cream, ices, etc. 0.50–1.0 ppm Candy 7.3 ppm Baked goods 2.2 ppm	Non-alcoholic beverages 10 ppm Ice cream, ices, etc. 0.50 ppm Candy 24 ppm Baked goods 0.50–20 ppm
Regulatory status	FDA 121.1164; FEMA No. 2584	FDA 121.1164; FEMA No. 2585

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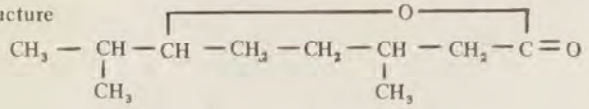
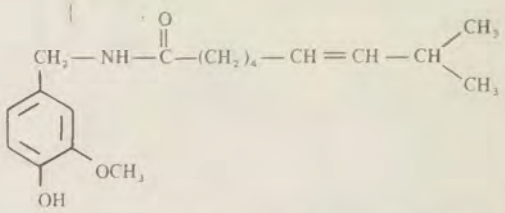
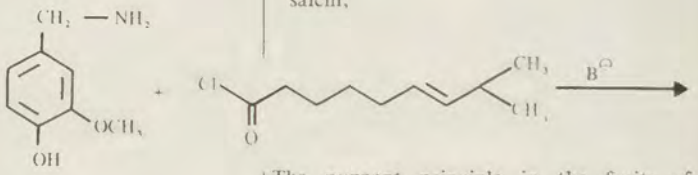
For References 1–5, see end of Part III.

	Hydroxycitronellol	4-Hydroxy-2,5-dimethyl-3(2H)-furanone
Other names	3,7-Dimethyloctane-1,7-diol 3,7-Dimethyl-1,7-octanediol	2,5-Dimethyl-4-hydroxy-2,3-dihydrofuran-3-one
Empirical formula	$C_{10}H_{22}O_2$	$C_6H_8O_3$
Structure		
Physical/chemical characteristics[5]		
Appearance	Colorless, viscous oil	Colorless or white solid
Molecular weight	174.29	128
Boiling point	156 C at 15 mm Hg; 124–125°C at 1 mm Hg	
Melting point		70°C (75–78°C)
Flash point	100 C	
Specific gravity	0.922–0.930 at 25/25 C; 0.935 at 20 C	
Refractive index	1.4550–1.4600 (1.4610) at 20 C	
Optical rotation	−1.9′ at 20 C	
Aldehyde content	Not more than 10% (as hydroxycitronellal)	
Solubility	Slightly soluble in toluene and benzene; 1:1 in 60% alcohol	Slightly soluble in water; soluble in alcohol and oils
Organoleptic characteristics	Odor reminiscent of rose and grape hyacinth	Fruity caramel or "burnt pineapple" aroma
Synthesis	By hydrogenation (under pressure in presence of Raney Ni) of 3,7-dimethyl-7-hydroxy-octan-1-al;[6] also in good yields by catalytic hydrogenation (using Raney Ni) of 1,2-epoxy-3,7-dimethyl-octan-7-ol[7]	From dimethyl-3,4-dihydroxyfuran-2,5-dicarboxylate[8]
Natural occurrence	Not reported found in nature	Reported as a constituent of pineapple aroma
Reported uses[3]	Non-alcoholic beverages 2.0 ppm Ice cream, ices, etc. 1.6 ppm Candy 3.6 ppm Baked goods 3.5 ppm Gelatins and puddings 0.30 ppm Chewing gum 0.30 ppm	Ice cream, ices, etc. 5.0 ppm Candy 10.0 ppm Baked goods 10.0 ppm Gelatins and puddings 5.0 ppm
Regulatory status	FDA 121.1164; FEMA No. 2586	FEMA No. 3174

REFERENCES

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

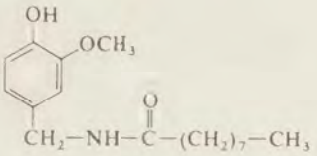
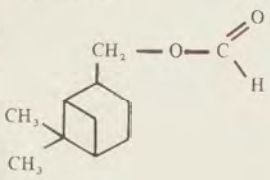
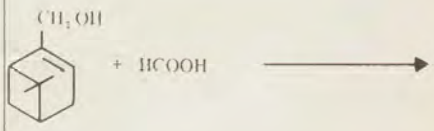
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8. **Henry and Silverstein,** *J. Org. Chem.*, 31, 2391, 1966.

	6-Hydroxy-3,7-dimethyl octanoic acid, lactone	N-(4-Hydroxy-3-methoxybenzyl)-8-methyl-6-nonenamide
Other names	6-Hydroxy-3,7-dimethyl caprylic acid, lactone 4-Methyl-7-isopropyl-2-oxoepanone	Capsaicin Isodecenoic acid, vanillylamide *trans*-8-Methyl-N-vanillyl-6-nonenamide 7-Methyloct-5-ene-1-carboxylic acid, vanillylamide
Empirical formula	$C_{10}H_{18}O_2$	$C_{18}H_{27}NO_3$
Structure		
Physical/chemical characteristics[5]		
Appearance		Monoclinic rectangular scales or platelets (from petroleum ether)
Molecular weight	170.24	305.42
Melting point		65°C
Boiling point		210–220°C at 0.01 mm Hg
Solubility		Insoluble in water at room temperature; slightly soluble in warm water and carbon disulfide; soluble in alcohol, ether, benzene, and chloroform
Organoleptic characteristics		Mild, warm-herbaceous odor; burning pungent taste (10 ppm);[12] used in compounded flavors for sauces where the pungent note is desired
Synthesis		From 3-chloro-2-isopropyltetrahydropyran;[6] biosynthesis from *Capsicum frutescens*;[8,9] separation from *cis*-capsaicin, pelargonic acid vanilamide, and dihydrocapsaicin,[10] reaction of capsaicin;[11]
		
Natural occurrence		The pungent principle in the fruits of various *Capsicum* species (Solanaceae)[7]
Reported uses[3]	Non-alcoholic beverages 300.0 ppm Ice cream, ices, etc. 200.0 ppm Candy 200.0 ppm Baked goods 500.0 ppm Gelatins and puddings 500.0 ppm Syrups 1,000.0 ppm	Gelatins and puddings 7.0 ppm Meat, meat sauces, soups 5.0 ppm
Regulatory status	FEMA No. 3355	FEMA No. 3404

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	n-(4-Hydroxy-3-methoxybenzyl)-nonanamide	2-Hydroxymethyl-6,6-dimethyl bicyclo[3,1,1]hept-2-enyl formate
Other names	*n*-Nonanoyl-4-hydroxy-3-methoxybenzyl-amide Nonanoyl vanillylamide Pelargonyl vanillylamide	Myrtenyl formate
Empirical formula	$C_{17}H_{27}NO_3$	$C_{11}H_{16}O_2$
Structure		
Physical/chemical characteristics		
Appearance	White powder (colorless crystal)	
Molecular weight	293.41	180.24
Solubility	Slightly soluble in water; soluble in alcohol	
Organoleptic characteristics	Odorless; pungent, burning taste	
Synthesis	From nonanyl chloride and vanillylamine	
Natural occurrence	Not reported found in nature	
Reported uses[3]		Non-alcoholic beverages 3.0 ppm Ice cream, ices, etc. 3.0 ppm Candy 3.0 ppm Baked goods 3.0 ppm Gelatins and puddings 3.0 ppm Condiments, pickles 3.0 ppm Preserves and spreads 3.0 ppm
Regulatory status	FDA 121.1164	FEMA No. 3405

REFERENCES

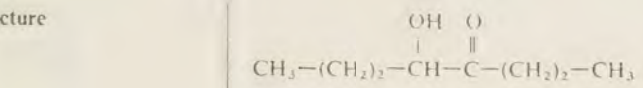
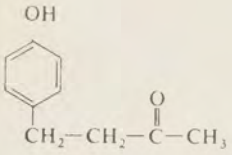
For References 1–5, see end of Part III.

	3-(Hydroxymethyl)-2-octanone		Hydroxynonanoic acid, Δ-lactone	
Other names			δ-Nonalactone α,n-Butyl-δ-valerolactone δ-Hydroxypelargonic acid, lactone 6-Butyltetrahydro-2H-pyran-2-one	
Empirical formula	$C_9H_{18}O_2$		$C_{19}H_{16}O_2$	
Structure	$CH_3-(CH_2)_4-\underset{\displaystyle CH_2OH}{\underset{\vert}{CH}}-CO-CH_3$			
Physical/chemical characteristics[5]				
Appearance	Colorless oily liquid		Colorless, very viscous liquid	
Molecular weight	158.24		156.23	
Boiling point			137.0–137.5°C at 11 mm Hg	
Congealing point			73°C at 0.095 mm Hg	
Specific gravity			0.9871 at 20°C	
Refractive index			1.4562 at 20°C	
Solubility	Almost insoluble in water; soluble in alcohol and oils		Almost insoluble in water; soluble in alcohol and oils	
Organoleptic characteristics	Musty-herbaceous, sweet, slightly earthy odor		Mild, nut-like odor; fatty, milk-creamy taste	
Synthesis	By condensation of methyl hexyl ketone with formaldehyde, followed by hydrogenation		By microbiological reduction of the corresponding keto acids;[6,7] by a patented process[8]	
Natural occurrence			Reported as responsible for the off-flavor in milk-fat[9]	
Reported uses[3]	Non-alcoholic beverages	0.3 ppm	Non-alcoholic beverages	2.0 ppm
	Ice cream, ices, etc.	0.3 ppm	Ice cream, ices, etc.	2.0 ppm
	Candy	5.0 ppm	Candy	4.0 ppm
	Baked goods	10.0 ppm	Baked goods	4.0 ppm
	Condiments, pickles	10.0 ppm	Gelatins and puddings	2.0 ppm
			Margarine	2.0 ppm
			Preserves	2.0 ppm
Regulatory status	FEMA No. 3292		FEMA No. 3356	

REFERENCES

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

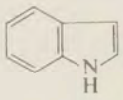
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8. Rosenmund and Bach, U.S. Patent 3,048,599, 1962.
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	5-Hydroxy-4-octanone	4-(*p*-Hydroxyphenyl)-2-butanone
Other names	Butyroin 5-Octanol-4-one	*p*-Hydroxybenzyl acetone
Empirical formula	$C_8H_{16}O_2$	$C_{10}H_{12}O_2$
Structure		
Physical chemical characteristics[5]		
Appearance	Yellowish liquid	Crystalline solid
Molecular weight	144.21	164.21
Melting point		82–83 C (84–85 C)
Boiling point	80–82 C (182 C) at 10 mm Hg	
Specific gravity	0.9231 (0.91) at 20 C	
Refractive index	1.4290 at 20 C	
Solubility	Almost insoluble in water; soluble in alcohol	Soluble in alcohol and ether; insoluble in ligroin at room temperature
Organoleptic characteristics	Sweet, slightly pungent, buttery, nut-like odor; sweet, buttery, oily taste	
Synthesis	By reacting sodium metal with ethyl butyrate in boiling ether[6,7] or in the same fashion starting from methyl butyrate[8]	By catalytic hydrogenation of *p*-hydroxybenzylidene acetone in the presence of platinum black in ether or methanol[9] or in the presence of palladium absorbed on charcoal[10]
Natural occurrence	Not reported found in nature	Reported found in raspberry aroma[11]
Reported uses[3]	Non-alcoholic beverages 0.50–5.0 ppm Ice cream, ices, etc. 1.0–20 ppm Candy 10 ppm Baked goods 7.8 ppm	Non-alcoholic beverages 16 ppm Ice cream, ices, etc. 34 ppm Candy 44 ppm Baked goods 54 ppm Gelatins and puddings 5.0–50 ppm Chewing gum 40–320 ppm
Regulatory status	FDA 121.1164; FEMA No. 2587	FDA 121.1164; FEMA No. 2588

REFERENCES

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

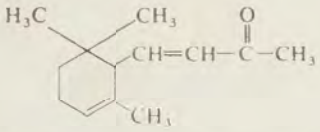
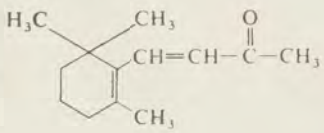
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11. Ruys, *Fr. Ses Parfums*, 9, 34, 1966.

	Indole
Other names	1-Benzazole 2,3-Benzopyrrole
Empirical formula	C_8H_7N
Structure	
Physical/chemical characteristics[5]	
Appearance	White, low-melting, crystalline solid
Molecular weight	117.14
Melting point	52 C
Boiling point	253–254 C; 123 C at 5 mm Hg
Congealing point	51 C (after being dried over sulfuric acid)[2]
Solubility	Readily soluble in most organic solvents; 1 gm in 2 ml of 70% alcohol[2]
Organoleptic characteristics	Almost floral odor when highly purified; otherwise exhibits characteristic odor of feces. Not very stable on exposure to light (turns red)
Synthesis	Obtained from the 220–260 C boiling fraction of coal tar[6] or by heating sodium phenylglycine-*o*-carboxylate with NaOH, saturating the aqueous solution of the melt with CO_2, and finally reducing with sodium amalgam;[7,8] can be prepared also by the reduction of indoxyl, indoxyl carboxylic acid, or indigo[2]
Natural occurrence	Reported occurring in several natural products as a complex compound that decomposes during enfleurage or steam distillation yielding free indole.[9,10] Reported found in the essential oil from flower of *Jasminum grandiflorum*,[11] in neroli oil,[12] and in the oil extracted from flowers of bitter orange;[13] also reported in the flowers of several plants: lemon and coffee,[14] *Hevea brasiliensis*, and *Randia formosa*,[15] in the oil extracted from flowers of *Jasminum odoratissimum* L.,[16] and in the oil of *Narcissus jonquilla*[17]
Reported uses[3]	Non-alcoholic beverages 0.26 ppm Ice cream, ices, etc. 0.28 ppm Candy 0.50 ppm Baked goods 0.58 ppm Gelatins and puddings 0.02–0.40 ppm
Regulatory status	FDA 121.1164; FEMA No. 2593

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	α-Ionone	β-Ionone
Other names	α-Cyclocitrylideneacetone 4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one	β-Cyclocitrylideneacetone 4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
Empirical formula	$C_{13}H_{20}O$	$C_{13}H_{20}O$
Structure		
Physical chemical characteristics	The composition of commercial ionones varies widely in the proportion of alpha and beta isomers. The specifications refer to the best grade of alpha and beta ionones and to a commercial grade that contains both alpha and beta ionones.[2]	
Appearance	Colorless to pale-yellow liquid	Colorless to pale-yellow liquid
Assay	~85%[2] (as alpha isomer); ~60%, comm.[2]	~95%[2] (as beta isomer)
Molecular weight	192.30	192.30
Boiling point	121–122 C at 10 mm Hg	128–129 C at 10 mm Hg
Flash point	115 C	
Specific gravity	0.927–0.933 at 25/25 C;[2] 0.927–0.936, comm.[2]	0.941–0.947 at 25/25 C;[2] 0.927–0.936, comm.[2]
Refractive index	1.4970–1.5020 at 20 C;[2] 1.4970–1.5060, comm.[2]	1.5190–1.5215 at 20 C;[2] 1.4970–1.5060, comm.[2]
Ketone content	~98%;[2] 90%, comm.[2]	~98%;[2] ~90%, comm.[2]
Solubility	1:3 in 70% alcohol[2]	1:3 in 70% alcohol[2]
Organoleptic characteristics	Characteristic violet-like odor	Characteristic violet-like odor, more fruity and woody than α-ionone
Synthesis	By condensing citral with acetone to form pseudoionone, which is then cyclized by acid-type reagents[2]	By condensing citral with acetone to form pseudoionone, which is then cyclized by acid-type reagents[2]
Natural occurrence	Not too common in nature; probably occurring in the absolute essence of *Acacia farnesiana*. Reported in the essential oil of *Sphaeranthus indicus* L. The *d*-, *l*-, and *dl*-isomers are known.[7]	Reported found in raspberry, in the distillate from flowers of *Boronia megatisima* Nees., and in few other essences
Reported uses[3]	Non-alcoholic beverages 2.5 ppm Ice cream, ices, etc. 3.6 ppm Candy 12 ppm Baked goods 6.7 ppm Gelatins and puddings 3.6 ppm Chewing gum 39 ppm Icings 50 ppm	Non-alcoholic beverages 1.6 ppm Ice cream, ices, etc. 3.4 ppm Candy 7.6 ppm Baked goods 5.2 ppm Gelatins and puddings 5.8 ppm Chewing gum 89 ppm Maraschino cherries 10 ppm
Regulatory status	FDA 121.1164; FEMA No. 2594	FDA 121.1164; FEMA No. 2595

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For α- and β-ionone: Naves and Bachmann, *Helv. Chim. Acta*, 26, 2151, 1943; 27, 645, 1944.

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