Compound Summary for CID 8914

1-Nonanol

Cite this Record

STRUCTURE VENDORS PHARMACOLOGY LITERATURE PATENTS BIOACTIVITIES

PubChem CID:	8914
Chemical Names:	1-Nonanol; Nonan-1-ol; Nonanol; N-Nonyl alcohol; 143-08-8; NONYL ALCOHOL More...
Molecular Formula:	$C_9H_{20}O$
Molecular Weight:	144.258 g/mol
InChI Key:	ZWRUINPWMLAQRD-UHFFFAOYSA-N
Substance Registry:	FDA UNII
Safety Summary:	Laboratory Chemical Safety Summary (LCSS)

1-Nonanol is found in citrus. 1-Nonanol is widespread in nature. 1-Nonanol occurs in oils of orange, citronella and lemon. Also found in cheese, prickly pears and bread. 1-Nonanol is a flavouring agent. 1-Nonanol is a straight chain fatty alcohol with nine carbon atoms and the molecular formula CH3(CH2)8OH. It is a colorless to slightly yellow liquid with a citrus odor similar to citronella oil

Metabolite Description from Human Metabolome Database (HMDB)

NONANOL is a colorless liquid with a rose or fruity odor. Floats on water. Freezing point 23°F. (USCG, 1999)

Physical Description from CAMEO Chemicals

PUBCHEM > COMPOUND > 1-NONANOL *Modify Date: 2018-01-13; Create Date: 2004-09-16*

Contents

1 2D Structure

Search Download Get Image

Magnify

from PubChem

2 3D Conformer

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fy

Show Hydrogens Show Atoms Animate

from PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

nonan-1-ol

from PubChem

3.1.2 InChI

InChI=1S/C9H20O/c1-2-3-4-5-6-7-8-9-10/h10H,2-9H2,1H3

from PubChem

3.1.3 InChI Key

ZWRUINPWMLAQRD-UHFFFAOYSA-N

from PubChem

3.1.4 Canonical SMILES

CCCCCCCCCO

from PubChem

3.2 Molecular Formula

$C_9H_{20}O$

from PubChem

3.3 Other Identifiers

3.3.1 CAS

143-08-8

from CAMEO Chemicals, ChemIDplus, DTP/NCI, EPA DSStox, European Chemicals Agency - ECHA, Human Meta...

28473-21-4

from ChemIDplus, DrugBank, EPA Chemicals under the TSCA, European Chemicals Agency - ECHA

3.3.2 EC Number

249-048-6

from European Chemicals Agency - ECHA

205-583-7

from European Chemicals Agency - ECHA

3.3.3 FEMA Number

2789

from Flavor & Extract Manufacturers Association - FEMA

3.3.4 NSC Number

5521

from DTP/NCI

3.3.5 UN Number

3082

from CAMEO Chemicals

3.3.6 UNII

NGK73Q6XMC

from DrugBank, FDA/SPL Indexing Data

3.3.7 Wikipedia

Title	nonyl alcohol
Description	chemical compound

from Wikipedia

3.4 Synonyms

3.4.1 MeSH Entry Terms

1-nonanol

from MeSH

3.4.2 Depositor-Supplied Synonyms

1. 1-Nonanol
2. Nonan-1-ol
3. Nonanol
4. n-Nonyl alcohol
5. 143-08-8
6. NONYL ALCOHOL
7. Pelargonic alcohol
8. Octyl carbinol
9. 1-Hydroxynonane
10. Nonalol
11. n-Nonanol
12. n-Nonan-1-ol
13. Alcohol C-9
14. Nonylalkohol
15. Pelargonalkohol
16. C9 alcohol
17. Fatty alcohol(C9)
18. UNII-NGK73Q6XMC
19. NSC 5521
20. Alcohol C9
21. FEMA No. 2789
22. HSDB 5145
23. EINECS 205-583-7
24. BRN 0969213
25. AI3-03962
26. 28473-21-4
27. CHEBI:35986
28. ZWRUINPWMLAQRD-UHFFFAOYSA-N
29. MFCD00002990
30. SBB059907
31. F09
32. EINECS 249-048-6
33. Nonanol-(1)
34. Nonyl alcohol, 8CI
35. ACMC-209cpi
36. 1-Nonanol, 98%
37. AC1L1RXY
38. DSSTox_CID_2008
39. NGK73Q6XMC
40. AC1Q2W9K
41.
42.
43.
44.
45.
46.
47.
48.
49.
50.

from PubChem

4 Chemical and Physical Properties

4.1 Computed Properties

Property Name	Property Value
Molecular Weight	144.258 g/mol
Hydrogen Bond Donor Count	1
Hydrogen Bond Acceptor Count	1
Rotatable Bond Count	7
Complexity	52.7
CACTVS Substructure Key Fingerprint	AAADceBwIAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA AAAAAAAAAAAAGgAACAAACACggAICAAAAAgAAAAAAA AAAAAAAAAAAAAAAAAAAAEAIAAAAAQAAEAAAAAAGAw KAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA==
Topological Polar Surface Area	20.2 A^2
Monoisotopic Mass	144.151 g/mol
Exact Mass	144.151 g/mol
XLogP3	4.3
Compound Is Canonicalized	true
Formal Charge	0
Heavy Atom Count	10
Defined Atom Stereocenter Count	0
Undefined Atom Stereocenter Count	0
Defined Bond Stereocenter Count	0
Undefined Bond Stereocenter Count	0
Isotope Atom Count	0
Covalently-Bonded Unit Count	1

from PubChem

4.2 Experimental Properties

4.2.1 Physical Description

NONANOL is a colorless liquid with a rose or fruity odor. Floats on water. Freezing point 23°F. (USCG, 1999)

from CAMEO Chemicals

Liquid

from EPA Chemicals under the TSCA, Human Metabolome Database (HMDB)

4.2.2 Color

Colorless to yellowish liquid

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1196

from HSDB

4.2.3 Odor

Floral odor

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 801

from HSDB

Odor of citronella oil

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1196

from HSDB

4.2.4 Boiling Point

415° F at 760 mm Hg (USCG, 1999)

from CAMEO Chemicals

213.3 deg C

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V4: 3651

from HSDB

4.2.5 Melting Point

23° F (USCG, 1999)

from CAMEO Chemicals

-5 deg C

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V4: 3651

from HSDB

-5 °C

from Human Metabolome Database (HMDB)

4.2.6 Flash Point

165° F (USCG, 1999)

from CAMEO Chemicals

165 deg F

Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 801

from HSDB

4.2.7 Solubility

Miscible with alcohol, ether

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1196

from HSDB

Soluble in ethanol, ether; very soluble in carbon tetrachloride

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V4: 3651

from HSDB

In water, 140 mg/L at 25 deg C

Barton AFM; pp. 438 in Solubility Data Series Vol 15, p 392 (1984)

from HSDB

0.14 mg/mL at 25 °C

from Human Metabolome Database (HMDB)

4.2.8 Density

0.827 at 68° F (USCG, 1999)

from CAMEO Chemicals

0.8279 at 20 deg C/4 deg C

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1196

from HSDB

4.2.9 Vapor Pressure

0.0227 mm Hg at 25 deg C (est)

Daubert, T.E., R.P. Danner. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis, 1989.

from HSDB

4.2.10 LogP

log Kow = 3.77

Tewari YB et al; J Chem Eng Data 27: 451-4 (1982)

from HSDB

3.77

from Human Metabolome Database (HMDB)

4.2.11 Decomposition

When heated to decomposition it emits acid smoke and irritating fumes.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2740

from HSDB

4.2.12 Viscosity

11.7 centapoise at 20 deg C

Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V1: 868 (1991)

from HSDB

4.2.13 Heat of Combustion

5943.4 kJ/mol at 298.15 deg K (liquid)

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 5-84

from HSDB

4.2.14 Heat of Vaporization

76.86 kJ/mol at 25 deg C

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 6-121

from HSDB

4.2.15 Odor Threshold

Odor and taste perception threshold is 0.1 mg/L.

Sheftel, V.O.; Indirect Food Additives and Polymers. Migration and Toxicology. Lewis Publishers, Boca Raton, FL. 2000., p. 774

from HSDB

4.2.16 Kovats Retention Index

Standard non-polar	1149, 1149, 1151, 1154.5, 1163, 1166, 1169, 1171, 1155, 1153, 1163.3, 1156.7, 1156.8,

	1156.8, 1156.9, 1160, 1156.9, 1157.2, 1161.3, 1161.9, 1153.6, 1140, 1140, 1143, 1147, 1149, 1154, 1167, 1151, 1152, 1160, 1162, 1161, 1163, 1160, 1162, 1166, 1160, 1160, 1171, 1154, 1154, 1158, 1156, 1166, 1157, 1161, 1159, 1158.4, 1160, 1154, 1152, 1158.9, 1152, 1155, 1155, 1159.2, 1157, 1159, 1157, 1161, 1155, 1161, 1161, 1164, 1155, 1156.7, 1153, 1160, 1163.3, 1156, 1156, 1161.3, 1161.9, 1168, 1166, 1153, 1153, 1153, 1166, 1154, 1130, 1156, 1156, 1161, 1161, 1156, 1156, 1155, 1155, 1162, 1157
Semi-standard non-polar	1171.6, 1179, 1172, 1173.9, 1172, 1169.2, 1181, 1175, 1168, 1171, 1180, 1173, 1171.4, 1171, 1137, 1172, 1175, 1174, 1171, 1169, 1170, 1169, 1186, 1172, 1173, 1143, 1155, 1174, 1173, 1180, 1173, 1175, 1150, 1173, 1181, 1156, 1176, 1181, 1174, 1173, 1170, 1171, 1171, 1172, 1173, 1174, 1176, 1171, 1174, 1186, 1169, 1176, 1182, 1182, 1183, 1172, 1156, 1163, 1171, 1180, 1173, 1178, 195.98, 197.48, 196.63, 1171, 1172, 1171, 1185, 1172, 1171, 1172, 1169, 1176, 1171, 1170, 1164, 1164, 1184, 1173, 1140, 1167, 1172, 1173, 1171, 1169, 1166, 1168, 1171, 1176, 1171, 1147.4, 1158, 1158, 1160, 1154, 1133
Standard polar	1663, 1668, 1673, 1658, 1656, 1654, 1639, 1643, 1653, 1640, 1668, 1649, 1682, 1665, 1661, 1663, 1649, 1681.2, 1681.2, 1644, 1653, 1671, 1668, 1663.3, 1663.9, 1663.9, 1664.8, 1665, 1665, 1666, 1645, 1662, 1663, 1666, 1666, 1627, 1649, 1652, 1658, 1659, 1663, 1664, 1680, 1662, 1666, 1624, 1624, 1630, 1635, 1640, 1647, 1665, 1624, 1629, 1655, 1655, 1661, 1676, 1653, 1685, 1645, 1653, 1661, 1661, 1649, 1695, 1652, 1660, 1654, 1660, 1669, 1665, 1695, 1660, 1625, 1647, 1658, 1662, 1647, 1650, 1644.9, 1661, 1665, 1658, 1664, 1619, 1657, 1636, 1665, 1658, 1674, 1624, 1664, 1664, 1664, 1665, 1666, 1636, 1672, 1658, 1663, 1636, 1654, 1662, 1665, 1665, 1630, 1630, 1664, 1664, 1658, 1668, 1636, 1676, 1664, 1663, 1658, 1624, 1670, 1664, 1664, 1658, 1654, 1664, 1661, 1665, 1685, 1659, 1665, 1653.6, 1664, 1659, 1631, 1631, 1651, 1632, 1698, 1630, 1630

▸ *from NIST*

4.3 Spectral Properties

Index of refraction = 1.4338 at 20 deg C/D

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1196

▸ *from HSDB*

IR: 1491 (Sadtler Research Laboratories Prism Collection)

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V4: 3651

▸ *from HSDB*

1H NMR: 102 (Sadtler Research Laboratories Spectral Collection)

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V4: 3651

▸ *from HSDB*

MASS: 4034 (NIST/EPA/MSDC Mass Spectral database, 1990 version); 803 (Atlas of Mass Spectral Data, John Wiley & Sons, New York)

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V4: 3651

▸ *from HSDB*

4.3.1 Infrared Spectra

Infrared Spectra: 1 of 5 (FTIR Spectra)	
Technique	CAPILLARY CELL: NEAT
Source of Sample	MCB MANUFACTURING CHEMISTS, NORWOOD, OHIO
Copyright	Copyright © 1980, 1981-2017 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	CLICK TO LOAD...

from SpectraBase

Infrared Spectra: 2 of 5 (FTIR Spectra)	
Technique	CAPILLARY CELL: NEAT
Source of Sample	MCB MANUFACTURING CHEMISTS, NORWOOD, OHIO
Copyright	Copyright © 1980, 1981-2017 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	CLICK TO LOAD...

from SpectraBase

Infrared Spectra: 3 of 5 (Vapor Phase IR Spectra)	
Instrument Name	DIGILAB FTS-14
Technique	VAPOR PHASE
Copyright	Copyright © 1980, 1981-2017 Bio-Rad Laboratories, Inc. All Rights Reserved.

Infrared Spectra: 3 of 5 (Vapor Phase IR Spectra)	
Thumbnail	CLICK TO LOAD...

from SpectraBase

View All 5 Infrared Spectra

4.3.2 1D NMR Spectra

1D NMR Spectra: 1 of 6 (1H NMR Spectra)	
1H NMR Spectra	1D NMR Spectrum 3838 - 1H NMR Spectrum (HMDB0031265)
13C NMR Spectra	1D NMR Spectrum 4105 - 13C NMR Spectrum (HMDB0031265)

from Human Metabolome Database (HMDB)

1D NMR Spectra: 2 of 6 (13C NMR Spectra)	
Source of Sample	MCB Manufacturing Chemists, Norwood, Ohio
Copyright	Copyright © 1980, 1981-2017 Bio-Rad Laboratories, Inc. All Rights Reserved.
Thumbnail	CLICK TO LOAD...

from SpectraBase

1D NMR Spectra: 3 of 6 (13C NMR Spectra)	
Copyright	Copyright © 2016 W. Robien, Inst. of Org. Chem., Univ. of Vienna. All Rights Reserved.

1D NMR Spectra: 3 of 6 (13C NMR Spectra)	
Thumbnail	CLICK TO LOAD...

from SpectraBase

View All 6 1D NMR Spectra

4.3.3 Mass Spectrometry

4.3.3.1 GC-MS

1. GC-MS Spectrum 1011 - GC-MS (1 TMS)
2. GC-MS Spectrum 3216
3. GC-MS Spectrum 26993
4. GC-MS Spectrum 28476
5. GC-MS Spectrum 28866
6. GC-MS Spectrum 31614
7. GC-MS Spectrum 42407

from Human Metabolome Database (HMDB)

<< < 1 of 6 > >>	
NIST Number	229864
Library	Main library
Total Peaks	67
m/z Top Peak	56
m/z 2nd Highest	55
m/z 3rd Highest	43

Thumbnail	CLICK TO LOAD...

1 of 6

from NIST

4.3.3.2 MS-MS

1. MS-MS Spectrum 73158
2. MS-MS Spectrum 73159
3. MS-MS Spectrum 73160
4. MS-MS Spectrum 132264
5. MS-MS Spectrum 132265
6. MS-MS Spectrum 132266

from Human Metabolome Database (HMDB)

4.3.3.3 EI-MS

EI-MS Spectrum 1580

from Human Metabolome Database (HMDB)

4.3.4 Other Spectra

Other Spectra: 1 of 1 (Raman Spectra)	
Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	Alfa Aesar, Thermo Fisher Scientific
Catalog Number	A12510
Lot Number	10183990
Copyright	Copyright © 2016-2017 Bio-Rad Laboratories, Inc. All Rights Reserved.

Other Spectra: 1 of 1 (Raman Spectra)	
Thumbnail	CLICK TO LOAD...

from SpectraBase

5 Related Records

CLICK TO LOAD...

from NCBI

5.1 Related Compounds with Annotation

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from PubChem

5.2 Related Compounds

Same Connectivity	8 records
Same Parent, Connectivity	35 records
Same Parent, Exact	27 records
Mixtures, Components, and Neutralized Forms	61 records
Similar Compounds	899 records
Similar Conformers	914 records

from PubChem

5.3 Substances

5.3.1 Related Substances

All	239 records
Same	136 records
Mixture	103 records

from PubChem

5.3.2 Substances by Category

CLICK TO LOAD...

from PubChem

5.4 Entrez Crosslinks

PubMed	810 records
Protein Structures	18 records
Taxonomy	2 records
Gene	2 records

from PubChem

6 Chemical Vendors

CLICK TO LOAD...

from PubChem

7 Food Additives and Ingredients

7.1 Food Additive Classes

Flavoring Agents

from EU Food Improvement Agents

JECFA Functional Classes

Flavouring Agent: FLAVOURING_AGENT

from FAO/WHO Food Additive Evaluations - JECFA

7.2 FEMA Flavor Profile

Fat, Floral, Green, Oil

from Flavor & Extract Manufacturers Association - FEMA

7.3 Evaluations of the Joint FAO/WHO Expert Committee on Food Additives - JECFA

Evaluations of the Joint FAO/WHO Expert Committee on Food Additives - JECFA: 1 of 1 (JECFA Chemical)	
Chemical Name	ALCOHOL C-9
ADI	No safety concern at current levels of intake when used as a flavouring agent
Evaluation Year	1997
Report	TRS 884-JECFA 49/29

from FAO/WHO Food Additive Evaluations - JECFA

8 Pharmacology and Biochemistry

8.1 Absorption, Distribution and Excretion

Skin absorption is low; the dermal flux of 1-nonanol in human skin (epidermis) in vitro is 0.003 mg/sq cm/hr.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:482

from HSDB

8.2 Metabolism/Metabolites

Nonanol, like other primary alcohols, undergoes two general reactions in vivo. The first is oxidation to the carboxylic acid derivative and next the direct conjugation with glucuronic acid. It was reported that nonanol undergoes direct glucuronic conjugation to the extent of 4.1%. This oxidation proceeds with very little inhibition as opposed to that shown by methyl amyl alcohol and 2-ethyl butyl alcohol which form ester glucuronides.

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. Second Edition. Volume 3 Alcohols and Esters. New York, NY: Elsevier, 1992., p. 186

from HSDB

8.3 Mechanism of Action

... Intermediate-chain alcohols (pentanol to octanol) caused channel currents to fluctuate between the fully open and closed state level so that openings occurred in bursts interrupted by brief gaps ... The number of gaps within a burst was dependent on alcohol concentration whereas gap duration was independent of concentration but increased with increasing chain length of the alcohol up to octanol. Nonanol and decanol reduced the mean duration of bursts of openings but did not cause an increase in the number of short closed intervals within a burst. Beyond decanol there was a decline in the ability of the n-alcohols to affect channel function. A saturated solution of undecanol (0.07 mM) reduced the mean open time by 33 + or - 17%, whereas a saturated solution of dodecanol had no significant effect. The current integral per burst was reduced by all the n-alcohols between pentanol and undecanol. The IC50s were as follows: hexanol, 0.53 + or - 0.14 mM; heptanol, 0.097 + or - 0.02 mM; octanol, 0.04 mM and nonanol, 0.16 + or - 0.035 mM ... Blocking rate constants (k+B) for pentanol through to nonanol were calculated to be between 2.8 and 5.7 X 10(6) /M/sec ... Equilibrium dissociation constants (KD), calculated from the blocking and unblocking rate constants (KD = k-B/k+B), decreased with increasing chain length from 8 mM for pentanol to 0.15 mM for octanol. The standard free energy per methylene group for adsorption to the site of action was calculated to be about -3.3 kJ/mol.[Murrell RD et al; J Physiol 437: 431-48 (1991)] Full text: PMC1180056
Abstract: PubMed

from HSDB

8.4 Human Metabolite Information

8.4.1 Metabolite Description

1-Nonanol is found in citrus. 1-Nonanol is widespread in nature. 1-Nonanol occurs in oils of orange, citronella and lemon. Also found in cheese, prickly pears and bread. 1-Nonanol is a flavouring agent. 1-Nonanol is a straight chain fatty alcohol with nine carbon atoms and the molecular formula CH3(CH2)8OH. It is a colorless to slightly yellow liquid with a citrus odor similar to citronella oil

from Human Metabolome Database (HMDB)

8.4.2 Biofluid Locations

Feces

from Human Metabolome Database (HMDB)

8.4.3 Cellular Locations

1. Extracellular
2. Membrane

from Human Metabolome Database (HMDB)

9 Use and Manufacturing

9.1 Uses

EPA Safer Chemical Functional Use Classes

Fragrances

from EPA Safer Choice

Food additives -> Flavoring Agents

from EU Food Improvement Agents

JECFA Functional Classes

Flavouring Agent: FLAVOURING_AGENT

from FAO/WHO Food Additive Evaluations - JECFA

9.1.1 Industry Uses

Ion exchange agents

from EPA Chemicals under the TSCA

9.2 Methods of Manufacturing

By sodium or high-pressure catalytic reduction of esters of pelargonic acid; hydroformylation of C8 linear alpha-olefins or internal olefins (occurs in a mixt); natural constituent of rose, grapefruit & orange oils.

SRI

from HSDB

Preparation by reduction of ethyl delta (superscript 1)-nonylenate ... by reduction of pelargonic aldehyde ... by oxo process: Russum, Hengstebeck, US patent 2,638,487 (1953 to Standard Oil of Indiana); by reductive cleavage of oleic acid ozonide ... from diborane and propylene trimer: Marshall, Smith, British patent 879,242(1961 to I.C.I.).

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. 13th Edition, Whitehouse Station, NJ: Merck and Co., Inc., 2001., p. 1196-7

from HSDB

... Oxo synthesis from dimeric 1-butene and 2-butene (mixture known as raffinate II) or from dimeric isobutene. /C9 Alcohol mixtures/

Ullmann's Encyclopedia of Industrial Chemistry. 6th ed.Vol 1: Federal Republic of Germany: Wiley-VCH Verlag GmbH & Co. 2003 to Present, p. V2 32 (2003)

from HSDB

9.3 U.S. Production

(1977) PROBABLY GREATER THAN 4.54X10+5 GRAMS

SRI

▸ *from HSDB*

(1979) PROBABLY GREATER THAN 4.54X10+5 GRAMS

SRI

▸ *from HSDB*

(2002) >1 million-10 million pounds

US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). Nonyl Alcohol (143-08-8). Available from, as of May 16, 2006: http://www.epa.gov/oppt/iur/tools/data/2002-vol.html

▸ *from HSDB*

10 Identification

10.1 OSHA Chemical Sampling

Nonyl Alcohol

from OSHA Chemical Sampling Information

11 Safety and Hazards

11.1 Hazards Identification

11.1.1 GHS Classification

Signal: Warning
GHS Hazard Statements
Aggregated GHS information provided by 1214 companies from 10 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.

Reported as not meeting GHS hazard criteria by 7 of 1214 companies. For more detailed information, please visit ECHA C&L website

Of the 9 notification(s) provided by 1207 of 1214 companies with hazard statement code(s):

H315 (16.82%): Causes skin irritation [Warning Skin corrosion/irritation]
H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]
H411 (81.19%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.

Precautionary Statement Codes
P264, P273, P280, P302+P352, P305+P351+P338, P321, P332+P313, P337+P313, P362, P391, and P501
(The corresponding statement to each P-code can be found here.)

from European Chemicals Agency - ECHA

View all (2) GHS Classification entries

11.1.2 EPA Safer Chemical

1-Nonanol - Green half-circle - The chemical is expected to be of low concern based on experimental and modeled data. Additional data would strengthen EPA's confidence in the chemical's safer status.

from EPA Safer Choice

11.1.3 Health Hazard

Liquid irritates eyes. (USCG, 1999)

from CAMEO Chemicals

11.1.4 Fire Hazard

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: Some may burn but none ignite readily. Containers may explode when heated. Some may be transported hot. For UN3508, be aware of possible short circuiting as this product is transported in a charged state. (ERG, 2016)

from CAMEO Chemicals

11.1.5 Skin, Eye, and Respiratory Irritations

Based on the eye irritation scores that were reported, 1-nonanol would be considered an eye irritant using the EU criteria.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:481

from HSDB

11.2 Safety and Hazard Properties

11.2.1 LEL

0.8 % (USCG, 1999)

from CAMEO Chemicals

11.2.2 UEL

6.1 % (USCG, 1999)

from CAMEO Chemicals

11.2.3 Critical Temperature

Critical temperature = 671.5 K; Critial pressure = 2.63 MPa

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 6-64

from HSDB

11.2.4 Critical Pressure

Critical temperature = 671.5 K; Critial pressure = 2.63 MPa

Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 6-64

from HSDB

11.2.5 NFPA Fire Rating

2

from CAMEO Chemicals

11.2.6 NFPA Health Rating

2

from CAMEO Chemicals

11.3 First Aid Measures

11.3.1 First Aid

Flush eyes and skin with water for at least 15 min. (USCG, 1999)

from CAMEO Chemicals

11.4 Fire Fighting Measures

11.4.1 Fire Fighting

Fire Extinguishing Agents Not to Be Used: Water may be ineffective Fire Extinguishing Agents: Alcohol foam, dry chemical, or carbon dioxide (USCG, 1999)

from CAMEO Chemicals

11.5 Accidental Release Measures

11.5.1 Isolation and Evacuation

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: As an immediate precautionary measure, isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids. SPILL: Increase, in the downwind direction, as necessary, the isolation distance shown above. FIRE: If tank, rail car or tank truck is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2016)

from CAMEO Chemicals

11.5.2 Cleanup Methods

AEROBIC: Nonyl alcohol degraded fast in aerobic biodegradation screening tests(1-3). In one 5-day BOD test using acclimated mixed cultures, 47.9% of theoretical BOD was consumed(1). In the other test which used an activated sludge inoculum, nonyl alcohol's half-life was 1.2 days(SRC), calculated from a biodegradation rate of 2.36X10-2/hr(3). In a third test, 62% of its theoretical BOD in a grab sample of freshwater incubated at 18-19 deg C was expended in 4 days(2).

(1) Vaishnav DD et al; Chemosphere 16: 695-703 (1987) (2) Hammerton C; J Appl Chem 5: 517-24 (1955) (3) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 11: 77-82 (1981)

from HSDB

11.5.3 Disposal Methods

SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.

from HSDB

11.6 Handling and Storage

11.6.1 Nonfire Spill Response

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: Do not touch or walk through spilled material. Stop leak if you can do it without risk. Prevent dust cloud. Avoid inhalation of asbestos dust. SMALL DRY SPILL: With clean shovel, place material into clean, dry container and cover loosely; move containers from spill area. SMALL SPILL: Pick up with sand or other non-combustible absorbent material and place into containers for later disposal. LARGE SPILL: Dike far ahead of liquid spill for later disposal. Cover powder spill with plastic sheet or tarp to minimize spreading. Prevent entry into waterways, sewers, basements or confined areas. (ERG, 2016)

from CAMEO Chemicals

11.7 Exposure Control and Personal Protection

11.7.1 Protective Equipment and Clothing

Goggles or face shield; rubber gloves. (USCG, 1999)

from CAMEO Chemicals

11.8 Stability and Reactivity

11.8.1 Air and Water Reactions

No rapid reaction with air. No rapid reaction with water.

from CAMEO Chemicals

11.8.2 Reactive Group

Alcohols and Polyols

from CAMEO Chemicals

11.8.3 Reactivity Profile

NONANOL is an alcohol. Flammable and/or toxic gases are generated by the combination of alcohols with alkali metals, nitrides, and strong reducing agents. They react with oxoacids and carboxylic acids to form esters plus water. Oxidizing agents convert them to aldehydes or ketones. Alcohols exhibit both weak acid and weak base behavior. They may initiate the polymerization of isocyanates and epoxides.

from CAMEO Chemicals

11.9 Transport Information

11.9.1 DOT Label

Class 9

from CAMEO Chemicals

11.10 Regulatory Information

11.10.1 FDA Requirements

Nonyl alcohol is a food additive permitted for direct addition to food for human consumption as a synthetic flavoring substance and adjuvant in accordance with the following conditions: a) they are used in the minimum quantity required to produce their intended effect, and otherwise in accordance with all the principles of good manufacturing practice, and 2) they consist of one or more of the following, used alone or in combination with flavoring substances and adjuvants generally recognized as safe in food, prior-sanctioned for such use, or regulated by an appropriate section in this part.

21 CFR 172.515; U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of June 21, 2006: http://www.ecfr.gov

from HSDB

12 Toxicity

12.1 Toxicological Information

12.1.1 Interactions

... Maximum permeation of MT was observed when fatty alcohol carbon chain length was 10. As the level of unsaturation increased from one to two double bonds, there was an increase in the permeation of MT both in porcine and human skin. However, a decrease in the permeation was observed with three double bonds. Regression analysis using the steady state flux data showed a significant positive correlation between porcine and human skin for saturated fatty alcohols (r(2)=0.8868, P=0.0005).
More information...

Andega S et al; J Control RElease 77 (1-2): 17-25 (2001)

from HSDB

12.1.2 Antidote and Emergency Treatment

Basic Treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary ... . Monitor for pulmonary edema and treat if necessary ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal ... . /Higher alcohols (>3 carbons) and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 232-3

from HSDB

Advanced Treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques, with a bag-valve-mask device, may be beneficial. Consider drug therapy for pulmonary edema ... . Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start IV administration of D5W /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Consider vasopressors if patient is hypotensive with a normal fluid volume. Watch for signs of fluid overload ... . Monitor for signs of hypoglycemia (decreased LOC, tachycardia, pallor, dilated pupils, diaphoresis, and/or dextrose strip or glucometer readings below 50 mg) and administer 50% dextrose if necessary ... . Treat seizures with diazepam or lorazepam ... . Use proparacaine hydrochloride to assist eye irrigation ... . /Higher alcohols (>3 carbons) and related compounds/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3Rd edition, Elsevier Mosby, St. Louis, MO 2005, p. 233

from HSDB

12.1.3 Human Toxicity Excerpts

/HUMAN EXPOSURE STUDIES/ 1-Nonanol (2% in petrolatum) was reportedly neither a skin irritant nor a skin sensitizer to humans. /1-Nonanol, 2% in petrolatum/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:482

from HSDB

12.1.4 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ Fatal intoxication following nonyl alcohol rich in trimethyl hexanol.../given rats, single oral dose 1.4-1.75 ml/kg; rabbits single oral dose 1.4-2.1 mg/kg or iv 0.015-0.021 g/kg/. ... There were slight degenerative changes in myocardium. /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4626

▸ *from HSDB*

/LABORATORY ANIMALS: Acute Exposure/ There were no deaths among rats exposed /SRP: by inhalation/ to either 215 or 730 ppm for 6 hr.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:482

▸ *from HSDB*

/LABORATORY ANIMALS: Acute Exposure/ An inhalation experiment conducted with rats at "saturated vapor" for 8 hours resulted in no deaths /Nonyl alcohols; from table/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4628

▸ *from HSDB*

/LABORATORY ANIMALS: Acute Exposure/ Inhalation experiments conducted with rats, guinea pigs, or mice at 21.7 mg/L aerosol for 6 hours resulted in 2/10, 0/10, or 1/10 deaths, respectively /Nonyl alcohols; from table/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4628

▸ *from HSDB*

/LABORATORY ANIMALS: Acute Exposure/ Aspiration of 0.2 mL of 1-nonanol produced deaths among 10 out of 10 rats; death was instant and was due to respiratory arrest.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:481

▸ *from HSDB*

/LABORATORY ANIMALS: Acute Exposure/ Based on the eye irritation scores that were reported, 1-nonanol would be considered an eye irritant using the EU criteria.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:481

▸ *from HSDB*

/LABORATORY ANIMALS: Acute Exposure/ Upon rabbit eye contact, conjunctival irritation but no corneal effects were noted with lower molecular weight alcohols /Nonyl alcohols; from table/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4628

▸ *from HSDB*

/LABORATORY ANIMALS: Acute Exposure/ Fatal intoxication following nonyl alcohol rich in trimethylhexanols revealed degenerative changes in neurons in all parts of brain and brain stem /in rats given single oral dose 1.4-1.75 mL/kg and rabbits single oral dose 1.4-2.1 mL/kg or iv 0.015-0.021 g/kg/. Hepatocellular degeneration... renal damage... /were observed/. /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4626

▸ *from HSDB*

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Application of 5 mL (1.6 to 2.0 g/kg) of nonyl alcohol to the skin of rabbits for 1 hr/day on each of 50 days over period of 75 days resulted in retarded growth & erythema of the treated skin but no mortality. /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4629

▸ *from HSDB*

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ Rabbits were exposed by inhalation to vapor containing 84 mg/cu m (14.2 ppm) nonyl alcohol for 6 months. Electron microscopy examination of the retina of the eye revealed ultrastructural changes in the photoreceptor cells and Muller fibers. /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4629

▸ *from HSDB*

/LABORATORY ANIMALS: Subchronic or Prechronic Exposure/ In rabbits and rats exposed to conc of 0.8, 0.6, or 0.2 mg/L (136, 99, or 33 ppm) nonyl alcohol for 2 hr/day for 2 months, small amt of deformed or degenerate glial elements diffusely scattered in the cerebral cortex and subcortex were observed. /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4629

▸ *from HSDB*

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ Embryotoxicity and delayed fetal development (including retardation of ossification) was reported in a study in which female rats were dosed orally with a 40% solution of 1-nonanol during days 1 through 15 of pregnancy. /40% solution of 1-nonanol/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:482

▸ *from HSDB*

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ Exposure of female rats to saturated vapors of 1-nonanol (25 ppm or 150 mg/cu m) 7 hr/day on days 1 to 19 of gestation did not result in maternal or developmental toxicity.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:482

▸ *from HSDB*

/LABORATORY ANIMALS: Developmental or Reproductive Toxicity/ As part of a large study evaluating the developmental toxicology of industrial alcohols administered by inhalation, groups of approximately 15 pregnant female Sprague-Dawley rats were exposed for 7 hr/day on gestation days 1-19 (sperm= 0) to one of three long-chain alcohols at the maximum concentrations that could be generated as a vapor. These concentrations were 400 mg/cu m 1-octanol, 150 mg/ cu m 1-nonanol, and 100 mg/cu m 1-decanol. Dams were weighed daily for the first week of exposure, and weekly thereafter. On gestation day 20, rats were sacrificed. Fetuses were serially removed, blotted dry, examined for external malformations, sexed, weighed, placed in appropriated fixatives,and subsequently examined for visceral or skeletal abnormalities. No treatment-related effects were observed in pregnant females, frequency of resorptions, fetal weights, or skeletal/visceral malformations. Thus, long-chain alcohols at these vapor concentration appear not to be toxic as evidenced by these fetal and maternal parameters.

Nelson BK et al; J of The Am College of Toxicol 9 (1): 93-7 (1990)

▸ *from HSDB*

/GENOTOXICITY/ Mutagenic and genotoxic substances were determined in the offgassing products of particle board ... (TA 100) was more sensitive than (TA 98), (TA 1535), and (TA 1537) ... Compounds found were formaldehyde ... benzene ... toluene ... xylenes, styrene ... alpha-pinene ... camphene ... limonene ... nonanal ... tetradecane ... and n-butanol ... Camphene was present in the highest concentrations, 1336 to 3418 ng/L. The amount of nonanal was also high, while benzene was found in two samples and styrene in one.
Abstract: PubMed

Glass LR et al; Toxicol Lett 31 (1): 75-83 (1986)

from HSDB

12.1.5 Non-Human Toxicity Values

LC50 Mouse inhalation 5500 mg/cu m/2 hr

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. Second Edition. Volume 3 Alcohols and Esters. New York, NY: Elsevier, 1992., p. 186

from HSDB

LD50 Rat oral 3.56 g/kg

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. Second Edition. Volume 3 Alcohols and Esters. New York, NY: Elsevier, 1992., p. 186

from HSDB

LD50 Rabbit dermal 5.66 ml/kg for 24 hr

Snyder, R. (ed.). Ethel Browning's Toxicity and Metabolism of Industrial Solvents. Second Edition. Volume 3 Alcohols and Esters. New York, NY: Elsevier, 1992., p. 187

from HSDB

LD50 Mouse ip 0.8 g/kg /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4628

from HSDB

LD50 Rat ip 0.8 mg/kg /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4628

from HSDB

LD50 Rabbit iv 15 mg/kg /Nonyl alcohols/

Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 4628

from HSDB

LD50 Guinea pig dermal >10 mL/kg

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:482

from HSDB

LD50 Rabbit dermal 2.96 g/kg

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:481

from HSDB

LD50 Rat oral 3.2 g/kg /Nonyl alcohol containing 2% 2-propylheptanol/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:481

from HSDB

LD50 Mouse oral 6.4 g/kg /Nonyl alcohol containing 2% 2-propylheptanol/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:481

from HSDB

12.1.6 Ecotoxicity Values

LC50 Pimephales promelas (Fathead minnow, weight 0.12 g) 5.7 mg/L 96 hr flow-through bioassay, water hardness 45.5 mg/L CaCO3, temp: 25 +/- 1 deg C, pH 7.5, dissolved oxygen >60% of saturation

Veith GD et al; Canadian J Fisheries Aquat Sci 40 (6): 743-8 (1983)

from HSDB

LC50 Pimephales promelas (Fathead minnow, age 30-31 days, mean weight 0.124 g, mean length 20.0 mm) 5.7 mg/L/96 hr (95% confidence limit: 5.4-6.0 mg/L); flow through bioassay, temp 24.8 deg C, pH 7.63, dissolved oxygen 7.2 mg/L, hardness 44.3 mg/L CaCO3, alkalinity 43.0 mg/L CaCO3 /purity 97%/

Brooke, L.T., D.J. Call, D.T. Geiger and C.E. Northcott (eds.). Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Superior, WI: Center for Lake Superior Environmental Studies Univ. of Wisconsin Superior, 1984., p. 353

from HSDB

LC50 Alburnus alburnus (Bleak) 18 mg/L/96 hr (95% confidence limit: 16-20 mg/L); static /formulated product/

Linden E et al; Chemosphere 8 (11/12): 843-851 (1979) Available from, as of April 27, 2006: http://cfpub.epa.gov/ecotox/quick_query.htm

from HSDB

LC50 Nitocra spinipes (Harpacticoid copepod) 25 mg/L/96 hr (95% confidence limit: 21-30 mg/L); static /formulated product/

Linden E et al; Chemosphere 8 (11/12): 843-851 (1979) Available from, as of April 27, 2006: http://cfpub.epa.gov/ecotox/quick_query.htm

from HSDB

EC50 Ceriodaphnia dubia (Water flea; intoxication, immobilization) 2.5 umol/L/48 hr (95% confidence limit: 1.5-4.3 umol/L/48 hr); static /formulated product/

Rose RM et al; Arch Environ Contam Toxicol 34 (3): 248-252 (1998) Available from, as of April 27, 2006: http://cfpub.epa.gov/ecotox/quick_query.htm

from HSDB

EC50 Tetrahymena pyriformis (Ciliate; growth inhibition) 24.35 mg/L/48 hr (95% confidence limit: 19.94-28.91 mg/L); static /formulated product/

Schultz TW et al; Ecotoxicol Environ Saf 19 (3): 247-53 (1990) Available from, as of April 27, 2006: http://cfpub.epa.gov/ecotox/quick_query.htm

from HSDB

12.1.7 TSCA Test Submissions

1-Nonanol (CAS # 142-08-8) was evaluated for acute oral toxicity. The test substance was administered by gavage to Sprague-Dawley albino rats. Dosage and mortality data are as follows: 2,000 mg/kg (0/3 M, 0/2 F); 2,510 mg/kg (0/2 M, 2/3 F); 3,160 mg/kg (0/3 M, 2/2 F); 3,980 mg/kg (0/2 M, 3/3 F); 5,010 mg/kg (3/3 M, 2/2 F); and 6,310 mg/kg (2/2 M, 3/3 F). Signs of intoxication included weight loss, increasing weakness, ocular discharge, collapse, and death. Gross autopsy revealed hemorrhagic lungs, liver discoloration, and acute gastrointestinal inflammation.

MONSANTO CO; Initial Submission: Toxicity Studies with Nonyl Alcohol in Rats and Rabbits with Cover Letter Dated 08/13/92; 02/28/79; EPA No. 88-920007147; Fiche No. OTS0545486

from HSDB

1-Nonanol (CAS # 142-08-8) was evaluated for acute dermal toxicity. The test substance was administered to New Zealand albino rabbits. Dosage and mortality data are as follows: 398 mg/kg (0/1 M); 631 mg/kg (0/1 F); 1,000 mg/kg (0/1 M, 1/1 F); 1,260 mg/kg (1/1 F); 2,000 mg/kg (0/1 M); 3,160 mg/kg (1/1 F); and 5,010 mg/kg (1/1 M). Signs of intoxication included weight loss, increasing weakness, ocular discharge, collapse, and death. Gross autopsy revealed hemorrhagic areas of the lungs, discoloration of the liver and kidneys, enlarged gall bladder, darkened spleen, and gastrointestinal inflammation.

MONSANTO CO; Initial Submission: Toxicity Studies with Nonyl Alcohol in Rats and Rabbits with Cover Letter Dated 08/13/92; 02/28/79; EPA No. 88-920007147; Fiche No. OTS0545486

▸ *from HSDB*

1-Nonanol (CAS # 143-08-8) was evaluated for dermal sensitization using standard methods. The test substance was administered to 10 guinea pigs with an initial reaction rating of slight to very slight in 2 animals and a final patch rating of slight in 1 animal. The test substance was determined to be a non-sensitizer. No further information was available.

E.I. DUPONT DE NEMOURS & CO; Primary Toxicity Tests on 15 Compounds; 12/18/47; EPA No. 86-870001072; Fiche No. OTS0514975

▸ *from HSDB*

1-Nonanol (CAS # 142-08-8) was evaluated for primary dermal irritation. The test substance was administered to 6 New Zealand albino rabbits receiving 0.5 ml of undiluted test substance for a 24 hour exposure period. Average irritation score was 5.8/8.0. Irritation consisted of a defatting effect (skin sloughed off in 10-14 days). There was no in depth injury.

MONSANTO CO; Initial Submission: Toxicity Studies with Nonyl Alcohol in Rats and Rabbits with Cover Letter Dated 08/13/92; 02/28/79; EPA No. 88-920007147; Fiche No. OTS0545486

▸ *from HSDB*

1-Nonanol (CAS # 142-08-8) was evaluated for primary eye irritation. The test substance was administered to 6 New Zealand albino rabbits receiving 0.1 ml of undiluted test substance for a 24 hour exposure period. Average irritation score was 33.3/110. Immediate discomfort was moderate with eyes tightly closed. Irritation consisted of slight erythema, copious discharge, and corneal dullness.

MONSANTO CO; Initial Submission: Toxicity Studies with Nonyl Alcohol in Rats and Rabbits with Cover Letter Dated 08/13/92; 02/28/79; EPA No. 88-920007147; Fiche No. OTS0545486

▸ *from HSDB*

12.2 Ecological Information

12.2.1 Environmental Fate/Exposure Summary

1-Nonanol's production and use in perfumery and as a flavoring ingredient may result in its release to the environment through various waste streams. 1-nonanol is also a plant volatile and has been identified in several foods. If released to air, a vapor pressure of 2.27X10-2 mm Hg at 25 deg C indicates 1-nonanol will exist solely as a vapor in the atmosphere. Vapor-phase 1-nonanol will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 28 hours. If released to soil, 1-nonanol is expected to have moderate mobility based upon an estimated Koc of 290. Volatilization from moist soil surfaces is expected to be an important fate process based upon an estimated Henry's Law constant of 3.08X10-5 atm-cu m/mole. 1-Nonanol is not expected to volatilize from dry soil surfaces based upon its vapor pressure. 1-Nonanol has been shown to biodegrade in mixed culture and sludge screening tests. If released into water, 1-nonanol is expected to adsorb to suspended solids and sediment based upon the estimated Koc. Biodegradation of 1-nonanol has been shown to occur in freshwater grab samples. Volatilization from water surfaces is expected to be an important fate process based upon this compound's estimated Henry's Law constant. Estimated volatilization half-lives for a model river and model lake are 1.6 days and 15 days, respectively. An estimated BCF of 160 suggests the potential for bioconcentration in aquatic organisms is high. Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions. Occupational exposure to 1-nonanol may occur through dermal contact with this compound at workplaces where 1-nonanol is produced or used. Monitoring data indicate that the general population

may be exposed to 1-nonanol via ingestion of food and drinking water, and dermal contact with this compound and other consumer products in which 1-nonanol is used as a fragrance. (SRC)

▸ *from HSDB*

12.2.2 Natural Occurring Sources

1-Nonanol is a plant volatile(1) occurring, for example in oil of orange(2), kiwi fruit flowers(3), nectarines(4) and earth almonds (Cyperus esculentus L.)(5).

(1) Graedel TE; Chemical Compounds In The Atmosphere NY, NY: Academic Press (1978) (2) Budavari D et al; The Merck Index 11th ed Rahway, NJ: Merck & Co Inc p. 1056 (1989) (3) Tatsuka K et al; J Agric Food Chem 38: 2176-80 (1990) (4) Takeoka GR et al; J Agric Food Chem 36: 553-60 (1988) (5) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997)

▸ *from HSDB*

12.2.3 Artificial Sources

1-Nonanol may be released to the environment during its manufacture, transport, disposal, and use in perfumery and as a flavoring ingredient (lemon flavoring)(1).

(1) Sax NI, Lewis RJ Jr; Hawley's Condensed Chemical Dictionary 11th ed NY, NY: Van Nostrand Reinhold Co p 836 (1987)

▸ *from HSDB*

12.2.4 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of 290(SRC), determined from a water solubility of 140 mg/L(2) and a regression-derived equation(3), indicates that 1-nonanol is expected to have moderate mobility in soil(SRC). Volatilization of 1-nonanol from moist soil surfaces is expected to be an important fate process(SRC) given an estimated Henry's Law constant of 3.08X10-5 atm-cu m/mole(SRC), derived from its vapor pressure, 2.27X10-2 mm Hg(4) and water solubility(2). 1-Nonanol is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(4). 1-Nonanol has been demonstrated to be readily biodegradable in aerobic screening tests(5-7) and therefore may readily biodegrade in soil(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Barton AFM; pp. 438 in Solubility Data Series Vol 15 (1984) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990) (4) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds NY, NY: Amer Inst for Phys Prop Data (1989) (5) Vaishnav DD et al; Chemosphere 16: 695-703 (1987) (6) Hammerton C; J Appl Chem 5: 517-24 (1955) (7) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 11: 77-82 (1981)

▸ *from HSDB*

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 290(SRC), determined from a water solubility of 140 mg/L(2) and a regression-derived equation(3), indicates that 1-nonanol is expected to adsorb to suspended solids and sediment(SRC). Volatilization from water surfaces is expected(3) based upon an estimated Henry's Law constant of 3.08X10-5 atm-cu m/mole(SRC), derived from its vapor pressure, 2.27X10-2 mm Hg(4), and water solubility(2). Using this Henry's Law constant and an estimation method(3), volatilization half-lives for a model river and model lake are 1.6 days and 15 days, respectively(SRC). 1-Nonanol has been demonstrated to be readily biodegradable in aerobic screening tests(5-7) and therefore may biodegrade in natural water(SRC). According to a classification scheme(8), an estimated BCF of 160(SRC), from a log Kow of 3.77(9) and a regression-derived equation(10), suggests the potential for bioconcentration in aquatic organisms is high(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Barton AFM; pp. 438 in Solubility Data Series Vol 15 (1984) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9, 15-1 to 15-29 (1990) (4) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds NY, NY: Amer Inst for Phys Prop Data (1989) (5) Vaishnav DD et al; Chemosphere 16: 695-703 (1987) (6) Hammerton C; J Appl Chem 5: 517-24 (1955) (7) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 11: 77-82 (1981) (8) Franke C et al; Chemosphere 29: 1501-14 (1994) (9) Tewari YB et al; J Chem Eng Data 27: 451-4 (1982) (10) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999)

from HSDB

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), 1-nonanol, which has a vapor pressure of 2.27X10-2 mm Hg at 25 deg C(2), is expected to exist solely as a vapor in the ambient atmosphere. Vapor-phase 1-nonanol is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be 28 hours(SRC), calculated from its rate constant of 1.4X10-11 cu cm/molecule-sec at 25 deg C(SRC) that was derived using a structure estimation method(3).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds NY, NY: Amer Inst for Phys Prop Data (1989) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)

from HSDB

12.2.5 Biodegredation

AEROBIC: 1-Nonanol degraded fast in aerobic biodegradation screening tests(1-3). In one 5-day BOD test using acclimated mixed cultures, 47.9% of theoretical BOD was consumed(1). In the other test which used an activated sludge inoculum, 1-nonanol's half-life was 1.2 days(SRC), calculated from a biodegradation rate of 2.36X10-2/hr(2). In a third test, 62% of its theoretical BOD in a grab sample of freshwater incubated at 18-19 deg C was expended in 4 days(3).

(1) Vaishnav DD et al; Chemosphere 16: 695-703 (1987) (2) Hammerton C; J Appl Chem 5: 517-24 (1955) (3) Yonezawa Y et al; Kogai Shigen Kenkyusho Iho 11: 77-82 (1981)

from HSDB

12.2.6 Abiotic Degredation

The rate constant for the vapor-phase reaction of 1-nonanol with photochemically-produced hydroxyl radicals has been estimated as 1.4X10-11 cu cm/molecule-sec at 25 deg C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 28 hr at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). 1-Nonanol is not expected to undergo hydrolysis in the environment due to the lack of functional groups that hydrolyze under environmental conditions(2).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 7-4, 7-5, 8-12 (1990)

from HSDB

12.2.7 Bioconcentration

An estimated BCF of 160 was calculated for 1-nonanol(SRC), using a log Kow of 3.77(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC), provided the compound is not metabolized by the organism(SRC).

(1) Tewari YB et al; J Chem Eng Data 27: 451-4 (1982) (2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

from HSDB

12.2.8 Soil Adsorption/Mobility

An estimated BCF of 160 was calculated for 1-nonanol(SRC), using a log Kow of 3.77(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high(SRC), provided the compound is not metabolized by the organism(SRC).

(1) Barton AFM; pp. 438 in Solubility Data Series Vol 15 (1984) (2) Meylan WM et al; Environ Sci Technol 26: 1560-7 (1992) (3) Swann RL et al; Res Rev 85: 17-28 (1983) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods, NY: McGraw-Hill Chapt 4, Eqn 4-5 (1982)

▸ *from HSDB*

12.2.9 Volatilization from Water/Soil

The Henry's Law constant for 1-nonanol estimated as 3.08X10-5 atm-cu m/mol(SRC) derived from its vapor pressure, 2.27X10-2 mm Hg at 25 deg C(1), and water solubility, 140 mg/L(2). This Henry's Law constant indicates that 1-nonanol is expected to volatilize from water surfaces(3). Based on this Henry's Law constant, the volatilization half-life from a model river (1 m deep, flowing 1 m/sec, wind velocity of 3 m/sec)(3) is estimated as 1.6 days(SRC). The volatilization half-life from a model lake (1 m deep, flowing 0.05 m/sec, wind velocity of 0.5 m/sec)(3) is estimated as 15 days(SRC). 1-Nonanol's Henry's Law constant indicates that volatilization from moist soil surfaces may occur(SRC). 1-Nonanol is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(1).

(1) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds NY, NY: Amer Inst for Phys Prop Data (1989) (2) Barton AFM; pp. 438 in Solubility Data Series Vol 15 (1984) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)

▸ *from HSDB*

12.2.10 Water Concentrations

DRINKING WATER: 1-Nonanol, isomer non specified, was identified in drinking water(1). It was identified (maximum concn 100 ng/L) in finished drinking water in The Netherlands that was from bank-filtered Rhine River water(2).

(1) Kool HJ et al; CRC Crit Rev Env Control 12: 307-57 (1982) (2) Piet GH, Morra CF; pp. 31-42 in Artificial Groundwater Recharge Huisman L, Olsthorn TN, eds Pitman Publ (1983)

▸ *from HSDB*

DRINKING WATER: 1-Nonanol, isomer non specified, was identified in drinking water(1). It was identified (maximum concn 100 ng/L) in finished drinking water in The Netherlands that was from bank-filtered Rhine River water(2).

(1) Great Lakes Water Quality Board; An Inventory of Chemical Substances Identified in the Great Lakes Ecosystem Vol 1 Windsor, Ontario, Canada (1983) (2) Ewing BB et al; Monitoring to Detect Previously Unrecognized Pollutants in Surface Water. Washington, DC: US EPA. EPA-560/6-77-015 (1977)

▸ *from HSDB*

SNOW: Eight surface snow samples taken during 1987/88, 1988/89, and 1990/91 antartic expeditions were analyzed for pollutants using capillary column GC and GC/MS(1). 1-Nonanol was found in one sample of surface snow from 1990/91 at 27 ng/L (standard deviation 5 ng/L), but was below the detection limit in the other samples(1). The positive sample was taken from the area closest to the Italian base camp and the coast(1).

(1) Desederi PG et al; J Environ Anal Chem 55: 33-46 (1994)

▸ *from HSDB*

12.2.11 Food Survey Values

1-Nonanol has been identified in a variety of foods including nectarines(1), oil of orange(7), cassava(2), duck(3), peanut oil(4), earth almonds (Cyperus esculentus L.)(5), and a French mountain cheese(6). Unspecified nonyl alcohol isomers have been identified in pork and beef(7,8).

(1) Takeoka GR et al; J Agric Food Chem 36: 553-60 (1988) (2) Dougan J et al; J Sci Food Agric 34: 874-84 (1983) (3) Wu CM, Liou SE; J Agric Food Chem 40: 838-41 (1992) (4) Chung TY et al; J Agric Food Chem 41: 1467-70 (1993) (5) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997) (6) Budavari D et al; The Merck Index. 11th ed., Rahway, NJ: Merck & Co Inc, p. 1056 (1989) (7) King MF et al; J Agric Food Chem 41: 1974-81 (1993) (8) Shahidi F et al; CRC Crit Rev Food Sci Nature 24: 141-243 (1986)

from HSDB

12.2.12 Plant Concentrations

1-Nonanol has been identified in kiwi fruit flowers(1), nectarines(2) and earth almonds (Cyperus esculentus L.)(3).

(1) Tatsuka K et al; J Agric Food Chem 38: 2176-80 (1990) (2) Takeoka GR et al; J Agric Food Chem 36: 553-60 (1988) (3) Cantalejo MJ; J Agric Food Chem 45: 1853-60 (1997)

from HSDB

12.2.13 Fish/Seafood Concentrations

1-Nonanol was detected in lake trout from Lake Michigan near Saugatuck, MI(1). Although the concns were not reported, the gas chromatography peaks indicate that moderate concns were present.

(1) Hesselberg RJ, Seelye JG; p. 49 in ADMEN Rep 82-1 Ann Arbor, MI: US Fish Wildlife Soc (1982)

from HSDB

12.2.14 Probable Routes of Human Exposure

NIOSH (NOES Survey 1981-1983) has statistically estimated that 1557 workers (276 of these are female) are potentially exposed to 1-nonanol in the US(1). Occupational exposure to 1-nonanol may occur through dermal contact with this compound at workplaces where 1-nonanol is produced or used(SRC). Monitoring data indicate that the general population may be exposed to 1-nonanol via ingestion of food and drinking water, and dermal contact with this compound and other consumer products in which 1-nonanol is used as a fragrance(SRC).

(1) NIOSH; International Safety Cards. Nonyl alcohol. 143-08-8. Available at http://www.cdc.gov/niosh/ipcs/nicstart.html as of Jun 8, 2006.

from HSDB

13 Literature

13.1 Depositor Provided PubMed Citations

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13.2 NLM Curated PubMed Citations

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from PubChem

13.3 Metabolite References

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1 to 5 of 6 View More

PMID	Reference
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16902246	Watson AD: Thematic review series: systems biology approaches to metabolic and cardiovascular disorders. Lipidomics: a global approach to lipid analysis in biological systems. J Lipid Res. 2006 Oct;47(10):2101-11. Epub 2006 Aug 10.
17374880	Sethi JK, Vidal-Puig AJ: Thematic review series: adipocyte biology. Adipose tissue function and plasticity orchestrate nutritional adaptation. J Lipid Res. 2007 Jun;48(6):1253-62. Epub 2007 Mar 20.
20044567	Lingwood D, Simons K: Lipid rafts as a membrane-organizing principle. Science. 2010 Jan 1;327(5961):46-50. doi: 10.1126/science.1174621.

PMID	Reference
	Yannai, Shmuel. (2004) Dictionary of food compounds with CD-ROM: Additives, flavors, and ingredients. Boca Raton: Chapman & Hall/CRC.

from Human Metabolome Database (HMDB)

13.4 Springer Nature References

CLICK TO LOAD...

from Springer Nature

14 Patents

14.1 Depositor-Supplied Patent Identifiers

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from PubChem

15 Biomolecular Interactions and Pathways

15.1 Protein Bound 3-D Structures

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from PubChem

15.2 DrugBank Interactions

Target	ATP synthase subunit c, sodium ion specific
General Function	Lipid binding
Specific Function	F(1)F(0) ATP synthase produces ATP from ADP in the presence of a proton or sodium gradient. F-type ATPases consist of two structural domains, F(1) containing the extramembraneous catalytic core and F(0) containing the membrane sodium channel, linked together by a central stalk and a peripheral stalk. During catalysis, ATP synthesis in the catalytic domain of F(1) is coupled via a rotary mechanism of the central stalk subunits to sodium translocation.Key component of the F(0) channel; it plays a direct role in translocation across the membrane. A homomeric c-ring of between 10-14 subunits forms the central stalk rotor element with the F(1) delta and epsilon subunits (Probable).
Reference	Overington JP, Al-Lazikani B, Hopkins AL: How many drug targets are there? Nat Rev Drug Discov. 2006 Dec;5(12):993-6. Abstract: PubMed
Reference	Imming P, Sinning C, Meyer A: Drugs, their targets and the nature and number of drug targets. Nat Rev Drug Discov. 2006 Oct;5(10):821-34. Abstract: PubMed

from DrugBank

16 Biological Test Results

16.1 BioAssay Results

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17 Classification

17.1 Ontologies

17.1.1 MeSH Tree

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from MeSH

17.1.2 ChEBI Ontology

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from ChEBI

17.1.3 LIPID MAPS Classification

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from LIPID MAPS

17.1.4 WIPO IPC

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from WIPO

17.1.5 EPA Safer Choice

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from EPA Safer Choice

17.1.6 ChemIDplus

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18 Information Sources

1. CAMEO Chemicals /source/CAMEO Chemicals
   NONANOL
   https://cameochemicals.noaa.gov/chemical/8911 https://cameochemicals.noaa.gov/chemical/8911

2. ChemIDplus /source/ChemIDplus
   Nonanol
   https://chem.nlm.nih.gov/chemidplus/sid/0028473214 https://chem.nlm.nih.gov/chemidplus/sid/0028473214
   Nonyl alcohol
   https://chem.nlm.nih.gov/chemidplus/sid/0000143088 https://chem.nlm.nih.gov/chemidplus/sid/0000143088
   ChemIDplus Chemical Information Classification
   https://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp https://chem.sis.nlm.nih.gov/chemidplus/chemidheavy.jsp

3. DTP/NCI /source/DTP/NCI
   1-Nonanol
   https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=5521
   https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=5521

4. DrugBank /source/DrugBank
   Nonan-1-Ol
   http://www.drugbank.ca/drugs/DB03143 http://www.drugbank.ca/drugs/DB03143
   http://www.drugbank.ca/drugs/DB03143#targets http://www.drugbank.ca/drugs/DB03143#targets

5. EPA Chemicals under the TSCA /source/EPA Chemicals under the TSCA
   Nonanol
   http://www.epa.gov/chemical-data-reporting http://www.epa.gov/chemical-data-reporting

6. EPA DSStox /source/EPA DSStox
   1-Nonanol
   https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID6022008 https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID6022008

7. European Chemicals Agency - ECHA /source/European Chemicals Agency - ECHA
   Nonan-1-ol
   https://www.echa.europa.eu https://www.echa.europa.eu
   Nonan-1-ol
   https://www.echa.europa.eu/web/guest/information-on-chemicals/cl-inventory-database/-/discli/details/84236
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8. Human Metabolome Database (HMDB) /source/Human Metabolome Database (HMDB)
   1-Nonanol
   http://www.hmdb.ca/metabolites/HMDB0031265 http://www.hmdb.ca/metabolites/HMDB0031265

9. HSDB /source/HSDB
   1-NONANOL
   https://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+@rel+143-08-8 https://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+@rel+143-08-8

10. FDA/SPL Indexing Data /source/FDA/SPL Indexing Data
    NGK73Q6XMC
    https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/
    https://www.fda.gov/ForIndustry/DataStandards/SubstanceRegistrationSystem-UniqueIngredientIdentifierUNII/

11. EPA Safer Choice /source/EPA Safer Choice

1-Nonanol
https://www.epa.gov/saferchoice/safer-ingredients https://www.epa.gov/saferchoice/safer-ingredients
EPA Safer Chemical Ingredients Classification
https://www.epa.gov/saferchoice https://www.epa.gov/saferchoice

12. EU Food Improvement Agents /source/EU Food Improvement Agents

Nonan-1-ol
http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32012R0872 http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32012R0872

13. FAO/WHO Food Additive Evaluations - JECFA /source/FAO/WHO Food Additive Evaluations - JECFA

ALCOHOL C-9
http://apps.who.int/food-additives-contaminants-jecfa-database/chemical.aspx?chemID=485 http://apps.who.int/food-additives-contaminants-jecfa-database/chemical.aspx?chemID=485

14. NITE-CMC /source/NITE-CMC

Nonan-1-ol
http://www.safe.nite.go.jp/english/ghs/08-meti-0047e.html http://www.safe.nite.go.jp/english/ghs/08-meti-0047e.html

15. Flavor & Extract Manufacturers Association - FEMA /source/Flavor & Extract Manufacturers Association - FEMA

NONYL ALCOHOL
https://www.femaflavor.org/flavor-library/nonyl-alcohol https://www.femaflavor.org/flavor-library/nonyl-alcohol

16. SpectraBase /source/SpectraBase

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https://spectrabase.com/compound/6ExYfQORYhy#HGCFeSGhfia https://spectrabase.com/compound/6ExYfQORYhy#HGCFeSGhfia
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https://spectrabase.com/compound/6ExYfQORYhy#2SKxClPSyC4 https://spectrabase.com/compound/6ExYfQORYhy#2SKxClPSyC4
https://spectrabase.com/compound/6ExYfQORYhy#JXyHBCePK9L https://spectrabase.com/compound/6ExYfQORYhy#JXyHBCePK9L
https://spectrabase.com/compound/6ExYfQORYhy#1Y3ZqApk3Ce https://spectrabase.com/compound/6ExYfQORYhy#1Y3ZqApk3Ce
https://spectrabase.com/compound/6ExYfQORYhy#7Wh0pPGXElU https://spectrabase.com/compound/6ExYfQORYhy#7Wh0pPGXElU
https://spectrabase.com/compound/6ExYfQORYhy#FalintqXONS https://spectrabase.com/compound/6ExYfQORYhy#FalintqXONS
https://spectrabase.com/compound/6ExYfQORYhy#Kl1Eqdh7awE https://spectrabase.com/compound/6ExYfQORYhy#Kl1Eqdh7awE

17. NIST /source/NIST

1-Nonanol
http://www.nist.gov/srd/nist1a.cfm http://www.nist.gov/srd/nist1a.cfm

18. OSHA Chemical Sampling Information /source/OSHA Chemical Sampling Information

Nonyl Alcohol
https://www.osha.gov/dts/chemicalsampling/data/CH_258375.html
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19. Springer Nature /source/Springer Nature

nonanol
https://pubchem.ncbi.nlm.nih.gov/substance/341141889 https://pubchem.ncbi.nlm.nih.gov/substance/341141889

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Data deposited in or computed by PubChem

https://pubchem.ncbi.nlm.nih.gov https://pubchem.ncbi.nlm.nih.gov

22. MeSH /source/MeSH

1-nonanol
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MeSH Tree
http://www.nlm.nih.gov/mesh/meshhome.html http://www.nlm.nih.gov/mesh/meshhome.html

23. ChEBI /source/ChEBI

ChEBI Ontology
http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology
http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

24. LIPID MAPS /source/LIPID MAPS

LIPID MAPS classification system for lipids
http://www.lipidmaps.org/data/classification/LM_classification_exp.php
http://www.lipidmaps.org/data/classification/LM_classification_exp.php

25. WIPO /source/WIPO

International Patent Classification
http://www.wipo.int/classifications/ipc/ http://www.wipo.int/classifications/ipc/

26. NCBI

LinkOut is a service that allows one to link directly from NCBI databases to a wide range of information and services beyond NCBI systems.
https://www.ncbi.nlm.nih.gov/projects/linkout https://www.ncbi.nlm.nih.gov/projects/linkout