Valeraldehyde:

The following information was generated from the
Hazardous Substances Data Bank (HSDB),
a database of the National Library of Medicine's TOXNET system
(http://toxnet.nlm.nih.gov) on October 30, 2006.

Query: The chemical name valeraldehyde was identified.
The following terms were added from ChemIDplus:
pentanal
valerylaldehyde
valeric aldehyde
butyl formal
amyl aldehyde
CAS Registry Number: 110-62-3

1
NAME: PENTANAL

HSN: 851

RN: 110-62-3

HUMAN HEALTH EFFECTS:

HUMAN TOXICITY EXCERPTS:

A MILD IRRITANT. [The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 1272]**PEER REVIEWED**

/CNS depressant/ and irritation common to aldehydes, but they are mild. [ITII. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1988., p. 551]**PEER REVIEWED**

SKIN, EYE AND RESPIRATORY IRRITATIONS:

Vapor may irritate eyes. [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

PROBABLE ROUTES OF HUMAN EXPOSURE:

The general population may be exposed to pentanal in both indoor and outdoor air via inhalation and by ingesting food in which pentanal naturally occurs. (SRC) **PEER REVIEWED**

NIOSH (NOES Survey 1981-1983) has statistically estimated that 1,557 workers, including 276 females, are exposed to pentanal in the USA(1). [(1) NIOSH; National Occupational Exposure Survey (1989)]**PEER REVIEWED**

BODY BURDEN:

As part of EPA's pilot Total Exposure Assessment Methodology (TEAM) study, the breaths of 12 subjects were analyzed. Only one contained pentanal(1). The concn was not reported. In EPA's National Human Adipose Tissue Survey (NHATS) for 1982, all 46 composite samples analyzed contained pentanal(2). Pentanal was detected, but not quantified, in 7 of 8 samples of mother's milk analyzed from 4 U.S. urban areas(3). [(1) Wallace LA et al; Environ Res 35: 293-319 (1984) (2) Onstot JD et al; Characterization of HRGC/MS Unidentified Peaks from the Broad Scan Analysis of the FY82 NHATS Composites Vol.I USEPA 68-02-4252 (1987) (3) Pellizzari ED et al; Bull Environ Contam Toxicol 28: 322-8 (1982)]**PEER REVIEWED**

AVERAGE DAILY INTAKE:

AIR INTAKE: (Assume mean concn 0.05-1.07 ppb(1,2)) 0.0036-0.765 ug; WATER INTAKE: 0 ug; FOOD: Insufficient Data. [(1) Guicherit K, Schulting FL; Sci Total Environ 43: 193-219 (1985) (2) Jonsson A et al; Environ Intl 11: 383-92 (1985)]**PEER REVIEWED**

EMERGENCY MEDICAL TREATMENT:

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EMT COPYRIGHT DISCLAIMER:

Portions of the POISINDEX(R) and MEDITEXT(R) database have been provided here for general reference. THE COMPLETE POISINDEX(R) DATABASE OR MEDITEXT(R) DATABASE SHOULD BE CONSULTED FOR ASSISTANCE IN THE DIAGNOSIS OR TREATMENT OF SPECIFIC CASES. The use of the POISINDEX(R) and MEDITEXT(R) databases is at your sole risk. The POISINDEX(R) and MEDITEXT(R) databases are provided "AS IS" and "as available" for use, without warranties of any kind, either expressed or implied. Micromedex makes no representation or warranty as to the accuracy, reliability, timeliness, usefulness or completeness of any of the information contained in the POISINDEX(R) and MEDITEXT(R) databases. ALL IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE OR USE ARE HEREBY EXCLUDED. Micromedex does not assume any responsibility or risk for your use of the POISINDEX(R) or MEDITEXT(R) databases. Copyright 1974-2006 Thomson MICROMEDEX. All Rights Reserved. Any duplication, replication, "downloading," sale, redistribution or other use for commercial purposes is a violation of Micromedex' rights and is strictly prohibited.<p>The following Overview, *** ACETALDEHYDE ***, is relevant for this HSDB record chemical.

LIFE SUPPORT:

- This overview assumes that basic life support measures have been instituted.

CLINICAL EFFECTS:

0.2.1 SUMMARY OF EXPOSURE

0.2.1.1 ACUTE EXPOSURE

A) This agent is a skin and mucous membrane irritant which causes a burning sensation of the nose, throat, and eyes. Prolonged exposure to high concentrations may injure the corneal epithelium causing persistent lacrimation, photophobia, and foreign body sensation.

B) Fatalities, following inhalation, are due to anesthesia when prompt and pulmonary edema when delayed. Very large exposures may cause death due to respiratory paralysis.

C) Prolonged skin contact may cause dermal erythema and burns. Repeated exposures may cause dermatitis due to primary irritation or sensitization.

D) Sympathomimetic effects of acetaldehyde include tachycardia, hypertension, and increased respiration. Bradycardia and hypotension occur at higher levels of acetaldehyde exposure.

0.2.3 VITAL SIGNS

0.2.3.1 ACUTE EXPOSURE

A) Increased ventilation, hypertension, and tachycardia are sympathomimetic effects which may develop at low levels of exposure.

B) Higher levels produce bradycardia and hypotension.

0.2.4 HEENT

0.2.4.1 ACUTE EXPOSURE

A) Human eye irritation begins to occur at 50 ppm in the air and becomes excessive at 200 ppm. Splash contacts produce painful but superficial corneal injury. Changes in auditory sensitivity were noted in one foreign study of vapor exposures.

0.2.5 CARDIOVASCULAR

0.2.5.1 ACUTE EXPOSURE

A) In humans, systemic poisoning can result in sympathomimetic effects of tachycardia and hypertension.

B) Ventricular dysrhythmias have occurred in halothane anesthetized animals given acetaldehyde.

0.2.6 RESPIRATORY

0.2.6.1 ACUTE EXPOSURE

- A) Acetaldehyde is a pulmonary irritant and may cause bronchitis and pulmonary edema when inhaled. Very high concentrations may result in respiratory paralysis.

0.2.7 NEUROLOGIC

0.2.7.1 ACUTE EXPOSURE

- A) High serum concentrations have caused narcosis in animals.

0.2.8 GASTROINTESTINAL

0.2.8.1 ACUTE EXPOSURE

- A) Liquid acetaldehyde is an emetic.

0.2.9 HEPATIC

0.2.9.1 ACUTE EXPOSURE

- A) Acetaldehyde can impair mitochondrial respiration in the liver, similar to effects seen with ethanol.

0.2.14 DERMATOLOGIC

0.2.14.1 ACUTE EXPOSURE

- A) Prolonged contact causes erythema and burns. Repeated exposures may cause dermatitis.

0.2.20 REPRODUCTIVE HAZARDS

- A) No human reproductive effects were found at the time of this review. Acetaldehyde was detected in 4 out of 8 samples of human breast milk. Embryotoxicity and malformations have been seen in animals.

0.2.21 CARCINOGENICITY

0.2.21.1 IARC CATEGORY

- A) IARC Carcinogenicity Ratings for CAS75-07-0 (IARC, 2004):
  - 1) IARC Classification
    - a) Listed as: Acetaldehyde
    - b) Carcinogen Rating: 2B
      - 1) The agent (mixture) is possibly carcinogenic to humans. The exposure circumstance entails exposures that are possibly carcinogenic to humans. This category is used for agents, mixtures and exposure circumstances for which there is limited evidence of carcinogenicity in humans and less than sufficient evidence of carcinogenicity in experimental animals. It may also be used when there is inadequate evidence of carcinogenicity in humans but there is sufficient evidence of carcinogenicity in experimental animals. In some instances, an agent, mixture or exposure circumstance for which there is inadequate evidence of carcinogenicity in humans but limited evidence of carcinogenicity in experimental animals together with supporting evidence from other relevant data may be placed in this group.

0.2.21.2 HUMAN OVERVIEW

- A) Acetaldehyde has been implicated as a cocarcinogen in the workplace. There was an increased incidence of total cancers in acetaldehyde production workers as compared with the general population, although this study failed to adjust for confounders.

0.2.21.3 ANIMAL OVERVIEW

- A) Acetaldehyde is a carcinogen in rats and hamsters.

0.2.22 GENOTOXICITY

- A) Acetaldehyde has been active in short-term assays for DNA damage and repair, mutagenicity, chromosome aberrations, sister chromatid exchanges, micronucleus test, and oncogenic transformation (HSDB , 2001; RTECS , 2001).

LABORATORY:

- A) No toxic levels have been established. For significant exposures, base-line liver and kidney function tests may be indicated.
- B) Monitor vital signs and chest x-ray in all significant exposures.
- C) Monitor for signs of CNS depression following significant exposures.

TREATMENT OVERVIEW:

0.4.2 ORAL EXPOSURE

- A) GASTRIC LAVAGE: Consider after ingestion of a potentially life-threatening amount of poison if it can be performed soon after ingestion (generally within 1 hour). Protect airway by placement in Trendelenburg and left lateral decubitus position or by endotracheal intubation. Control any seizures first.
  - 1) CONTRAINDICATIONS: Loss of airway protective reflexes or decreased level of consciousness in unintubated patients; following ingestion of corrosives; hydrocarbons (high aspiration potential); patients at risk of hemorrhage or gastrointestinal perforation; and trivial or non-toxic ingestion.
- B) ACTIVATED CHARCOAL: Administer charcoal as a slurry (240 mL water/30 g charcoal). Usual dose: 25 to 100 g in adults/adolescents, 25 to 50 g in children (1 to 12 years), and 1 g/kg in infants less than 1 year old.
- C) EMESIS: Ipecac-induced emesis is not recommended because of the potential for CNS depression.
- D) ACUTE LUNG INJURY: Maintain ventilation and oxygenation and evaluate with frequent arterial blood gas or pulse oximetry monitoring. Early use of PEEP and mechanical ventilation may be needed.
- E) Acetaldehyde in high concentrations may result in narcosis; patients should be monitored for possible coma and respiratory depression.

0.4.3 INHALATION EXPOSURE

- A) INHALATION: Move patient to fresh air. Monitor for respiratory distress. If cough or difficulty breathing develops, evaluate for respiratory tract irritation, bronchitis, or pneumonitis. Administer oxygen and assist ventilation as required. Treat bronchospasm with inhaled beta2 agonist and oral or parenteral corticosteroids.
- B) ACUTE LUNG INJURY: Maintain ventilation and oxygenation and evaluate with frequent arterial blood gas or pulse oximetry monitoring. Early use of PEEP and mechanical ventilation may be needed.
- C) Acetaldehyde in high concentrations may result in narcosis so patients should be monitored for possible coma and respiratory depression.

0.4.4 EYE EXPOSURE

- A) DECONTAMINATION: Irrigate exposed eyes with copious amounts of room temperature water for at least 15 minutes. If irritation, pain, swelling, lacrimation, or photophobia persist, the patient should be seen in a health care facility.

0.4.5 DERMAL EXPOSURE

- A) OVERVIEW
  - 1) DECONTAMINATION: Remove contaminated clothing and wash exposed area thoroughly with soap and water. A physician may need to examine the area if irritation or pain persists.

RANGE OF TOXICITY:

- A) 50 ppm for 15 minutes will cause eye irritation in the majority of subjects.
- B) Fatalities have occurred in animals exposed to levels of 16,000 ppm for four hours.

ANIMAL TOXICITY STUDIES:

NON-HUMAN TOXICITY EXCERPTS:

3 OUT OF 3 RATS DIED AFTER INHALATION EXPOSURE TO 48,000 PPM FOR 1.2 HR; 0 OUT OF 3 RATS DIED AFTER EXPOSURE TO 1,400 PPM FOR 6 HR. COMPOUND PRODUCED SEVERE IRRITANT EFFECT ON SKIN OF GUINEA PIGS & ON EYE OF RABBITS. /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. 2643]**PEER REVIEWED**

Rated 5 on rabbit eyes. The compound was tested externally on the eyes of rabbits, and according to the degree of injury observed after 24 hours, and rated on a scale of 1 to 10. The most severely injurious substances have been rated 10. [Grant, W.M. Toxicology of the Eye. 3rd ed. Springfield, IL: Charles C. Thomas Publisher, 1986., p. 1063]**PEER REVIEWED**

Inhalation of n-valeraldehyde vapor at 4000 ppm for 4 hours was lethal to three of six rats. [American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1675]**PEER REVIEWED**

n-Valeraldehyde is reported to be severely irritating to guinea pig. [American Conference of Governmental Industrial Hygienists, Inc.

Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1675]**PEER REVIEWED**

In a study of the relative inhalation toxicity of 13 aliphatic saturated and unsaturated aldehydes, mice (50), guinea pigs (20), or rabbits (5) were exposed to the aerosols for periods of 10 hours or until death. Two mice died during exposure at 670 ppm n-valeraldehyde. Five guinea pigs and two mice died subsequent to cessation of exposure. No rabbits died during or after exposure. ... All aldehydes employed in this study were irritant substances, with the main pathologic changes occurring in the respiratory tract. n-Valeraldehyde was considered less toxic than the lower saturated aldehydes. [American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1675]**PEER REVIEWED**

The sensory irritation potential of n-valeraldehyde was investigated in B6C3F1 and Swiss Webster mice. Groups of three or four mice were exposed in a head-only exposure chamber for 10 minutes to varying conc of n-valeraldehyde. Respiratory rates were recorded during a 5 min pre-exposure, a 10 min exposure, and a 5 min recovery period. The average maximum reduction in respiratory rate for 1 min was computed from the response of each group of animals. RD50 values (conc eliciting a 50% decrease in respiratory rate) were 1190 and 1121 ppm for B6C3F1 and Swiss Webster mice, respectively. [American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1675]**PEER REVIEWED**

NON-HUMAN TOXICITY VALUES:

LD50 Mouse oral 6,400 mg/kg [Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2716]**PEER REVIEWED**

LD50 Guinea pig skin 20 mg/kg [Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2716]**PEER REVIEWED**

LD50 Rat oral 3,200 mg/kg [Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2716]**PEER REVIEWED**

LD50 Rabbit skin 6,000 mg/kg [Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2716]**PEER REVIEWED**

ECOTOXICITY VALUES:

LC50 Pimephales promelas (fathead minnow) 12.4 mg/l/96 hr (95% confidence limit 11.3-13.6 mg/l), flow-through bioassay with measured concentrations, 24.5 deg C, dissolved oxygen 6.1 mg/l, hardness 37.5 mg/l calcium carbonate, alkalinity 44.1 mg/l calcium carbonate, and pH 7.52. [Geiger D.L., Poirier S.H., Brooke L.T., Call D.J., (eds). Acute Toxicities of Organic Chemicals to Fathead Minnows (Pimephales Promelas). Vol. II. Superior, Wisconsin: University of Wisconsin-Superior, 1985., p. 61]**PEER REVIEWED**

METABOLISM/PHARMACOKINETICS:

METABOLISM/METABOLITES:

Hydrogeration, oxidation, and aminating hydrogeration to corresponding alcohol, acid, and amine. [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA1 328]**PEER REVIEWED**

PHARMACOLOGY:

ENVIRONMENTAL FATE & EXPOSURE:

ENVIRONMENTAL FATE/EXPOSURE SUMMARY:

Pentanal is a natural product and is emitted into the atmosphere by plants and microorganisms and from animal wastes and forest fires. Pentanal may

also be released to the environment during its production, use as a chemical intermediate, and during its transport, storage and disposal. Anthropogenic sources include emissions from gasoline, diesel, turbine engines, burning logs, and some building products such as carpet-covered pressed board and polyurethane-coated plywood. Pentanal has a high Henry's Law constant, high vapor pressure, and a very low soil adsorptivity and if released on soil, it would readily volatilize as well as leach into the ground. If release in water, pentanal will be lost to the atmosphere by volatilization. Its estimated volatilization half-life from a model river is 8.3 hr. It may also undergo direct photolysis in surface waters. Based on laboratory biodegradability tests and the behavior of similar chemicals, pentanal would be expected to readily biodegrade both in soil and water. In the atmosphere, pentanal will react with photochemically-produced hydroxyl radicals. It's half-life resulting from its reaction with hydroxyl radicals is 13.5 hr. Direct photolysis is also expected to be an important degradative process in the atmosphere. However, pentanal's rate of direct photolysis is unknown. The general population may be exposed to pentanal in both indoor and outdoor air via inhalation and by ingesting food in which pentanal naturally occurs. (SRC)
PEER REVIEWED

PROBABLE ROUTES OF HUMAN EXPOSURE:

The general population may be exposed to pentanal in both indoor and outdoor air via inhalation and by ingesting food in which pentanal naturally occurs. (SRC) **PEER REVIEWED**

NIOSH (NOES Survey 1981-1983) has statistically estimated that 1,557 workers, including 276 females, are exposed to pentanal in the USA(1).
[(1) NIOSH; National Occupational Exposure Survey (1989)]**PEER REVIEWED**

BODY BURDEN:

As part of EPA's pilot Total Exposure Assessment Methodology (TEAM) study, the breaths of 12 subjects were analyzed. Only one contained pentanal(1).

The concn was not reported. In EPA's National Human Adipose Tissue Survey (NHATS) for 1982, all 46 composite samples analyzed contained pentanal(2). Pentanal was detected, but not quantified, in 7 of 8 samples of mother's milk analyzed from 4 U.S. urban areas(3). [(1) Wallace LA et al; Environ Res 35: 293-319 (1984) (2) Onstot JD et al; Characterization of HRGC/MS Unidentified Peaks from the Broad Scan Analysis of the FY82 NHATS Composites Vol.I USEPA 68-02-4252 (1987) (3) Pellizzari ED et al; Bull Environ Contam Toxicol 28: 322-8 (1982)]**PEER REVIEWED**

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NATURAL POLLUTION SOURCES:

Pentanal is a plant volatile(1-2). It is also an emission product of microorganisms and animal waste(1). It may be emitted from burning logs(3) and therefore, forest fires would be a source of pentanal. [(1) Graedel TE et al; Atmospheric Chemical Compounds NY: Academic Press (1986) (2) Isidorov VA et al; Atmos Environ 19: 1-8 (1985) (3) Lipari F et al; Environ Sci Technol 18: 326-30 (1984)]**PEER REVIEWED**

REPORTED FOUND AMONG CONSTITUENTS OF SEVERAL ESSENTIAL OILS: BRAZILIAN SASSAFRAS, BULGARIAN ROSE, BULGARIAN CLARY SAGE, & OTHERS; ALSO IN DISTILLATES FROM LEAVES OF VARIOUS EUCALYPTUS SPECIES: E CINEREA, E GLOBULUS, E DIVES, E MAIDENI,& E HEMILAMPRA. [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 558]**PEER REVIEWED**

ARTIFICIAL POLLUTION SOURCES:

Pentanal may be released to the environment during its production, use as a chemical intermediate primarily in the production of the corresponding alcohol, acid and amine, transport, storage and disposal(1). It is an emission product of gasoline, diesel, and turbine engines(2). Pentanal is a product of the photooxidation of 1-hexene(2). Pentanal may be emitted from fireplaces. Emission appears to be inversely proportional to the burn rate(3). In eight tests, the pentanal emission rate from a fireplace with different types of logs ranged from nondetectable to 0.010 g/kg of wood(3). [(1) Falbe J et al; Ullman's Encyclopedia of Industrial Chemistry A1: 321-52 (1985) (2) Graedel TE et al; Atmospheric Chemical Compounds NY: Academic Press (1986) (3) Lipari F et al; Environ Sci Technol 18: 326-30 (1984)]**PEER REVIEWED**

ENVIRONMENTAL FATE:

TERRESTRIAL FATE: Pentanal is estimated to have a very low soil adsorptivity and if released on soil, it would readily leach. It has a high vapor pressure(2) and Henry's Law constant(1) and should volatilize from the upper layers of soil. Based on laboratory tests and the behavior of similar chemicals, pentanal would be expected to readily biodegrade(SRC). [(1) Buttery RG et al; J Agric Food Chem 17: 385-9 (1969) (2) Flick EW; Industrial Solvents Handbook 4th ed. p. 511 Noyes Publishing Co. (1991)]**PEER REVIEWED**

AQUATIC FATE: If release in water, pentanal will be released to the atmosphere by volatilization. Using its Henry's Law constant(1), one estimates a volatilization half-life from a model river of 8.3 hours(2). Based on laboratory biodegradability tests(3) and the behavior of similar chemicals, pentanal would be expected to readily biodegrade(SRC). [(1) Buttery RG et al; J Agric Food Chem 17: 385-9 (1969) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill Chapt 15, 16 (1982) (3) Gerhold RM, Malaney GW; J Water Pollut Contr Fed 38: 562-79 (1966)]**PEER REVIEWED**

ATMOSPHERIC FATE: In the atmosphere, pentanal will react with photochemically-produced hydroxyl radicals and undergo direct photolysis(2). It's half-life resulting from its reaction with hydroxyl radicals is 13.5 hr(1,SRC). Its rate of direct photolysis, while believed to be important in the atmosphere, is unknown. Photolysis may also occur in the surface layers of water. However, estimates of photolysis half-lives for pentanal cannot be made because of lack of data on quantum yields and photolysis rates(SRC). [(1) Atkinson R; J Chem Phys Ref Data Monograph 1 (1989) (2) Lloyd AC; Tropospheric Chemistry of Aldehydes Wash DC: Natl Bur Standards NTIS PB-299-439 pp. 27-48 (1978)]**PEER REVIEWED**

ENVIRONMENTAL BIODEGRADATION:

Aldehydes, especially straight chain ones, are readily oxidized in biodegradability tests(2). The oxygen uptake in a biodegradability test using sludge from different wastewater treatment plants was 12.7, 16.5, and 17.8 percent of theoretical oxygen demand after 6, 12, and 24 hr, respectively(2). These results are supported by the fact that the analogous chemical, butyraldehyde, is similarly readily biodegradable in laboratory tests(1,3,4,5). While no information was located concerning the anaerobic biodegradability of pentanal, the analogous chemical, butyraldehyde, was readily biodegradable under anaerobic conditions(6) and it is therefore likely that pentanal would show similar behavior(SRC). [(1) Heukelekian H, Rand MC; J Water Pollut Contr Assoc 29: 1040-53 (1955) (2) Gerhold RM, Malaney GW; J Water Pollut Contr Fed 38: 562-79 (1966) (3) Dore M et al; Trib Cebedeau 28: 3-11 (1975) (4) Ettinger MB; Ind Eng Chem 48: 256-9 (1956) (5) Urano K, Kato Z; J Hazard Mater 13: 147-59 (1986) (6) Chou WL et al; Biotech Bioeng Symp 8: 391-414 (1979)]**PEER REVIEWED**

ENVIRONMENTAL ABIOTIC DEGRADATION:

In the atmosphere, pentanal reacts with photochemically-produced hydroxyl radicals with a rate constant of 2.85X10-11 cu cm/molecule-sec(1). Assuming a hydroxyl radical concn of 5X10+5 radicals/cu cm, the half-life of pentanal in the atmosphere would be 13.5 hr(SRC). Aldehydes absorb UV radiation > 290 nm, and investigations with formaldehyde and acetaldehyde indicate that direct photolysis together with reaction with hydroxyl radicals are the major sinks for pentanal in the lower atmosphere(2). Photolysis may also occur in the surface layers of water. However, estimates of photolysis half-lives for pentanal cannot be made because of lack of data on quantum yields and photolysis rates(SRC). [(1) Atkinson R; J Chem Phys Ref Data Monograph 1 (1989) (2) Lloyd AC; Tropospheric Chemistry of Aldehydes Wash DC: Natl Bur Standards NTIS PB-299-439 pp. 27-48 (1978)]**PEER REVIEWED**

ENVIRONMENTAL BIOCONCENTRATION:

Using its estimated log Kow, 1.31(1), one can estimate a BCF of 5.8 for pentanal using a recommended regression equation(2,SRC). Therefore, pentanal would not be expected to bioconcentrate in aquatic organisms. [(1) Meylan WM, Howard PH; Group Contribution Method for Estimating Octanol-Water Partition Coefficients. SETAC Meeting Cincinnati, OH. Nov 8-12, (1992) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill Chapt 5 (1982)]**PEER REVIEWED**

SOIL ADSORPTION/MOBILITY:

Using the water solubility for pentanal, 13.5 mg/L(1), one can estimate a Koc of 1,040 for pentanal(2,SRC). According to a suggested classification scheme(3), a Koc of this magnitude would indicate that pentanal would have low mobility in soil. [(1) Dean JA; Lange's Handbook of Chemistry 13th ed. NY: McGraw-Hill (1985) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill Chapt 4 (1982) (3) Swann RL et al; Res Rev 85: 17-28 (1983)]**PEER REVIEWED**

VOLATILIZATION FROM WATER/SOIL:

The Henry's Law constant for pentanal is 1.47X10-4 atm-cu m/mole(1). Using this value for the Henry's Law constant one can estimate that the the volatilization half-life of pentanal from a 1 m deep model river flowing at 1 m/s with a 3 m/s wind is 8.3 hours(2,SRC). Similarly, the volatilization half-life of pentanal from a model lake 1 m deep, with a 0.05 m/s current and a 0.5 m/s wind is estimated to be 5.4 days(3,SRC). Its high Henry's Law constant and low adsorptivity to soil indicates that it should readily volatilize from moist soil(2). Pentanal has a high vapor pressure, 26 mm Hg at 20 deg C(3) and would therefore readily volatilize from dry soil and other surfaces. [(1) Buttery RG et al; J Agric Food Chem 17: 385-9 (1969) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill Chapt 15, 16 (1982) (3) Flick EW; Industrial Solvents Handbook 4th ed. p. 511 Noyes Publishing Co. (1991)]**PEER REVIEWED**

ENVIRONMENTAL WATER CONCENTRATIONS:

DRINKING WATER: In an EPA survey of drinking water in 10 cities, pentanal was found in the drinking water of Ottumwa, IA at approximately 0.5 ug/L, but was not detected in the drinking water of Miami, FL, Seattle, WA, Philadelphia, PA, Cincinnati, OH, Grand Forks, MI, Lawrence, MA, New York, NY, Terrebonne Parrish, LA, and Tuscon, AZ(1). [(1) Keith LH et al; pp. 327-373 in Ident Anal Org Pollut Water Keith LH, ed Ann Arbor, MI: Ann Arbor Press (1976)]**PEER REVIEWED**

EFFLUENT CONCENTRATIONS:

Pentanal was emitted from samples of particle board with glued-on carpet and plywood coated with polyurethane at rates of 0.031 and 0.014 mg/sq m-hr, respectively(1). [(1) Colombo A et al; Sci Total Environ 91: 237-49 (1990)]**PEER REVIEWED**

ATMOSPHERIC CONCENTRATIONS:

SOURCE DOMINATED: Levels of pentanal ranging from not detectable to 38 ug/cu m were found in ambient air surrounding the Kin-Buc Waste Disposal Site in New Jersey(1). [(1) Pellizzari ED; Environ Sci Technol 16: 781-5 (1982)]**PEER REVIEWED**

URBAN/SUBURBAN: Air concns of pentanal were determined between 1979 and 1981 at three sites in The Netherlands, an unpolluted island, a small city, and a heavily industrialized area(1). The mean and maximum concns of pentanal in air at these sites in the Netherlands were 0.05 and 0.40 ppb, respectively(1). The mean, minimum, and maximum 1-hr pentanal concns ranged from 0.15-1.07, 0.04-0.37, and 0.33-1.88 ppb, respectively(2) at four urban sites in Stockholm, Sweden. The corresponding concns at a recreational site 12 km outside the central city were 0.49, 0.12, and 1.99 ppb. Ambient levels of pentanal measured on September 11-19, 1985 on the Pomona College campus in Claremont, CA ranged from < 0.1 to 0.6 ppb, with a median of 0.1 ppb(3). These levels were much lower than those measured previously during a photochemical smog episode. Pentanal was detected in one of ten samples in the Kanawha Valley, WV and four of nine air samples in the Shenandoah Valley, VA in the fall of 1977(4). [(1) Guicherit K, Schulting FL; Sci Total Environ 43: 193-219 (1985) (2) JonssonA et al; Environ Intl 11: 383-92 (1985) (3) Grosjean D; Atmos Environ 22: 1637-48 (1988) (4) Erickson MD, Pellizzari ED; Analysis of Organic Air Pollutants in the Kanawha Valley, WV & the Shenandoah Valley VA USEPA-903/9-78-007 (1978)]**PEER REVIEWED**

INDOOR AIR: In a study of air quality in three EPA headquarters' buildings following health complaints, it was found that 18 of the 20 samples contained pentanal above the 0.06 ug/cu m quantitation limit(3). The mean and maximum pentanal concn were 0.5, 0.7, 1.9 ug/cu m and 0.8, 0.9, 2.0 ug/cu m, respectively(3) in the three buildings. Pentanal was found in two of six samples of indoor air analyzed in Italy at concns of 8 and 15 ug/cu m(1). Pentanal was present in two preschools in Stockholm, Sweden(2) and one of four Swedish dwellings that were part of a study on emissions from floor finishes(4). Its concn was not reported. PERSONAL AIR: As part of EPA's pilot Total Exposure Assessment Methodology (TEAM) study, personal air of 8 subjects in New Jersey were monitored(5). None contained pentanal. [(1) De Bortoli M et al; Environ Internat 12: 343-50 (1986) (2) Noma E et al; Atmos Environ 22: 451-60 (1988) (3) USEPA; Indoor Air Quality & Work Environment Study. EPA Headquarters' Buildings. Volume 2. Results of Indoor Air Environmental Monitoring Study. Research Triangle Park, NC: Atmos Res & Exposure Assessment Lab (1990) (4) Van Netten C et al; Bull Environ Contam Toxicol 40: 672-7 (1988) (5) Wallace LA et al; Environ Res 35: 293-319 (1984)]**PEER REVIEWED**

FOOD SURVEY VALUES:

Pentanal has been identified as a volatile in the following foods: Korean chamchwi(1), baked potatoes(2), cassava(3), French mountain cheese(4), raw beef(5,10), roasted filberts(6), boiled short-necked clams and clams(7), scrambled eggs(8), Delicious apples(9), and fried chicken(11). [(1) Chung TY et al; J Agric Food Chem 41: 1693-7 (1993) (2) Coleman EC et al; JAgric Food Chem 29: 42-9 (1981) (3) Dougan J et al; J Sci Food Agric 34: 874-84 (1983) (4) Dumont JP, Adda J; J Agric Food Chem 26: 364-7 (1978) (5) King MF et al; J Agric Food Chem 41: 1974-81 (1993) (6) Kinlin TE et al; J Agric Food Chem 20: 1021-8 (1972) (7) Kubota K et al; J Agric Food Chem 39: 1127-30 (1991) (8) Matiella JE, Hsieh TCY; J Food Sci 56: 387-90, 426 (1991) (9) Mattheis JP et al; J Agric Food Chem 39: 1902-6 (1991) (10) Shahidi F et al; CRC Crit Rev Food Sci Nature 24: 141-243 (1986) (11) Tang J et al; J Agric Food Chem 31: 1287-92 (1983)]**PEER REVIEWED**

PLANT CONCENTRATIONS:

Pentanal is a plant volatile(1). The concentration of pentanal is relatively high in undeveloped apples but then decreases to undetectable levels as the harvest approaches(2). The concentration of pentanal decreases to undetectable levels as the fruit ripens(2). These changes may reflect the use of pentanal in ester synthesis as ripening begins(2). [(1) Graedel TE et al; Atmospheric Chemical Compounds NY: Academic Press (1986) (2) Mattheis JP et al; J Agric Food Chem 39: 1902-6 (1991)]**PEER REVIEWED**

MILK CONCENTRATIONS:

Pentanal was detected, but not quantified, in 7 of 8 samples of mother's milk analyzed from 4 U.S. urban areas(1). [(1) Pellizzari ED et al; Bull Environ Contam Toxicol 28: 322-8 (1982)]**PEER REVIEWED**

OTHER ENVIRONMENTAL CONCENTRATIONS:

Pentanal was detected, but not quantified, in gasoline and diesel fuel(1).

[(1) Hampton CV et al; Environ Sci Technol 16: 287-98 (1982)]**PEER REVIEWED**

ENVIRONMENTAL STANDARDS & REGULATIONS:

TSCA REQUIREMENTS:

Section 8(a) of TSCA requires manufacturers of this chemical substance to report preliminary assessment information concerned with production, use, and exposure to EPA as cited in the preamble in 51 FR 41329. [40 CFR 712.30 (7/1/92)]**PEER REVIEWED**

Pursuant to section 8(d) of TSCA, EPA promulgated a model Health and Safety Data Reporting Rule. The section 8(d) model rule requires manufacturers, importers, and processors of listed chemical substances and mixtures to submit to EPA copies and lists of unpublished health and safety studies. Pentanal is included on this list. [40 CFR 716.120 (7/1/92)]**PEER REVIEWED**

CHEMICAL/PHYSICAL PROPERTIES:

MOLECULAR FORMULA:

C5-H10-O **PEER REVIEWED**

MOLECULAR WEIGHT:

86.13 [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989., p. 1558]**PEER REVIEWED**

COLOR/FORM:

COLORLESS LIQUID [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 55]**PEER REVIEWED**

Colorless liquid. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 94-116. Washington, D.C.: U.S. Government Printing Office, June 1994., p. 326]**QC REVIEWED**

ODOR:

POWERFUL, ACRID, PUNGENT ODOR [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 558]**PEER REVIEWED**

Strong, acrid, pungent odor. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 94-116. Washington, D.C.: U.S. Government Printing Office, June 1994., p. 326]**QC REVIEWED**

TASTE:

WARM, SLIGHTLY FRUITY, & NUT-LIKE AT LOW LEVELS [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 558]**PEER REVIEWED**

PLEASANT, CHOCOLATE AROMA & TASTE [Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Volume 2. Boca Raton, Florida: CRC Press, Inc., 1980., p. 306]**PEER REVIEWED**

... IT HAS SHARP, PENETRATING FLAVOR [Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 510]**PEER REVIEWED**

BOILING POINT:

103 DEG C @ 760 MM HG [Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 71st ed. Boca Raton, FL: CRC Press Inc., 1990-1991., p. 3-513]**PEER REVIEWED**

MELTING POINT:

-91.5 DEG C [Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 71st ed. Boca Raton, FL: CRC Press Inc., 1990-1991., p. 3-513]**PEER REVIEWED**

DENSITY/SPECIFIC GRAVITY:

0.8095 @ 20 DEG C/4 DEG C [Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 71st ed. Boca Raton, FL: CRC Press Inc., 1990-1991., p. 3-513]**PEER REVIEWED**

SOLUBILITIES:

SOL IN ETHANOL, ETHER [Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 71st ed. Boca Raton, FL: CRC Press Inc., 1990-1991., p. 3-513]**PEER REVIEWED**

SOL IN PROPYLENE GLYCOL; OILS [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 558]**PEER REVIEWED**

1.35% in water [Dean JA; Lange's Handbook of Chemistry 13th ed p. 7-576 1985]**PEER REVIEWED**

water solubility = 1.17X10+4 mg/l @ 20 deg C [Yalkowsky SH, Dannenfelser RM; The AQUASOL dATAbASE of Aqueous Solubility. Fifth Ed, Tucson, AZ: Univ Az, College of Pharmacy (1992)]**QC REVIEWED**

SPECTRAL PROPERTIES:

INDEX OF REFRACTION: 1.3944 @ 20 DEG C/D; MAX ABSORPTION (GAS): 178 NM, 182 NM, 184 NM [Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-413]**PEER REVIEWED**

SADTLER REFERENCE NUMBER: 9199 (IR, PRISM) [Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc., 1979., p. C-679]**PEER REVIEWED**

IR: 9490 (Sadtler Research Laboratories Prism Collection) [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985., p. V2 11]**PEER REVIEWED**

NMR: 17142 (Sadtler Research Laboratories Spectral Collection) [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985., p. V2 11]**PEER REVIEWED**

MASS: 22 (Aldermaston, Eight Peak Index of Mass Spectra, UK) [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985., p. V2 11]**PEER REVIEWED**

Refractive index = 1.3942 @ 20 deg C [Dean JA; Lange's Handbook of Chemistry 13th ed p. 7-576 1985]**PEER REVIEWED**

SURFACE TENSION:

27.4 mN/m @ 20 deg C [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA1 323]**PEER REVIEWED**

VAPOR DENSITY:

3.0 (AIR= 1) [Patty, F. (ed.). Industrial Hygiene and Toxicology: Volume II: Toxicology. 2nd ed. New York: Interscience Publishers, 1963., p. 1967]**PEER REVIEWED**

VAPOR PRESSURE:

26 MM HG AT 20 DEG C [American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1675]**PEER REVIEWED**

VISCOSITY:

0.54 mPa-s @ 20 deg C [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA1 323]**PEER REVIEWED**

OTHER CHEMICAL/PHYSICAL PROPERTIES:

CONVERSION FACTORS: 1 MG/L EQUALS 284 PPM; 1 PPM EQUALS 3.5 MG/CU M [Patty, F. (ed.). Industrial Hygiene and Toxicology: Volume II: Toxicology. 2nd ed. New York: Interscience Publishers, 1963., p. 1967]**PEER REVIEWED**

Henry's Law Constant: 1.47X10-4 atm-cu m/mole [Buttery RG et al; J Agr Food Chem 17: 385-9 (1969)]**PEER REVIEWED**

hydroxyl radical rate constant = 2.85X10-11 cu-cm/molc sec @ 25 deg C [Atkinson R; Journal of Physical And Chemical Reference Data. Monograph No 1 (1989)]**QC REVIEWED**

CHEMICAL SAFETY & HANDLING:

DOT EMERGENCY GUIDELINES:

Fire or explosion: Highly flammable: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low confined areas (sewers, basements, tanks). Vapor explosion hazard indoors, outdoors or in sewers. Those substances labeled "P" may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. [U.S. Department of Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

Health: May cause toxic effects if inhaled or absorbed through skin. Inhalation or contact with material may irritate or burn skin and eyes. Fire will produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. [U.S. Department of Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

Public safety: Call Emergency Response Telephone Number. ... Isolate spill or leak area immediately for at least 50 to lOO meters (160 to 330 feet) in all directions. Keep unauthorized personnel away. Stay upwind. Keep out of low areas. Ventilate closed spaces before entering. [U.S. Department of Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

Protective clothing: Wear positive pressure self-contained breathing apparatus (SCBA). Structural firefighters' protective clothing will only provide limited protection. [U.S. Department of Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

Evacuation: ... 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. [U.S. Department of Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

Fire: Caution: All these products have a very low flash point: Use of water spray when fighting fire may be inefficient. Small fires: Dry chemical, CO2, water spray or alcohol-resistant foam. Do not use dry chemical extinguishers to control fires involving nitromethane or nitroethane. Large fires: Water spray, fog or alcohol-resistant foam. Do not use straight streams. Move containers from fire area if you can do it without risk. Fire involving tanks or car/trailer loads: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. Always stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. [U.S. Department of Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

Spill or leak: Eliminate all ignition sources (no smoking, flares, sparks or flames in immediate area). All equipment used when handling the product must be grounded. Do not touch or walk through spilled material. Stop leak if you can do it without risk. Prevent entry into waterways, sewers, basements or confined areas. A vapor suppressing foam may be used to reduce vapors. Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers. Use clean non-sparking tools to collect absorbed material. Large spills: Dike far ahead of liquid spill for later disposal. Water spray may reduce vapor; but may not prevent ignition in closed spaces. [U.S. Department of

Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

First aid: Move victim to fresh air. Call 911 or emergency medical service. Apply artificial respiration if victim is not breathing. Administer oxygen if breathing is difficult. Remove and isolate contaminated clothing and shoes. In case of contact with substance, immediately flush skin or eyes with running water for at least 20 minutes. Wash skin with soap and water. Keep victim warm and quiet. Effects of exposure (inhalation, ingestion or skin contact) to substance may be delayed. Ensure that medical personnel are aware of the material(s) involved, and take precautions to protect themselves. [U.S. Department of Transportation. 2000 Emergency Response Guidebook. RSPA P 5800.8 Edition. Washington, D.C: U.S. Government Printing Office, 2000,p. G-129]**QC REVIEWED**

SKIN, EYE AND RESPIRATORY IRRITATIONS:

Vapor may irritate eyes. [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

FIRE POTENTIAL:

FIRE HAZARD: DANGEROUS [Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2716]**PEER REVIEWED**

NFPA HAZARD CLASSIFICATION:

Health: 1. 1= Materials that, on exposure, would cause irritation, but only minor residual injury, including those requiring the use of an approved air-purifying respirator. These materials are only slightly hazardous to health and breathing protection is needed. [National Fire Protection Guide. Fire Protection Guide on Hazardous Materials. 10 th ed. Quincy, MA: National Fire Protection Association, 1991., p. 325M-92]**PEER REVIEWED**

Flammability: 3. 3= Includes Class IB and IC flammable liquids and materials that can be easily ignited under almost all normal temp conditions. Water may be ineffective in controlling or extinguishing fires in such materials. [National Fire Protection Guide. Fire Protection Guide on Hazardous Materials. 10 th ed. Quincy, MA: National Fire Protection Association, 1991., p. 325M-92]**PEER REVIEWED**

Reactivity: 0. 0= Includes materials that are normally stable, even under fire exposure conditions, and that do not react with water. Normal fire fighting procedures may be used. [National Fire Protection Guide. Fire Protection Guide on Hazardous Materials. 10 th ed. Quincy, MA: National Fire Protection Association, 1991., p. 325M-92]**PEER REVIEWED**

FLASH POINT:

53.6 DEG F (Closed cup) [Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2716]**PEER REVIEWED**

54 deg F (Open cup) [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

AUTOIGNITION TEMPERATURE:

432 deg F (222 deg C) [National Fire Protection Guide. Fire Protection Guide on Hazardous Materials. 10 th ed. Quincy, MA: National Fire Protection Association, 1991., p. 325M-92]**PEER REVIEWED**

FIRE FIGHTING PROCEDURES:

Foam, dry chemical, or carbon dioxide. Water may be ineffective. [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

FIREFIGHTING HAZARDS:

Burning Rate: 1.9 mm/min [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

Flashback along vapor trail may occur. [U.S. Coast Guard, Department of

Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

EXPLOSIVE LIMITS & POTENTIAL:

Vapor may explode if ignited in an enclosed area. [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

HAZARDOUS DECOMPOSITION:

When heated to decomposition it emits acrid smoke and fumes. [Sax, N.I. Dangerous Properties of Industrial Materials. 6th ed. New York, NY: Van Nostrand Reinhold, 1984., p. 2716]**PEER REVIEWED**

PROTECTIVE EQUIPMENT & CLOTHING:

Goggles or face shield; rubber gloves and boots. [U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5., p.]**PEER REVIEWED**

Wear appropriate personal protective clothing to prevent skin contact. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 327]**QC REVIEWED**

Wear appropriate eye protection to prevent eye contact. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 327]**QC REVIEWED**

Eyewash fountains should be provided in areas where there is any possbility that workers could be exposed to the substance; this is irrespective of the recommendation involving the wearing of eye protection. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 327]**QC REVIEWED**

Facilities for quickly drenching the body should be provided within the immediate work area for emergency use where there is a possibility of exposure. [Note: It is intended that these facilities provide a sufficient quantity or flow of water to quickly remove the substance from any body areas likely to be exposed. The actual determination of what constitutes an adequate quick drench facility depends on the specific circumstances. In certain instances, a deluge shower should be readily available, whereas in others, the availability of water from a sink or hose could be considered adequate.][NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 327]**QC REVIEWED**

PREVENTIVE MEASURES:

SRP: The scientific literature for the use of contact lenses in industry is conflicting. The benefit or detrimental effects of wearing contact lenses depend not only upon the substance, but also on factors including the form of the substance, characteristics and duration of the exposure, the uses of other eye protection equipment, and the hygiene of the lenses. However, there may be individual substances whose irritating or corrosive properties are such that the wearing of contact lenses would be harmful to the eye. In those specific cases, contact lenses should not be worn. In any event, the usual eye protection equipment should be worn even when contact lenses are in place. **PEER REVIEWED**

The worker should immediately wash the skin when it becomes contaminated. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 327]**QC REVIEWED**

Work clothing that becomes wet should be immediately removed due to its flammability hazard. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 327]**QC REVIEWED**

Contact lenses should not be worn when working with this chemical. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 327]**QC REVIEWED**

SHIPMENT METHODS AND REGULATIONS:

No person may /transport,/ offer or accept a hazardous material for transportation in commerce unless that person is registered in conformance ... and the hazardous material is properly classed, described, packaged, marked, labeled, and in condition for shipment as required or authorized by ... /the hazardous materials regulations (49 CFR 171-177)./ [49 CFR 171.2 (7/1/96)]**QC REVIEWED**

The International Air Transport Association (IATA) Dangerous Goods Regulations are published by the IATA Dangerous Goods Board pursuant to IATA Resolutions 618 and 619 and constitute a manual of industry carrier regulations to be followed by all IATA Member airlines when transporting hazardous materials. [IATA. Dangerous Goods Regulations. 38th ed. Montreal, Canada and Geneva, Switzerland: International Air Transport Association, Dangerous Goods Board, January, 1997., p. 228]**QC REVIEWED**

The International Maritime Dangerous Goods Code lays down basic principles for transporting hazardous chemicals. Detailed recommendations for individual substances and a number of recommendations for good practice are included in the classes dealing with such substances. A general index of technical names has also been compiled. This index should always be consulted when attempting to locate the appropriate procedures to be used when shipping any substance or article. [IMDG; International Maritime Dangerous Goods Code; International Maritime Organization p.3110 (1988)]**QC REVIEWED**

CLEANUP METHODS:

Absorb the spills with rags or other available absorbing materials.

Evaporate in a hood and dispose by burning the rag or the absorbing materials. [ITII. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1988., p. 551]**PEER REVIEWED**

DISPOSAL METHODS:

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices. **PEER REVIEWED**

Dissolve in a combustible solvent, thence spray the solvent into the furnace with afterburner. [ITII. Toxic and Hazardous Industrial Chemicals Safety Manual. Tokyo, Japan: The International Technical Information Institute, 1988., p. 551]**PEER REVIEWED**

OCCUPATIONAL EXPOSURE STANDARDS:

THRESHOLD LIMIT VALUES:

8 hr Time Weighted Avg (TWA): 50 ppm. [American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2005, p. 58]

Excursion Limit Recommendation: Excursions in worker exposure levels may exceed three times the TLV-TWA for no more than a total of 30 min during a work day, and under no circumstances should they exceed five times the TLV-TWA, provided that the TLV-TWA is not exceeded. [American Conference of Governmental Industrial Hygienists TLVs and BEIs. Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices. Cincinnati, OH, 2005, p. 5]

NIOSH RECOMMENDATIONS:

Recommended Exposure Limit: 10 Hr Time-Weighted Avg: 50 ppm (175 mg/cu m). [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication

No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 326]**QC REVIEWED**

Testing has not been completed to determine the carcinogenicity of n-valeraldehyde. However, the limited studies to date indicate that /n-valeraldehyde/ has chemical reactivity and mutagenicity similar to acetaldehyde and malonaldehyde. [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 326]**QC REVIEWED**

OTHER OCCUPATIONAL PERMISSIBLE LEVELS:

Australia: 50 ppm (1990) [American Conference of Governmental Industrial Hygienists, Inc. Documentation of the Threshold Limit Values and Biological Exposure Indices. 6th ed. Volumes I, II, III. Cincinnati, OH: ACGIH, 1991., p. 1676]**PEER REVIEWED**

MANUFACTURING/USE INFORMATION:

MAJOR USES:

IN FLAVORING COMPOUNDS, RESIN CHEMISTRY, & RUBBER ACCELERATORS [Budavari, S. (ed.). The Merck Index - Encyclopedia of Chemicals, Drugs and Biologicals. Rahway, NJ: Merck and Co., Inc., 1989., p. 1558]**PEER REVIEWED**

FLAVOR INGREDIENT FOR FOODS & BEVERAGES; MONOMER FOR ACETAL RESINS **PEER REVIEWED**

REPORTED USES: IN NON-ALCOHOLIC BEVERAGES @ 1.3 PPM; IN ICE CREAM, ICES, ETC @ 5.0 PPM; IN CANDY @ 4.2 PPM, & IN BAKED GOODS @ 5.4 PPM. [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 558]**PEER REVIEWED**

SYNTHETIC FLAVORING MATERIAL ... IT IS USED AS TOP NOTE /TOP NOTE GIVES IDENTITY TO FLAVORING ON FIRST IMPRESSION/ & PRODUCES FRUIT, NUT FLAVOR. [Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed.

Cleveland: The Chemical Rubber Co., 1972., p. 510]**PEER REVIEWED**

MANUFACTURERS:

Union Carbide Corporation, Hq, Old Ridgebury Road, Danbury, CT 06817, (203) 794-2000; Solvents and Coatings Materials Division; Production site: 3301 Fifth Ave, South, Texas City, TX 77590 [SRI. 1994 Directory of Chemical Producers -United States of America. Menlo Park, CA: SRI International, 1994., p. 992]**PEER REVIEWED**

METHODS OF MANUFACTURING:

CATALYTIC DEHYDROGENATION OF N-PENTANOL IN THE PRESENCE OF A COPPER OR A COPPER-CHROMITE CATALYST AT HIGH TEMPERATURES **PEER REVIEWED**

BY DISTILLATION OF CALCIUM VALERATE & CALCIUM FORMATE; BY REDN OF N-VALERIC ACID. [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed. Cleveland: The Chemical Rubber Co., 1975., p. 558]**PEER REVIEWED**

OXIDATION OF AMYL ALCOHOL; ALSO BY THE OXO PROCESS. [Sax, N.I. and R.J. Lewis, Sr. (eds.). Hawley's Condensed Chemical Dictionary. 11th ed. New York: Van Nostrand Reinhold Co., 1987., p. 1213]**PEER REVIEWED**

Hydroformylation of butene [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA1 328]**PEER REVIEWED**

GENERAL MANUFACTURING INFORMATION:

PATENTS: ...OLSEN, US PATENT 2,548,171 (1951 TO GENERAL ANILINE & FILM CORP)... [The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 1272]**PEER REVIEWED**

U. S. PRODUCTION:

(1972) PROBABLY GREATER THAN 4.54X10+5 GRAMS **PEER REVIEWED**

(1976) PROBABLY GREATER THAN 2.27X10+6 GRAMS **PEER REVIEWED**

LABORATORY METHODS:

ANALYTIC LABORATORY METHODS:

HPLC DETERMINATION OF ALDEHYDES IN AUTOMOTIVE EXHAUST GAS. LINEAR

CALIBRATION CURVE WAS OBTAINED FOR 5-50 UG/ML ALDEHYDE. [INOUE T ET AL; TOYOTA GIJUTSU 29 (4): 500 (1980)]**PEER REVIEWED**

GC PROCEDURE FOR DETERMINING SIMPLE MONOCARBONYLS IN CIGARET SMOKE AS BENZYLOXIME DERIVATIVES. [MAGIN DF; J CHROMATOGR 202 (2): 255 (1980)]**PEER REVIEWED**

OSHA Method No. 85. HPLC Reliable quantitation limit 174 ppb [Valeraldehyde Issue July 1990]**PEER REVIEWED**

NIOSH Method 2539 GC, FID & GC/MS Estimated limit of detection 2 ug aldehyde per sample [Aldehyde Screening Issue 5/15/89]**PEER REVIEWED**

NIOSH Method 2536. GC FID Working range 0.11 to 110 ppm for 10 L air sample. Estimated limit of detection 2 ug per sample [Valeraldehyde Issue 5/15/89]**PEER REVIEWED**

SPECIAL REFERENCES:

SYNONYMS AND IDENTIFIERS:

SYNONYMS:

AMYL ALDEHYDE [U.S. Department of Health and Human Services, Public Health Service, Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances 1979 edition. Volumes 1 and 2. Washington, DC: U.S. Government Printing Office, 1980., p. V2 691]**PEER REVIEWED**

BUTYL FORMAL [U.S. Department of Health and Human Services, Public Health Service, Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances 1979 edition. Volumes 1 and 2. Washington, DC: U.S. Government Printing Office, 1980., p. V2 691]**PEER REVIEWED**

FEMA NUMBER 3098. [Fenaroli's Handbook of Flavor Ingredients. Volume 2. Edited, translated, and revised by T.E. Furia and N. Bellanca. 2nd ed.

Cleveland: The Chemical Rubber Co., 1975., p. 558]**PEER REVIEWED**

N-PENTANAL **PEER REVIEWED**

VALERAL **PEER REVIEWED**

VALERALDEHYDE **PEER REVIEWED**

N-VALERALDEHYDE **PEER REVIEWED**

VALERIC ACID ALDEHYDE **PEER REVIEWED**

VALERIC ALDEHYDE **PEER REVIEWED**

VALERYLALDEHYDE **PEER REVIEWED**

SHIPPING NAME/ NUMBER DOT/UN/NA/IMO:
UN 2058; Valeraldehyde

IMO 3.2; Valeraldehyde

ADMINISTRATIVE INFORMATION:

HAZARDOUS SUBSTANCES DATABANK NUMBER: 851

LAST REVISION DATE: 20050823

LAST REVIEW DATE: Reviewed by SRP on 9/29/1994

UPDATE HISTORY:
Complete Update on 2005-08-23, 0 fields added/edited/deleted

Field Update on 2005-01-27, 2 fields added/edited/deleted

Complete Update on 02/14/2003, 1 field added/edited/deleted.

Complete Update on 11/08/2002, 1 field added/edited/deleted.

Complete Update on 10/16/2002, 1 field added/edited/deleted.

Complete Update on 07/22/2002, 1 field added/edited/deleted.

Complete Update on 02/13/2002, 1 field added/edited/deleted.

Complete Update on 01/14/2002, 1 field added/edited/deleted.

Complete Update on 08/09/2001, 1 field added/edited/deleted.

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Complete Update on 02/08/2000, 1 field added/edited/deleted.

Complete Update on 02/02/2000, 1 field added/edited/deleted.

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Complete Update on 12/27/1999, 1 field added/edited/deleted.
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Complete Update on 07/27/1999, 3 fields added/edited/deleted.
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Complete Update on 09/04/1996, 5 fields added/edited/deleted.
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Complete Update on 11/10/1995, 1 field added/edited/deleted.
Complete Update on 01/24/1995, 1 field added/edited/deleted.
Complete Update on 01/12/1995, 69 fields added/edited/deleted.
Field Update on 12/22/1994, 1 field added/edited/deleted.
Field Update on 11/02/1994, 1 field added/edited/deleted.
Field Update on 08/04/1994, 1 field added/edited/deleted.
Field Update on 03/21/1994, 1 field added/edited/deleted.
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Field update on 12/16/1992, 1 field added/edited/deleted.
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Field Update on 05/05/1989, 1 field added/edited/deleted.
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Complete Update on 03/08/1988, 2 fields added/edited/deleted.

Complete Update on 06/04/1985

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