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Query: Records containing the term 120 57 0

1  
NAME: PIPERONAL

HSN: 581

RN: 120-57-0

#### HUMAN HEALTH EFFECTS:

#### HUMAN TOXICITY EXCERPTS:

Moderately toxic by ingestion and intraperitoneal routes. Can cause central nervous system depression. A human skin irritant. [Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 2716]\*\*PEER REVIEWED\*\*

#### HUMAN TOXICITY VALUES:

LD50 Mouse ip > 0.5 g/kg /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. 2664]\*\*PEER REVIEWED\*\*

#### SKIN, EYE AND RESPIRATORY IRRITATIONS:

A human skin irritant. [Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 2716]\*\*PEER REVIEWED\*\*

#### PROBABLE ROUTES OF HUMAN EXPOSURE:

NIOSH (NOES Survey 1981-1983) has statistically estimated that 15,846 workers (6,568 of these are female) are potentially exposed to piperonal in the US(1). Occupational exposure to piperonal may occur through inhalation and dermal contact with this compound at workplaces where piperonal is produced or used(SRC). Since this compound is used in the perfume and fragrance industry, the general population may be exposed to piperonal through the use of consumer products containing this compound(SRC). Piperonal is also used as a flavorant and exposure may occur through ingestion of foods that contain this compound(SRC). [(1) NIOSH; National Occupational Exposure Survey (NOES) (1983)]\*\*PEER REVIEWED\*\*

#### MINIMUM FATAL DOSE LEVEL:

3. 3= MODERATELY TOXIC: PROBABLE ORAL LETHAL DOSE (HUMAN) IS 0.5-5 G/KG; BETWEEN 1 OZ & 1 PINT (OR 1 LB) FOR 70 KG PERSON (150 LB). [Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-169]\*\*PEER REVIEWED\*\*

EMERGENCY MEDICAL TREATMENT:

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LIFE SUPPORT:

- o 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) Whether a substance is labeled a "corrosive" or "irritant" depends on several factors: the nature of the substance, concentration, viscosity, pH, molarity, oxidation-reduction potential, complexing affinity toward bivalent ions etc. It is difficult to determine if a substance is a corrosive or irritant at a particular concentration.
- B) Irritants are substances that cause inflammation and swelling, but not cellular death and tissue damage; a corrosive causes cellular damage and death.
- C) Exposure via inhalation may result in headache, rhinorrhea, cough, shortness of breath, chest pain, bronchospasm and rarely, upper airway swelling or acute lung injury.
- D) Ingestion may cause irritation of the oral mucous

membranes and esophagus.

#### 0.2.4 HEENT

##### 0.2.4.1 ACUTE EXPOSURE

- A) Irritants may cause swelling, redness and pain at any site, especially at mucous membranes. The mouth, nose, and eyes are susceptible to these effects.

#### 0.2.6 RESPIRATORY

##### 0.2.6.1 ACUTE EXPOSURE

- A) Cough, tachypnea, and wheezing are common after inhalation.

#### 0.2.8 GASTROINTESTINAL

##### 0.2.8.1 ACUTE EXPOSURE

- A) Nausea, vomiting and diarrhea are possible if ingested.

#### 0.2.14 DERMATOLOGIC

##### 0.2.14.1 ACUTE EXPOSURE

- A) Redness, swelling and pain may occur.

#### 0.2.20 REPRODUCTIVE HAZARDS

- A) Pregnant female rats were exposed to N-methylpyrrolidone. Exposed offspring had normal motor function, activity levels, and low-level learning abilities. On higher-level learning tests, their performance was impaired compared to unexposed offspring.

#### 0.2.21 CARCINOGENICITY

##### 0.2.21.2 HUMAN OVERVIEW

- A) Development of sinonasal neoplasms has been associated with exposure to wood dust and other irritants.

#### LABORATORY:

- A) No specific laboratory tests are necessary with the possible exception of testing the pH of the irritant substance and the pH of the ocular cul de sac with wide range pH paper.

#### TREATMENT OVERVIEW:

##### 0.4.2 ORAL EXPOSURE

- A) EMESIS - Not indicated due to the irritant nature of these agents.
- B) Charcoal - Not recommended; it may promote vomiting and make endoscopic evaluation difficult.
- C) DILUTION: Immediately dilute with 4 to 8 ounces (120 to 240 mL) of water or milk (not to exceed 4 ounces/120 mL in a child).
- D) NEUTRALIZATION - Neutralization is not indicated.
- E) Although these agents are irritants, and therefore should not produce tissue damage, it is almost impossible to assure that a particular substance under a particular set of circumstances would not cause damage. Therefore, each patient should be examined with the idea that mucous membrane damage might have occurred.

##### 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.

#### 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.
- B) If in a medical facility, sterile saline should be used to irrigate the eyes until the cul de sac is returned to neutrality. Some alkali exposures may require prolonged irrigation.

#### RANGE OF TOXICITY:

- A) The extent of damage will depend on a number of factors including concentration, mechanism of action, pH, free acidity and alkalinity, molarity and oxidation-reduction potential. In most cases these factors are more important than volume. Besides its irritant effect, a substance may also have some type of systemic effect. Observe for any potential systemic effects as is appropriate for each compound.

#### ANTIDOTE AND EMERGENCY TREATMENT:

/SRP:/ Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if necessary ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline 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 ... . Cover skin burns with dry sterile dressings after decontamination ... . /Poison A and B/ [Bronstein, A.C., P.L. Currance; Emergency Care for Hazardous Materials Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 139]\*\*PEER REVIEWED\*\*

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in respiratory arrest. Positive pressure ventilation techniques with a bag valve mask device may be beneficial. Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start an IV with D5W /SRP: "To keep open", minimal flow rate/. Use lactated Ringer's if signs of hypovolemia are present. Watch for signs of fluid overload. Consider drug therapy for pulmonary edema ... . For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload ... . Treat seizures with diazepam (Valium) ... . Use

proparacaine hydrochloride to assist eye irrigation ... . /Poison A and B/  
[Bronstein, A.C., P.L. Currence; Emergency Care for Hazardous Materials  
Exposure. 2nd ed. St. Louis, MO. Mosby Lifeline. 1994., p. 139]\*\*PEER  
REVIEWED\*\*

#### ANIMAL TOXICITY STUDIES:

#### NON-HUMAN TOXICITY EXCERPTS:

AT 1000 AND 10,000 PPM IN THE DIET FOR 28 AND 16 WEEKS, RESPECTIVELY, NO  
ADVERSE EFFECTS WERE SEEN IN RATS [Gosselin, R.E., H.C. Hodge, R.P. Smith,  
and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed.  
Baltimore: Williams and Wilkins, 1976., p. II-169]\*\*PEER REVIEWED\*\*

Moderately toxic by ingestion and intraperitoneal routes. Can cause  
central nervous system depression. [Lewis, R.J. Sax's Dangerous Properties  
of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand  
Reinhold, 1996., p. 2716]\*\*PEER REVIEWED\*\*

#### NON-HUMAN TOXICITY VALUES:

LD50 Rat oral 2700 mg/kg [Lewis, R.J. Sax's Dangerous Properties of  
Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand  
Reinhold, 1996., p. 2716]\*\*PEER REVIEWED\*\*

#### TSCA TEST SUBMISSIONS:

Piperonal (CAS # 120-57-0) was evaluated for acute dermal toxicity. The  
test substance was applied at a dose of 5.0 g/kg body weight to the  
unoccluded scapular region of 8 male and 8 female albino rats  
(Sprague-Dawley CD strain). No clinical signs or deaths occurred. All of  
the animals remained healthy and gained weight, except for 1 female who  
lost 10 grams in 14 days. At necropsy, there were no treatment-related  
signs. The dermal LD50 was determined to be greater than 5.0 g/kg body  
weight.[Letter Submitting Three Enclosed Studies on  
1,3-Benzodioxole-5-Carboxaldehyde with Attachments (Sanitized); 11/25/91;  
EPA Doc No. 86-920000245S; Fiche No. OTS0535062]\*\*UNREVIEWED\*\*

Piperonal (CAS # 120-57-0) was evaluated for primary dermal irritation.  
The test substance was applied to the cuff of 8 guinea pigs (sex and  
strain not indicated) at a dose range of 0.25-1.0 mg/kg. Strong skin  
irritation was evident at 24 hours with slight to gross edema and slight  
to severe erythema. At 48 hours, slight to moderate edema and erythema was  
found with eschar formation and necrotic area over part or all of the  
patch. At 1-week and 2-week observation, desquamation and alopecia was  
evident.[EASTMAN KODAK CO; Letter From Eastman Kodak Co To USEPA  
Submitting Enclosed Material Safety Data Sheet and Toxicity Report on  
Piperonal with Attachments; 10/22/91; EPA Doc No. 86-920000085; Fiche No.  
OTS0533448]\*\*UNREVIEWED\*\*

Piperonal (CAS # 120-57-0) was evaluated for primary eye irritation.

Several dry crystals of the test substance were administered to 3 unwashed and 3 washed eyes of rabbits (sex and strain not indicated). Observations after 48 hours indicated that two rabbits (1 unwashed, 1 washed) had slight erythema on the nictating membrane. All animals were normal after 14 days.[EASTMAN KODAK CO; Letter From Eastman Kodak Co To USEPA Submitting Enclosed Material Safety Data Sheet and Toxicity Report on Piperonal with Attachments; 10/22/91; EPA Doc No. 86-920000085; Fiche No. OTS0533448]\*\*UNREVIEWED\*\*

#### METABOLISM/PHARMACOKINETICS:

#### METABOLISM/METABOLITES:

IN MAMMALS METHYLENEDIPOXYPHENYL COMPOUNDS /PIPERONAL IS ONE OF THIS CLASS/ UNDERWENT DEGRADATION LARGELY THROUGH OXIDATION OF THE METHYLENE GROUP TO CARBON DIOXIDE. [Menzie, C. M. Metabolism of Pesticides, An Update. U.S. Department of the Interior, Fish, Wild-life Service, Special Scientific Report - Wildlife No. 184, Washington, DC: U.S. Government Printing Office, 1974., p. 257]\*\*PEER REVIEWED\*\*

PATHS OF METABOLISM: PIPERONAL CONVERTED TO PIPERONYL ALCOHOL WHICH IS METABOLIZED TO GLUCOSIDE CONJUGATE. /FROM TABLE/ [Menzie, C. M. Metabolism of Pesticides, An Update. U.S. Department of the Interior, Fish, Wild-life Service, Special Scientific Report - Wildlife No. 184, Washington, DC: U.S. Government Printing Office, 1974., p. 258]\*\*PEER REVIEWED\*\*

IN HOUSEFLIES PIPERONAL IS METABOLIZED TO PIPERONYLIC ACID WHICH CAN BE CONVERTED TO A GLYCINE CONJUGATE OR TO AN ALANINE CONJUGATE OR A GLUTAMINE CONJUGATE. THE ALANINE CONJUGATE IS FURTHER CONVERTED TO A SERINE CONJUGATE AND THE GLUTAMINE CONJUGATE TO A GLUTAMATE CONJUGATE. /FROM TABLE/ [Menzie, C. M. Metabolism of Pesticides, An Update. U.S. Department of the Interior, Fish, Wild-life Service, Special Scientific Report - Wildlife No. 184, Washington, DC: U.S. Government Printing Office, 1974., p. 258]\*\*PEER REVIEWED\*\*

IN RATS PIPERONAL IS METABOLIZED TO PIPERONYLIC ACID WHICH IS CONVERTED TO GLUCURONIDE OR TO A GLYCINE CONJUGATE. /FROM TABLE/ [Menzie, C. M. Metabolism of Pesticides, An Update. U.S. Department of the Interior, Fish, Wild-life Service, Special Scientific Report - Wildlife No. 184, Washington, DC: U.S. Government Printing Office, 1974., p. 258]\*\*PEER REVIEWED\*\*

THE BETA-GLUCOSIDE OF PIPERONYL ALCOHOL HAS ALSO BEEN FOUND AFTER INJECTION OF...PIPERONAL INTO HOUSEFLIES. [Menzie, C. M. Metabolism of Pesticides, An Update. U.S. Department of the Interior, Fish, Wild-life Service, Special Scientific Report - Wildlife No. 184, Washington, DC: U.S. Government Printing Office, 1974., p. 259]\*\*PEER REVIEWED\*\*

WHEN PIPERONAL WAS FED TO MICE, PIPERONYLIC ACID, N-PIPERONYLGLYCINE &

2 UNIDENTIFIED COMPOUNDS WERE OBSERVED. [Menzie, C.M. Metabolism of Pesticides. U.S. Department of the Interior, Bureau of Sport Fisheries and Wildlife, Publication 127. Washington, DC: U.S. Government Printing Office, 1969., p. 250]\*\*PEER REVIEWED\*\*

## PHARMACOLOGY:

### MINIMUM FATAL DOSE LEVEL:

3. 3= MODERATELY TOXIC: PROBABLE ORAL LETHAL DOSE (HUMAN) IS 0.5-5 G/KG; BETWEEN 1 OZ & 1 PINT (OR 1 LB) FOR 70 KG PERSON (150 LB). [Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-169]\*\*PEER REVIEWED\*\*

## ENVIRONMENTAL FATE & EXPOSURE:

### ENVIRONMENTAL FATE/EXPOSURE SUMMARY:

Piperonal's production and use as an insecticide synergist and as an ingredient in perfumes and fragrances has resulted in its direct release to the environment. Piperonal is also found in many essential oils. If released to air, a vapor pressure of 0.01 mm Hg at 25 deg C indicates piperonal will exist solely as a vapor in the ambient atmosphere.

Vapor-phase piperonal is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 14 hours. If released to soil,

Piperonal is expected to have high mobility based upon an estimated Koc of 89. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of  $5.6 \times 10^{-7}$  atm-cu m/mole. Piperonal reached 88% of its theoretical BOD in 2 weeks using an activated sludge inoculum, suggesting that biodegradation will be an important environmental fate process in the environment. If released into water, piperonal is not expected to adsorb to suspended solids and sediment based upon its estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. Piperonal contains functional groups that may be susceptible to hydrolysis, but the rates of degradation are not known. An estimated BCF of 1 suggests the potential for bioconcentration in aquatic organisms is low. Occupational exposure to piperonal may occur through inhalation and dermal contact with this compound at workplaces where piperonal is produced or used. Since this compound is used in the perfume and fragrance industry, the general population may be exposed to piperonal through the use of consumer products containing this compound. Piperonal is also used as a flavorant and exposure may occur through ingestion of foods that contain this compound. (SRC) \*\*PEER REVIEWED\*\*

## PROBABLE ROUTES OF HUMAN EXPOSURE:

NIOSH (NOES Survey 1981-1983) has statistically estimated that 15,846 workers (6,568 of these are female) are potentially exposed to piperonal in the US(1). Occupational exposure to piperonal may occur through inhalation and dermal contact with this compound at workplaces where piperonal is produced or used(SRC). Since this compound is used in the perfume and fragrance industry, the general population may be exposed to piperonal through the use of consumer products containing this compound(SRC). Piperonal is also used as a flavorant and exposure may occur through ingestion of foods that contain this compound(SRC). [(1) NIOSH; National Occupational Exposure Survey (NOES) (1983)]\*\*PEER REVIEWED\*\*

## NATURAL POLLUTION SOURCES:

REPORTED FOUND IN THE ESSENTIAL OILS OF ROBINIA PSEUDO-ACACIA AND ERYNGIUM POTERIUM; IN THE OILS OF SPIREA ULMARIA AND OF LEAVES OF DORYPHORA SASSAFRAS. ALSO REPORTED FOUND IN TAHITIAN VANILLA, CAMPHOR WOOD OIL, AND VIOLET FLOWERS... [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. 489]\*\*PEER REVIEWED\*\*

Piperonal occurs in a number of oils, but never as the main component(1). [(1) Bauer K, Garbe D; Ullmann's Encycl Indust Chem. 5th ed Gerhartz W, ed. Deerfield Beach, FL: VCH Publ A11: 141-250 (1985)]\*\*PEER REVIEWED\*\*

## ARTIFICIAL POLLUTION SOURCES:

Piperonal's production and use as an insecticide synergist(1) and as an ingredient in perfumes and fragrances(2) has resulted in its direct release to the environment(SRC). [(1) Varagnat J; Kirk-Othmer Encycl Chem Technol. 3rd ed NY,NY: John Wiley and Sons 13: 39-69 (1981) (2) Lewis RJ Sr, ed; Hawley's Condensed Chemical Dictionary. 13th ed. NY, NY: Van Nostrand Reinhold Co., p. 885 (1997)]\*\*PEER REVIEWED\*\*

## ENVIRONMENTAL FATE:

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc of 89(SRC) determined from a log Kow of 1.05(2), and a regression-derived equation(3), indicates that piperonal will have high mobility in soil(SRC). Volatilization of piperonal from moist soil surfaces is not expected(SRC) based on its estimated Henry's Law constant of  $5.6 \times 10^{-7}$  atm-cu m/mol, calculated from its vapor pressure of 0.01 mm Hg(4) and water solubility of 3,500 mg/l(5). Piperonal is not expected to volatilize from dry soil surfaces(SRC) based on its vapor pressure(4). Piperonal reached 88% of its theoretical BOD in 2 weeks using an activated sludge inoculum(6), suggesting that biodegradation will be an important environmental fate process in soil(SRC). [(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 38 (1995) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990) (4) Perry RH, Green D; Perry's Chemical Engineer's Handbook 6th

ed. NY, NY: McGraw-Hill Inc p. 3-60 (1984) (5) Yalkowsky SH, Dannenfelser RM; Aquasol Database of Aqueous Solubility. Version 5. College of Pharmacy, University of Arizona - Tucson, AZ (1992) (6) Chemicals Inspection and Testing Institute. Japan Chemical Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1 (1992)]\*\*PEER REVIEWED\*\*

**AQUATIC FATE:** Based on a classification scheme(1), an estimated Koc of 89(SRC), determined from a log Kow of 1.05(2) and a regression-derived equation(3), indicates that piperonal is not expected to adsorb to suspended solids and sediment(SRC). Volatilization from water surfaces is not expected to be an important fate process based on an estimated Henry's Law constant of  $5.6 \times 10^{-7}$  atm-cu m/mole(SRC), calculated from its vapor pressure of 0.01 mm Hg(4) and water solubility of 3,500 mg/l(5). An estimated BCF value of 1(SRC), from its log Kow(2), and a regression-derived equation(7), suggests the potential for bioconcentration in aquatic organisms is low. Piperonal reached 88% of its theoretical BOD in 2 weeks using an activated sludge inoculum(8), suggesting that biodegradation will be an important environmental fate process in water(SRC). [(1) Swann RL et al; Res Rev 85: 23 (1983) (2) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Professional Reference Book. Heller SR (consult ed) Washington, DC: Amer Chem Soc p. 38 (1995) (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) Perry RH, Green D; Perry's Chemical Engineer's Handbook 6th ed. NY, NY: McGraw-Hill Inc p. 3-60 (1984) (5) Yalkowsky SH, Dannenfelser RM; Aquasol Database of Aqueous Solubility. Version 5 (1992) (6) Franke C et al; Chemosphere 29: 1501-14 (1994) (7) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (8) Chemicals Inspection and Testing Institute. Japan Chemical Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1 (1992)]\*\*PEER REVIEWED\*\*

**ATMOSPHERIC FATE:** According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), piperonal, which has a vapor pressure of 0.01 mm Hg at 25 deg C(2) is expected to exist solely as a vapor in the ambient atmosphere. Vapor-phase piperonal 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 14 hours(SRC), calculated from its estimated rate constant of  $2.85 \times 10^{-11}$  cu cm/molecule-sec at 25 deg C(SRC) determined using a structure estimation method(3). [(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) Perry RH, Green D; Perry's Chemical Engineer's Handbook 6th ed. NY, NY: McGraw-Hill Inc p. 3-60 (1984) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993)]\*\*PEER REVIEWED\*\*

#### ENVIRONMENTAL BIODEGRADATION:

Piperonal, present at 100 mg/l, reached 88% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/l and the Japanese MITI test(1). [(1) Chemicals Inspection and Testing Institute. Japan Chemical

Industry Ecology - Toxicology and Information Center. ISBN 4-89074-101-1  
(1992)]\*\*PEER REVIEWED\*\*

#### ENVIRONMENTAL ABIOTIC DEGRADATION:

The rate constant for the vapor-phase reaction of piperonal with photochemically-produced hydroxyl radicals has been estimated as  $2.85 \times 10^{-11}$  cu cm/molecule-sec at 25 deg C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about 14 hours at an atmospheric concentration of  $5 \times 10^5$  hydroxyl radicals per cu cm(1). Piperonal may undergo hydrolysis and photolysis in the environment(SRC) since this compound contains functional groups that hydrolyze and absorb light in the environmental UV spectrum(2), but the rates of these reactions are unknown. [(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 (1990)]\*\*PEER REVIEWED\*\*

#### ENVIRONMENTAL BIOCONCENTRATION:

An estimated BCF of 1 was calculated for piperonal(SRC), using a log Kow of 1.05(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low. [(1) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Professional Reference Book. Heller SR (consult ed) Washington, DC: Amer Chem Soc p. 38 (1995) (2) Meylan WM et al; Environ Toxicol Chem 18: 664-72 (1999) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)]\*\*PEER REVIEWED\*\*

#### SOIL ADSORPTION/MOBILITY:

The Koc of piperonal is estimated as 89(SRC), using a measured log Kow of 1.05(1) and a regression-derived equation(2). According to a classification scheme(3), this Koc value suggests that piperonal is expected to have high mobility in soil. [(1) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Professional Reference Book. Heller SR (consult ed) Washington, DC: Amer Chem Soc p. 38 (1995) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 4-9 (1990)(3) Swann RL et al; Res Rev 85: 17-28 (1983)]\*\*PEER REVIEWED\*\*

#### VOLATILIZATION FROM WATER/SOIL:

The Henry's Law constant for piperonal is estimated as  $5.6 \times 10^{-7}$  atm-cu m/mole(SRC)calculated from its vapor pressure of 0.01 mm Hg(1) and water solubility of 3,500 mg/l(2). This Henry's Law constant indicates that piperonal is expected to be essentially nonvolatile from water surfaces(3). Piperonal's estimated Henry's Law constant(1,2) indicates that volatilization from moist soil surfaces is not expected(SRC). Piperonal is not expected to volatilize from dry soil surfaces(SRC) based upon its vapor pressure(1). [(1) Perry RH, Green D; Perry's Chemical Engineer's Handbook 6th ed. NY,NY: McGraw-Hill Inc p. 3-60 (1984) (2) Yalkowsky SH, Dannenfelser RM; Aquasol Database of Aqueous Solubility.

Version 5 (1992) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990)  
(3) Lyman WJ; p. 31 in Environmental Exposure From Chemicals Vol I, Neely WB, Blau GE, eds, Boca Raton, FL: CRC Press (1985)]\*\*PEER REVIEWED\*\*

#### FOOD SURVEY VALUES:

Piperonal was identified, not quantified, as a volatile component of chicken(1). [(1) Shahidi F et al; CRC Crit Rev Food Sci Nature 24: 141-243 (1986)]\*\*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 (7/1/2000)]\*\*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. 1,3-Benzodioxole-5-carboxaldehyde is included on this list. [40 CFR 716.120 (7/1/2000)]\*\*PEER REVIEWED\*\*

##### FDA REQUIREMENTS:

Synthetic flavoring substances and adjuvants /for animal drugs, feeds, and related products/ that are generally recognized as safe for their intended use, within the meaning of section 409 of the Act. Piperonal is included on this list. [21 CFR 582.60 (4/1/2000)]\*\*PEER REVIEWED\*\*

Synthetic flavoring substances and adjuvants /for human consumption/ that are generally recognized as safe for their intended use, within the meaning of section 409 of the Act. Piperonal is included on this list. [21 CFR 182.60 (4/1/2000)]\*\*PEER REVIEWED\*\*

#### CHEMICAL/PHYSICAL PROPERTIES:

##### MOLECULAR FORMULA:

C8-H6-O3 \*\*PEER REVIEWED\*\*

##### MOLECULAR WEIGHT:

150.13 [Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1286]\*\*PEER REVIEWED\*\*

**COLOR/Form:**

Colorless, lustrous crystals [Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1286]\*\*PEER REVIEWED\*\*

**ODOR:**

Floral odor [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 885]\*\*PEER REVIEWED\*\*

**TASTE:**

BITTERSWEET TASTE [Fenaroli's Handbook of Flavor Ingredients. Edited, trans. and rev. by T.E. Furia and N. Bellanca Cleveland: The Chemical Rubber Co., 1971., p. 589]\*\*PEER REVIEWED\*\*

**BOILING POINT:**

263 deg C @ 760 mm Hg [Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1286]\*\*PEER REVIEWED\*\*

**MELTING POINT:**

37 deg C [Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1286]\*\*PEER REVIEWED\*\*

**OCTANOL/WATER PARTITION COEFFICIENT:**

log Kow = 1.05 [Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 38]\*\*PEER REVIEWED\*\*

**SOLUBILITIES:**

Soluble in 500 parts water; freely soluble in alcohol, ether [Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1286]\*\*PEER REVIEWED\*\*

Soluble in acetone [Lide, DR (ed.). CRC Handbook of Chemistry and Physics. 81st Edition. CRC Press LLC, Boca Raton: FL 2000, p. 3-67]\*\*PEER REVIEWED\*\*

SOMEWHAT SOLUBLE IN PROPYLENE GLYCOL [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. 489]\*\*PEER REVIEWED\*\*

Solubility in water:  $3.5 \times 10^{-3}$  mg/l [Yalkowsky SH, Dannenfelser RM; The AQUASOL dATABASE of Aqueous Solubility. Fifth ed, Tucson, AZ: Univ Az, College of Pharmacy (1992)]\*\*PEER REVIEWED\*\*

**SPECTRAL PROPERTIES:**

MAX ABSORPTION (ALCOHOL): 275 NM (LOG E= 3.8); 310 NM (LOG E= 3.9);  
SADTLER REFERENCE NUMBER: 3885 (IR, PRISM) [Weast, R.C. (ed.). Handbook of  
Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc.,  
1979., p. C-144]\*\*PEER REVIEWED\*\*

UV: 6719 (Sadtlter 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. V2 1321]\*\*PEER REVIEWED\*\*

<sup>1</sup>H NMR: SAD 6719 (Sadtlter 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. V2 1321]\*\*PEER  
REVIEWED\*\*

IR: SADG 10326 (Sadtlter Research Laboratories IR Grating 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. V2 1321]\*\*PEER  
REVIEWED\*\*

MS: NIST 70331 (NIST/EPA/MCDC Mass Spectral Database 1990 version) [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. V2 1321]\*\*PEER  
REVIEWED\*\*

#### VAPOR PRESSURE:

1X10<sup>-2</sup> mm Hg @ 25 deg C (extrapolated) [Perry RH, Green D; Perry's  
Chemical Engineer's Handbook 6th ed. NY, NY: McGraw-Hill, Inc. p.3-60  
(1984)]\*\*PEER REVIEWED\*\*

#### OTHER CHEMICAL/PHYSICAL PROPERTIES:

CONGEALING POINT: 35 DEG C MIN; ASSAY: 99.0% MIN [Fenaroli's Handbook of  
Flavor Ingredients. Edited, trans. and rev. by T.E. Furia and N. Bellanca  
Cleveland: The Chemical Rubber Co., 1971., p. 589]\*\*PEER REVIEWED\*\*

Vapor pressure = 1 mm Hg @ 87 deg C [Patty, F. (ed.). Industrial Hygiene  
and Toxicology: Volume II: Toxicology. 2nd ed. New York: Interscience  
Publishers, 1963., p. 1983]\*\*PEER REVIEWED\*\*

#### CHEMICAL SAFETY & HANDLING:

#### SKIN, EYE AND RESPIRATORY IRRITATIONS:

A human skin irritant. [Lewis, R.J. Sax's Dangerous Properties of  
Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand  
Reinhold, 1996., p. 2716]\*\*PEER REVIEWED\*\*

#### FIRE POTENTIAL:

COMBUSTIBLE WHEN EXPOSED TO HEAT OR FLAMES; CAN REACT WITH OXIDIZING  
MATERIALS. [Lewis, R.J. Sax's Dangerous Properties of Industrial

Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 2716]\*\*PEER REVIEWED\*\*

#### HAZARDOUS REACTIVITIES & INCOMPATIBILITIES:

CAN REACT WITH OXIDIZING MATERIALS. [Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 9th ed. Volumes 1-3. New York, NY: Van Nostrand Reinhold, 1996., p. 2716]\*\*PEER REVIEWED\*\*

#### STABILITY/SHELF LIFE:

TENDS TO YELLOW ON EXPOSURE TO AIR AND LIGHT [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. 489]\*\*PEER REVIEWED\*\*

#### STORAGE CONDITIONS:

KEEP IN COOL PLACE PROTECTED FROM LIGHT [The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 973]\*\*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\*\*

#### OCCUPATIONAL EXPOSURE STANDARDS:

#### MANUFACTURING/USE INFORMATION:

#### MAJOR USES:

HAS BEEN USED AS PEDICULICIDE [Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-169]\*\*PEER REVIEWED\*\*

Perfumery, suntan preparations, mosquito repellent, laboratory reagent, flavoring. [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 885]\*\*PEER REVIEWED\*\*

In perfumery, flavors, and organic syntheses [Budavari, S. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Whitehouse Station, NJ: Merck and Co., Inc., 1996., p. 1286]\*\*PEER REVIEWED\*\*

FLAVORING AGENT (VANILLA & CHERRY) IN NON-ALCOHOLIC BEVERAGES, ICE CREAM, CANDY, BAKED GOODS, GELATINS & PUDDINGS, CHEWING GUM; FRAGRANCE

INGREDIENT IN SOAPS & DETERGENTS, CREAMS & LOTIONS, PERFUME \*\*PEER REVIEWED\*\*

Synergist for pyrethrum and rotenone, and as an ingredient for insecticidal preparations. [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1-26. New York, NY: John Wiley and Sons, 1978-1984., p. V13 (81) 62]\*\*PEER REVIEWED\*\*

MANUFACTURERS:

Bell Flavor & Fragrances Inc., 500 Academy Dr., Northbrook, IL 60662, (847) 291-8300; Production site: Milwaukee, WI 53204 [SRI International. 2000 Directory of Chemical Producers -- United States. SRI Consulting, Menlo Park: CA 2000, p. 627]\*\*PEER REVIEWED\*\*

Penta Mfg Co., 50 Okner Pkwy., Livingston, NJ 07039-1604, (973) 740-2300; Production site: East Hanover, NJ 07936 [SRI International. 2000 Directory of Chemical Producers -- United States. SRI Consulting, Menlo Park: CA 2000, p. 627]\*\*PEER REVIEWED\*\*

METHODS OF MANUFACTURING:

ISOMERIZATION OF SAFROLE WITH BASE, RESULTING IN ISOSAFROLE, FOLLOWED BY ACID OXIDATION \*\*PEER REVIEWED\*\*

BY THE OXIDATION OF ISOSAFROLE WITH POTASSIUM DICHROMATE AND SULFURIC ACID AND SUBSEQUENT STEAM DISTILLATION OF PIPERONAL. [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. 489]\*\*PEER REVIEWED\*\*

GENERAL MANUFACTURING INFORMATION:

USE IN FLAVORING: NONALCOHOLIC BEVERAGES: 6.0 PPM; ICE CREAM, ICES, ETC: 7.0 PPM; CANDY: 7.4 PPM; BAKED GOODS: 1.8 PPM; GELATINS & PUDDINGS: 5.8 PPM; CHEWING GUM: 36 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. 489]\*\*PEER REVIEWED\*\*

FORMULATIONS/PREPARATIONS:

Grades: technical; FCC [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 885]\*\*PEER REVIEWED\*\*

CONSUMPTION PATTERNS:

APPROXIMATELY  $6.8 \times 10^7$  G AS A FRAGRANCE INGREDIENT (1974) \*\*PEER REVIEWED\*\*

U. S. PRODUCTION:

(1972)  $5.63 \times 10^7$  G \*\*PEER REVIEWED\*\*

(1975) GREATER THAN  $4.54 \times 10^5$  G \*\*PEER REVIEWED\*\*

#### U. S. IMPORTS:

(1972) 8.92X10+7 G \*\*PEER REVIEWED\*\*

(1975) 5.97X10+7 G \*\*PEER REVIEWED\*\*

(1983) 5.0X10+6 g [USITC. IMPORTS OF BENZENOID CHEM & PROD 1983 p.94]\*\*PEER REVIEWED\*\*

#### U. S. EXPORTS:

(1984) 1.5X10+9 g/HELIOTROPIN, EUGENOL, GERANIOL, CITRONELLAL, ISOEUGENOL AND HYDROXYCITRONELLAL/ [BUREAU OF THE CENSUS. U.S. EXPORTS, SCHEDULE E, 1984 p.2-83]\*\*PEER REVIEWED\*\*

#### LABORATORY METHODS:

#### SPECIAL REFERENCES:

#### SYNONYMS AND IDENTIFIERS:

#### SYNONYMS:

BENZALDEHYDE, 3,4-(METHYLENEDIOXY)- [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

1,3-BENZODIOXOLE-5-CARBOXALDEHYDE \*\*PEER REVIEWED\*\*

3,4-DIHYDROXYBENZALDEHYDE METHYLENE KETAL [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

3,4-DIMETHYLENEDIOXYBENZALDEHYDE \*\*PEER REVIEWED\*\*

DIOXYMETHYLENEPROTOCATECHUIC ALDEHYDE [The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 973]\*\*PEER REVIEWED\*\*

FEMA NUMBER 2911 [Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 917]\*\*PEER REVIEWED\*\*

5-FORMYL-1,3-BENZODIOXOLE \*\*PEER REVIEWED\*\*

## GELIOTROPIN \*\*PEER REVIEWED\*\*

HELIOTROPIN [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

HELIOTROPINE [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

3,4-METHYLENEDIHYDROXYBENZALDEHYDE [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

3,4-METHYLENEDIOXYBENZALDEHYDE [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

PIPERONALDEHYDE [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

PIPERONYLALDEHYDE [The Merck Index. 9th ed. Rahway, New Jersey: Merck & Co., Inc., 1976., p. 973]\*\*PEER REVIEWED\*\*

PROTOCATECHUIC ALDEHYDE METHYLENE ETHER [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1978 edition. Washington, DC: U.S. Government Printing Office, 1979., p. 996]\*\*PEER REVIEWED\*\*

## FORMULATIONS/PREPARATIONS:

Grades: technical; FCC [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 13th ed. New York, NY: John Wiley & Sons, Inc. 1997., p. 885]\*\*PEER REVIEWED\*\*

## ADMINISTRATIVE INFORMATION:

HAZARDOUS SUBSTANCES DATABANK NUMBER: 581

LAST REVISION DATE: 20030326

LAST REVIEW DATE: Reviewed by SRP on 5/10/2001

UPDATE HISTORY:

Complete Update on 03/26/2003, 34 fields added/edited/deleted.

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

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

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

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

Field Update on 05/15/2001, 1 field added/edited/deleted.

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

Complete Update on 11/18/1999, 1 field added/edited/deleted.

Complete Update on 08/26/1999, 1 field added/edited/deleted.

Complete Update on 02/27/1998, 1 field added/edited/deleted.

Complete Update on 10/17/1997, 1 field added/edited/deleted.

Complete Update on 08/07/1996, 39 fields added/edited/deleted.

Field Update on 01/19/1996, 1 field added/edited/deleted.

Field Update on 12/21/1994, 1 field added/edited/deleted.

Field Update on 11/03/1994, 1 field added/edited/deleted.

Field Update on 11/02/1994, 1 field added/edited/deleted.

Complete Update on 03/25/1994, 1 field added/edited/deleted.

Field update on 12/13/1992, 1 field added/edited/deleted.

Complete Update on 10/10/1990, 1 field added/edited/deleted.

Field update on 03/06/1990, 1 field added/edited/deleted.

Complete Update on 10/14/1986

### 1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Piperonal

Product Number : P49104  
Brand : Aldrich

Supplier : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052  
Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555

Preparation Information : Sigma-Aldrich Corporation  
Product Safety - Americas Region  
1-800-521-8956

### 2. HAZARDS IDENTIFICATION

#### Emergency Overview

##### OSHA Hazards

Irritant

##### GHS Classification

Acute toxicity, Oral (Category 5)

Skin irritation (Category 2)

Acute aquatic toxicity (Category 3)

##### GHS Label elements, including precautionary statements

Pictogram



Signal word

Warning

Hazard statement(s)

H303

May be harmful if swallowed.

H315

Causes skin irritation.

H402

Harmful to aquatic life.

Precautionary statement(s)

none

#### HMIS Classification

Health hazard: 2

Flammability: 1

Physical hazards: 0

#### NFPA Rating

Health hazard: 2

Fire: 1

Reactivity Hazard: 0

#### Potential Health Effects

##### Inhalation

May be harmful if inhaled. Causes respiratory tract irritation.

**Skin** May be harmful if absorbed through skin. Causes skin irritation.  
**Eyes** Causes eye irritation.  
**Ingestion** May be harmful if swallowed.

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : 1,3-Benzodioxole-5-carboxaldehyde  
Heliotropin  
3,4-(Methylenedioxy)benzaldehyde

Formula : C<sub>8</sub>H<sub>6</sub>O<sub>3</sub>  
Molecular Weight : 150.13 g/mol

Component	Concentration
<b>Piperonal</b>	
CAS-No.	120-57-0
EC-No.	204-409-7
	-

### 4. FIRST AID MEASURES

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 5. FIREFIGHTING MEASURES

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

#### Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

#### Hazardous combustion products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

### 6. ACCIDENTAL RELEASE MEASURES

#### Personal precautions

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

#### Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

#### Methods and materials for containment and cleaning up

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 7. HANDLING AND STORAGE

#### Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

### Conditions for safe storage

Keep container tightly closed in a dry and well-ventilated place.

Light sensitive.

---

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

### Personal protective equipment

#### Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Hand protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Eye protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin and body protection

impervious clothing, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### Appearance

Form	solid
Colour	colourless

### Safety data

pH	no data available
Melting point/freezing point	Melting point/range: 35 - 39 °C (95 - 102 °F) - lit.
Boiling point	264 °C (507 °F) - lit.
Flash point	> 113 °C (> 235 °F) - closed cup
Ignition temperature	no data available
Autoignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	1 hPa (1 mmHg) at 87 °C (189 °F)
Density	no data available
Water solubility	no data available
Partition coefficient: n-octanol/water	log Pow: 1.05
Relative vapour density	no data available

Odour	no data available
Odour Threshold	no data available
Evaporation rate	no data available

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## 10. STABILITY AND REACTIVITY

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Materials to avoid

Strong oxidizing agents, Strong bases

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - no data available

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## 11. TOXICOLOGICAL INFORMATION

### Acute toxicity

#### Oral LD50

LD50 Oral - rat - 2,700 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity). Behavioral:Excitement. Behavioral:Ataxia.

#### Inhalation LC50

no data available

#### Dermal LD50

LD50 Dermal - rat - > 5 mg/kg

#### Other information on acute toxicity

no data available

### Skin corrosion/irritation

Skin - guinea pig - Skin irritation - 48 h

### Serious eye damage/eye irritation

no data available

### Respiratory or skin sensitization

no data available

### Germ cell mutagenicity

Genotoxicity in vitro - Human - lymphocyte  
Sister chromatid exchange

Genotoxicity in vitro - Chicken - Embryo  
Sister chromatid exchange

### Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

## Reproductive toxicity

no data available

## Teratogenicity

no data available

## Specific target organ toxicity - single exposure (Globally Harmonized System)

no data available

## Specific target organ toxicity - repeated exposure (Globally Harmonized System)

no data available

## Aspiration hazard

no data available

## Potential health effects

<b>Inhalation</b>	May be harmful if inhaled. Causes respiratory tract irritation.
<b>Ingestion</b>	May be harmful if swallowed.
<b>Skin</b>	May be harmful if absorbed through skin. Causes skin irritation.
<b>Eyes</b>	Causes eye irritation.

## Signs and Symptoms of Exposure

Central nervous system depression, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

## Synergistic effects

no data available

## Additional Information

RTECS: TO1575000

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## 12. ECOLOGICAL INFORMATION

### Toxicity

no data available

### Persistence and degradability

no data available

### Bioaccumulative potential

no data available

### Mobility in soil

no data available

### PBT and vPvB assessment

no data available

### Other adverse effects

Harmful to aquatic life.

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

no data available

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## 13. DISPOSAL CONSIDERATIONS

### Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

### Contaminated packaging

Dispose of as unused product.

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**14. TRANSPORT INFORMATION****DOT (US)**

Not dangerous goods

**IMDG**

Not dangerous goods

**IATA**

Not dangerous goods

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**15. REGULATORY INFORMATION****OSHA Hazards**

Irritant

**SARA 302 Components**

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Acute Health Hazard

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

Piperonal

CAS-No.  
120-57-0

Revision Date

**New Jersey Right To Know Components**

Piperonal

CAS-No.  
120-57-0

Revision Date

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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**16. OTHER INFORMATION****Further information**

Copyright 2012 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only. The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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