

1. Material Identification

Product Name : Octachloronaphthalene

Catalog Number : io-2779

CAS Number : 2234-13-1

Identified uses : Laboratory chemicals, manufacture of chemical compounds

Company : IonZ

>> R&D Use only

2. Hazards Identification

GHS Classification:

Flammable liquid (category 2)

Acute toxicity, oral (Category 3)

Acute toxicity, dermal (Category 3)

Acute toxicity, inhalation (Category 3)

Specific target organ toxicity, single exposure (Category 1)

Note

>> Pictograms displayed are for 91.1% (41 of 45) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for 8.9% (4 of 45) of reports.

Pictogram(s)



>> Warning

GHS Hazard Statements

>> H302 (91.1%): Harmful if swallowed [Warning Acute toxicity, oral]

Precautionary Statement Codes

>> P264, P270, P301+P317, P330, and P501

Health Hazards:

>> Excerpt from NIOSH Pocket Guide for Octachloronaphthalene:

>> Exposure Routes: Inhalation, skin absorption, ingestion, skin and/or eye contact

>> Symptoms: Acne-form dermatitis; liver damage, jaundice

>> Target Organs: Skin, liver (NIOSH, 2024)

>> Literature sources indicate that this chemical is nonflammable. (NTP, 1992)

>> Not combustible. Gives off irritating or toxic fumes (or gases) in a fire.

3. Composition/Information On Ingredients

Chemical name : Octachloronaphthalene

CAS Number : 2234-13-1

Molecular Formula : C₁₀Cl₈

Molecular Weight : 403.7000 g/mol

4. First Aid Measures

First Aid:

- >> EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.
- >> SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. If symptoms such as redness or irritation develop, IMMEDIATELY call a physician and be prepared to transport the victim to a hospital for treatment.
- >> INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.
- >> INGESTION: DO NOT INDUCE VOMITING. If the victim is conscious and not convulsing, give 1 or 2 glasses of water to dilute the chemical and IMMEDIATELY call a hospital or poison control center. Be prepared to transport the victim to a hospital if advised by a physician. If the victim is convulsing or unconscious, do not give anything by mouth, ensure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital. (NTP, 1992)

First Aid Measures

Inhalation First Aid

- >> Fresh air, rest. Refer for medical attention.

Skin First Aid

- >> Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .

Eye First Aid

- >> First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Ingestion First Aid

- >> Rinse mouth. Refer for medical attention .

5. Fire Fighting Measures

- >> Fires involving this material can be controlled with a dry chemical, carbon dioxide or Halon extinguisher. (NTP, 1992)
- >> In case of fire in the surroundings, use appropriate extinguishing media.

6. Accidental Release Measures

Spillage Disposal:

Methods for containment and safety measures to protect workers dealing with a spillage of this chemical.

- >> Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

7. Handling And Storage

Storage Conditions:

- >> This material should be stored in a refrigerator.

8. Exposure Control/ Personal Protection

- >> TWA 0.1 mg/m³ ST 0.3 mg/m³ [skin]

- >> 0.1 [mg/m³]

- >> 0.1 [mg/m³]

TLV-STEL

- >> 0.3 [mg/m³]

- >> 0.1 mg/m

Effects of Short Term Exposure:

- >> The substance may cause effects on the liver. This may result in tissue lesions.

Effects of Long Term Exposure:

- >> The substance may have effects on the liver.

Exposure Prevention

- >> STRICT HYGIENE!

Inhalation Prevention

- >> Use local exhaust or breathing protection.

Skin Prevention

- >> Protective gloves. Protective clothing.

Eye Prevention

- >> Wear safety goggles, face shield or eye protection in combination with breathing protection.

Ingestion Prevention

- >> Do not eat, drink, or smoke during work. Wash hands before eating.

Exposure Control and Personal Protection

Exposure Summary

- >> TIH (Toxic Inhalation Hazard) – Term used to describe gases and volatile liquids that are toxic when inhaled. Some are TIH materials themselves, e.g., chlorine, and some release TIH gases when spilled in water, e.g., chlorosilanes. [ERG 2016].

9. Physical And Chemical Properties

Molecular Weight:

- >> 403.7

Exact Mass:

>> 403.744921

Physical Description:

- >> Octachloronaphthalene is a pale yellow solid with an aromatic odor. (NTP, 1992)
- >> WAXY YELLOW SOLID IN VARIOUS FORMS WITH CHARACTERISTIC ODOUR.

Color/Form:

- >> Crystals from cyclohexane

Odor:

- >> Aromatic odor

Boiling Point:

- >> 824 °F at 760 mmHg (NTP, 1992)
- >> 440 °C

Melting Point:

- >> 387 to 388 °F (NTP, 1992)
- >> 192 °C

Flash Point:

- >> flash point > 430 °C

Solubility:

- >> Insoluble (NTP, 1992)
- >> Solubility in water: none

Density:

- >> 2 (NTP, 1992) – Denser than water; will sink
- >> Relative density (water = 1): 2.0

Vapor Density:

- >> 13.9 (air=1 at boiling point of octachloronaphthalene) (NTP, 1992) – Heavier than air; will sink (Relative to Air)

Vapor Pressure:

- >> less than 1 mmHg at 68 °F (NTP, 1992)
- >> Vapor pressure, kPa at 20 °C:

LogP:

- >> log Kow = 8.5
- >> 5.88/6.2

Decomposition:

- >> The substance decomposes on heating producing toxic fumes (chlorine).

Collision Cross Section:

Collision cross section (CCS) represents the effective area for the interaction between an individual ion and the neutral gas through which it is traveling (e.g., in ion mobility spectrometry (IMS) experiments). It quantifies the probability of a collision taking place between two or more particles.

- >> 164 Å² [M]⁺ [CCS Type: TIMS, Method: calibration with PAHs]

10. Stability And Reactivity

- >> Insoluble in water.

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION: There are 75 possible congeners of chlorinated naphthalenes. Commercial products are generally mixtures of several congeners and range from thin liquids to hard waxes to high melting point solids. The higher chlorinated naphthalene products have been used as impregnants for condensers and capacitors and dipping encapsulating compd in electronic and automotive applications and as temporary binders in the manufacture of ceramic components, in paper coating and in precision casting of alloys, in electroplating, stop-off compd, as additive in gear oils and cutting compd, in flame proofing and insulation of electrical cable and conductors and moisture proof sealants, as separators in batteries, in refractive index testing oils, masking compd in electroplating and in grinding wheel lubricants. HUMAN EXPOSURE: The major sources of release of chlorinated naphthalenes into the environment are likely from waste incineration and disposal of items containing chlorinated naphthalenes to landfill. In the past, chlorinated naphthalene concn of up to 14.5 mg/cu m have been measured in the workplace, while levels of 25–2900 ng/cu m have been recorded in out door air in vicinity of manufacturing sites. More recently, monitoring studies have revealed chlorinated naphthalene concn up to 150 pg/cu m at semirural sites and 1–40 pg/cu m at remote sites. Chlorinated naphthalenes can be absorbed via oral, inhalative and dermal routes, with absorption and distribution over the whole body after oral admin. Chlorinated naphthalenes, especially the dioxin like congeners, have been detected in adipose tissue, liver, blood and breast milk samples from the general population at concn in the ng/kg lipid range. Severe skin reactions (chloracne) and liver disease have been reported after occupational exposure to chlorinated naphthalenes. Chloracne was common among workers who handling chlorinated naphthalenes in the 1930's to 1940's. A cohort study on workers exposed to chlorinated naphthalenes at a cable manufacturing plant found an excess of deaths from cirrhosis of the liver. However, individuals with chloracne did not show a higher mortality due to liver cirrhosis compared with other workers. The mortality from all cancers was slightly but significantly elevated among all exposed men (standardized mortality ratio =1.18), but was not more elevated in the subcohort with chloracne. This subcohort showed statistically significant excess mortality from cancer of the esophagus and from benign and unspecified neoplasms. Symptoms described in workers exposed to chlorinated naphthalenes included irritation of the eyes, fatigue, headache, anemia, hematuria, impotency, anorexia, vomiting and severe abdominal pain. ANIMAL STUDIES: Chlorinated naphthalenes have been shown to be highly bioaccumulative in fish, but less so in shrimp and algae. The amount of bioaccumulation observed incr with the degree of chlorination of the chlorinated naphthalenes. The most highly chlorinated naphthalenes do not appear to bioaccumulate. Chlorinated naphthalene concn in fish range up to a maximum of around 300 ug/kg lipid weight. 1,2,3,4-Tetrachloronaphthalene has demonstrated no mutagenicity in the Salmonella Ames test. Monitoring studies with seabird eggs have revealed a decr in chlorinated naphthalene levels between 1974 and 1987. Hydroxy metabolites have been identified mostly for the lower chlorinated naphthalenes (mono- to tetra-) in experimental animals. Cattle developed severe systemic disease (bovine hyperkeratosis) during a 5–10 day oral exposure to 1.7–2.4 mg/kg bw/day of penta-, hexa-hepta- or octachlorinated naphthalenes. There are also preliminary indications for the occurrence of methylthio- or methyl sulfoxide chloronaphthalene metabolites in the feces of rats. Elimination of the parent compounds and/or metabolites occurs via feces and urine. The higher chlorinated congeners appeared to be more toxic than the lower chlorinated ones. Long term and carcinogenicity studies with chlorinated naphthalenes have not been performed. Like related compd, chlorinated naphthalenes have been demonstrated to be inducers of the cytochrome p450 (CYP) dependent microsomal enzymes. Chlorinated naphthalenes were also found to change lipid peroxidation and antioxidant enzyme activities in rats in a manner indicative of oxidative stress. At least some of the biological and toxic responses of chlorinated naphthalenes are believed to be mediated via the cytosolic Ah receptor, resembling those of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) and related compd. All chlorinated naphthalenes tested cause skin irritations in laboratory animals. Chlorinated naphthalenes appear to be of moderate to high acute toxicity to aquatic organisms. The amount of bioaccumulation observed increases with the amount of chlorination of the chlorinated naphthalenes, but the most highly chlorinated naphthalenes (octachloronaphthalene) do not appear to bioaccumulate. /Chlorinated naphthalenes, Higher Chlorinated Naphthalenes/

Exposure Routes:

- >> The substance can be absorbed into the body by inhalation, through the skin and by ingestion.
- >> inhalation, skin absorption, ingestion, skin and/or eye contact

Skin Exposure

- >> MAY BE ABSORBED!
- >> Acne-form dermatitis; liver damage, jaundice

Target Organs:

Organs that are affected by exposure to this chemical. Information in this section reflects human data unless otherwise noted.

- >> Skin, liver

Adverse Effects:

An adverse effect is an undesired harmful effect resulting from a medical treatment or other intervention.

>> Occupational hepatotoxin – Primary hepatotoxins: the toxic effect to the liver is the principal adverse effect of the chemical.

>> Dermatotoxin – Chloracne.

Antidote and Emergency Treatment:

>> NAPHTHALENE toxicosis caused by vapor inhalation can usually be managed simply by removing the individual to fresh air. Skin contamination should be removed promptly by washing with soap and water. Eye contamination should be removed by flushing with copious amounts of clear water. Irritation may be severe, and if it persists, should receive medical attention. SRP: /It may be helpful to empty stomach and administer dose of activated charcoal/ Examine the plasma for evidence of hemolysis: a reddish-brown tinge. Examine the blood smear for "ghosts" and Heinz bodies. If /hemolysis is/ present, monitor red blood cell count and hematocrit for anemia, urine for protein, and cells. Measure direct- and indirect-reacting bilirubin in the plasma. Monitor fluid balance and blood electrolytes. If possible, monitor urinary excretion of naphthol to assess severity of poisoning and clinical progress. If hemolysis is clinically significant, administer intravenous fluids to accelerate urinary excretion of the naphthol metabolite and protect the kidney from products of hemolysis. Use Ringer's-lactate or sodium bicarbonate to keep urine pH above 7.5. Consider use of mannitol, or furosemide, to promote diuresis. If urine flow declines, intravenous infusions must be carefully monitored to avoid fluid overload. Institute hemodialysis. Consider charcoal hemoperfusion in tandem to extract naphthalene and end-products. If anemia is severe, blood transfusions may be needed. Hydrocortisone may be of some benefit if significant hemolysis is present. /Fumigant poisoning/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ Until 1957 there was general agreement that as the degree of chlorination increased, so did the acneigenic properties and the systemic toxicity of the chloronaphthalenes. ... as a result /of/ ... experiments on human volunteers, the unexpected fact emerged that whereas tri-, tetra-, hepta-, and octachloronaphthalenes were entirely nonacneigenic, the penta- and hexachloro derivatives produced very severe chloracne indeed.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ The lowest value was the 30-day LD50 of 2,3,6,7-tetrachloronaphthalene from the guinea pig. This was nearly the only experiment taking into account the prolonged time to death, which is typical for dioxin-like compounds the mean time to death for such substances is 2–3 weeks after a single exposure for most small laboratory animals and even longer for larger domestic animals, dogs, and non-human primates /Polychloronaphthalenes/

12. Ecological Information

ICSC Environmental Data:

>> Bioaccumulation of this chemical may occur along the food chain, for example in fish. It is strongly advised not to let the chemical enter into the environment because it is persistent.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: Although analyzed for, octachloronaphthalene was not detected (detection limit of several ng/kg) in surface sediments collected from 18 lakes in central Finland in 1988(1); tetra-, penta-, and hexachloronaphthalenes were detected, but hepta- and octachloronaphthalene were not(1). Analysis of sediment samples taken from an industrial outfall in the Calcasieu River, LA (sampling date not reported), found octachloronaphthalene concns of 12 ug/g in the bottom sediment and 0.81 ug/g in the suspended sediment(2); octachloronaphthalene was not detected (detection limit not reported) in the water-only phase(2). Surface sediments (upper 5 cm) from two polluted Mediterranean lagoons in Italy, Venice and Orbetello, were sampled in 1995 and analyzed for polychlorinated naphthalenes; octachloronaphthalene concentrations ranged from 0.95–9.31 pg/g dry weight for five sites in Venice, and from not quantified–1.78 pg/g dry weight for three sites in Orbetello(3). A site at the Albegua River was selected as a control and had an octachloronaphthalene concentration in surface sediments of 1.06 pg/g dry weight(3). In this study octachloronaphthalene made up 1.6% of the total polychlorinated naphthalenes(3). Concentrations of octachloronaphthalene ranged from <0.001 to 1.29 ng/g dry weight in surface sediments (0–30 cm) collected in Jun 1998 from the upper Detroit River at nine sites; from 0.007 to 0.01 ng/g dry weight from three sites in Lake Michigan; and 0.247 pg/g dry weight from one site in the upper Rouge River(4).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

- >> Octachloronaphthalene made up approximately less than 10% of the polychlorinated naphthalenes found in the whole body and fillets of fish collected from Michigan waters, including the Great Lakes during 1996–1997; concentrations of total polychlorinated naphthalenes ranged from 19 to 31,400 pg/g wet weight(1).

Animal Concentrations:

Concentrations of this compound in animals.

- >> Polychlorinated naphthalenes were analyzed in blubber, nuchal fat, liver, muscle, kidney, and brain of three male harbor porpoises (*Phocoena phocoena*) from the west coast of Sweden, and octachloronaphthalene was not detected in any tissues(1). Polychlorinated naphthalenes were measured in the eggs (white and yoke) of double-crested cormorants and herring gulls collected from Michigan waters of the Great Lakes and were in the ranges of 380–2,400 and 83–1,300 pg/g wet weight, respectively, of which octachloronaphthalenes made up approximately 0%(2).

13. Disposal Considerations

Spillage Disposal

- >> Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Disposal Methods

- >> SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational exposure or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal, aquatic, and plant life; and conformance with environmental and public health regulations.
- >> Incineration, preferably after mixing with another combustible fuel. Care must be exercised to assure complete combustion to prevent the formation of phosgene. An acid scrubber is necessary to remove the halo acids produced. Recommendable method: Incineration. Peer-review: Ensure plentiful supply of hydrocarbon fuel. (Peer-review conclusions of an IRPTC expert consultation (May 1985))

14. Transport Information

DOT

Octachloronaphthalene

IATA

Octachloronaphthalene

15. Regulatory Information

Clean Water Act Requirements:

The Clean Water Act (CWA) of 1972 establishes the basic structure for regulating discharges of pollutants into the waters of the United States and regulating quality standards for surface waters. Under CWA, the U.S. Environmental Protection Agency (EPA) developed the Toxic Pollutant List (40 CFR Part 401.15) and the Priority Pollutant List (40 CFR Part 423, Appendix A). These lists are to be used by EPA and States to develop the Effluent Guidelines regulations and ensure water quality criteria and standards.

- >> Toxic pollutant designated pursuant to section 307(a)(1) of the Federal Water Pollution Control Act and is subject to effluent limitations. /Chlorinated Naphthalene/

TSCA Requirements:

This section provides information on requirements concerning this chemical under the Toxic Substances Control Act (TSCA) of 1976. TSCA provides EPA with authority to require reporting, record-keeping and testing requirements, and restrictions relating to chemical substances and/or mixtures. Certain substances are generally excluded from TSCA, including, among others, food, drugs, cosmetics and pesticides.

- >> 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. Octachloronaphthalene is included on this list.

Regulatory Information

The Australian Inventory of Industrial Chemicals

- >> Chemical: Naphthalene, octachloro-

EPA TSCA Regulatory Flag

- >> SP - indicates a substance that is identified in a proposed Significant New Use Rule.

16. Other Information

Toxic Combustion Products:

Toxic products (e.g., gases and vapors) produced from the combustion of this chemical.

- >> Toxic gases and vapors (such as carbon monoxide and toxic chloride fumes) may be released in a fire involving octachloronaphthalene.

Other Safety Information

Chemical Assessment

- >> IMAP assessments - Naphthalene, octachloro-: Human health tier I assessment
- >> IMAP assessments - Naphthalene, octachloro-: Environment tier I assessment

"The information provided is believed to be accurate but is not comprehensive and should be used as a reference. It reflects our current knowledge and is intended for safety guidance related to the product. This document does not constitute a warranty of the product's properties. Ionz is not responsible for any damages resulting from handling or contact with the product incorrectly."