ionz

SAFETY DATA SHEET

Updated on 08/02/2025

1. Material Identification

Product Name : Hexachloronaphthalene
Catalog Number : io-2485
CAS Number : 1335-87-1
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)

Pictogram(s)

GHS Hazard Statements

>> H315: Causes skin irritation [Warning Skin corrosion/irritation]

>> H319: Causes serious eye irritation [Warning Serious eye damage/eye irritation]

>> H372: Causes damage to organs through prolonged or repeated exposure [Danger Specific target organ toxicity, repeated exposure]

>> H373: May causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure]

Precautionary Statement Codes

>> P260, P264, P264+P265, P270, P280, P302+P352, P305+P351+P338, P319, P321, P332+P317, P337+P317, P362+P364, and P501

Health Hazards:

>> Excerpt from NIOSH Pocket Guide for Hexachloronaphthalene:

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

>> Symptoms: Acne-form dermatitis, nausea, confusion, jaundice, coma

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

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

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

3. Composition/Information On Ingredients

Chemical name : Hexachloronaphthalene
CAS Number : 1335-87-1
Molecular Formula : $C_{10}H_2Cl_6$
Molecular Weight : 334.8000 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. IMMEDIATELY call a hospital or poison control center even if no symptoms (such as redness or irritation) develop. IMMEDIATELY transport the victim to a hospital for treatment after washing the affected areas.
- >> INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. 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: 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. Generally, the induction of vomiting is NOT recommended outside of a physician's care due to the risk of aspirating the chemical into the victim's lungs. However, if the victim is conscious and not convulsing and if medical help is not readily available, consider the risk of inducing vomiting because of the high toxicity of the chemical ingested. Ipecac syrup or salt water may be used in such an emergency. IMMEDIATELY transport the victim to a hospital. 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.

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)
- >> Use water spray, foam, powder, carbon dioxide.

6. Accidental Release Measures

Spillage Disposal:

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

>> Personal protection: chemical protection suit and particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment.

7. Handling And Storage

Safe Storage:

>> Separated from strong oxidants and food and feedstuffs.

Storage Conditions:

>> Storage and handling: ... Materials...which can decompose into toxic components due to contact with heat ... acids, or acid fumes, should be stored in cool, well-ventilated place, out of direct rays of sun, away from ... Fire hazard, and should be periodically inspected and monitored. Incompatible materials ... isolated from each other.

8. Exposure Control/ Personal Protection

>> TWA 0.2 mg/m3 [skin]

>> 0.2 [mg/m3]

>> 0.2 [mg/m3]

>> 0.2 mg/m

Inhalation Risk:

>> Evaporation at 20 °C is negligible; a harmful concentration of airborne particles can, however, be reached quickly.

Effects of Short Term Exposure:

>> The substance is irritating to the eyes and skin.

Effects of Long Term Exposure:

>> May cause chloracne. The substance may have effects on the liver. This may result in liver impairment.

Exposure Prevention

>> PREVENT DISPERSION OF DUST! STRICT HYGIENE! IN ALL CASES CONSULT A DOCTOR!

Inhalation Prevention

>> Use local exhaust or breathing protection.

Skin Prevention

>> Protective gloves. Protective clothing.

Eye Prevention

>> Wear face shield or eye protection in combination with breathing protection.

Ingestion Prevention

>> Do not eat, drink, or smoke during work.

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:

- 334.8

Exact Mass:

- 333.825816

Physical Description:

- Hexachloronaphthalene is a white solid with an aromatic odor. (NTP, 1992)
- WHITE SOLID IN VARIOUS FORMS WITH CHARACTERISTIC ODOUR.

Color/Form:

- White solid

Odor:

- Aromatic odor.

Boiling Point:

- 649 to 729 °F at 760 mmHg (NTP, 1992)
- 344-388 °C

Melting Point:

- 279 °F (NTP, 1992)
- 137 °C

Solubility:

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

Density:

- 1.78 (NIOSH, 2024) - Denser than water; will sink
- 1.78 g/cm^3

Vapor Density:

- 11.6 (Air= 1 at bp of Hexachloronaphthalene)
- Relative vapor density (air = 1): 11.6

Vapor Pressure:

- less than 1 mmHg at 68 °F (NTP, 1992)
- Vapor pressure, Pa at 25 °C:

LogP:

- log Kow = 7.0 /Estimated/
- 7.59

Decomposition:

- Toxic gases and vapors (such as hydrogen chloride and carbon monoxide) may be released when /hexachloronaphthalene/ decomposes.

Relative Evaporation Rate:

The rate at which a material will vaporize (evaporate, change from liquid to vapor), compared to the rate of vaporization of a specific known material.

- Much less than 1 (Butyl Acetate= 1)

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.

>> 153.4 Å² [M]+ [CCS Type: TIMS, Method: calibration with PAHs]

10. Stability And Reactivity

>> Insoluble in water.

11. Toxicological Information

Toxicity Summary:

>> 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 impregnates for condensers and capacitors and dipping encapsulating cmpd 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 cmpd, as additive in gear oils and cutting cmpd, in flame proofing and insulation of electrical cable and conductors and moisture proof sealants, as separators in batteries, in refractive index testing oils, masking cmpd in electroplating and in grinding wheel lubricants. 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 concentration 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 concentration up to 150 pg/cu m at semi-rural 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 administration. Chlorinated naphthalenes, especially the dioxin like congeners, have been detected in adipose tissue, liver, blood and breast milk samples from the general population at concentration 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. The polychlorinated naphthalenes congener/isomer pattern found in human samples was significantly different from the commercial polychlorinated naphthalenes mixtures. Two dominating congeners were 1,2,3,5,7/1,2,5,6,7-hexachloronapthalene. Analyses of human tissue samples and fluids confirmed the high retention potency of the 1,2,3,4,6,7-/1,2,3,5,6,7-hexachloronaphthalene isomers. Chlorinated naphthalenes can be absorbed via oral, inhalative and dermal routes, with absorption and distribution over the e badministeredoy after oral admin. The main target organs are the liver and fat tissue (besides the kidney and lung) showing a high retention, especially for the higher chlorinated congeners The amount of bioaccumulation observed incr with the degree of chlorination of the chlorinated naphthalenes. Elimination of the parent compounds and/or metabolites occurs via feces and urine. Lower chlorinated naphthalenes are less toxic than the higher chlorinated naphthalenes. Long term and carcinogenicity studies with chlorinated naphthalenes have not been performed. Like related cmpd, chlorinated naphthalenes have been demonstrated to be inducers of the cytochrome p450 (CYP) dependent microsomal enzymes. 1,2,3,4,6,7-Hexachloronaphthalene has been found to accelerate the onset of spermatogenesis in male offspring of rats. Cattle developed severe hyperkeratosis during a 5 to 10 day oral exposure of purified hexachloronaphthalenes. Hexachlorinated naphthalenes showed hyperkeratoic activity in the rabbit ear test and in hairless mice. Rats fed a mixture of penta/hexachloronaphthalenes dosed on alternate days for 26 days showed moderate liver changes (swollen and vacoulated liver cells, as well as necrosis and degeneration of scattered cells.Inhalation of a mixture containing penta-/hexachloronaphthalenes resulted in slight histological liver damage in rats. 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 cmpd. Two hexa-isomers , which are minor components of Halowax 1014 were given single oral doses of Halowax 1014 or a mixture of hexachloronaphthalenes (consisting of equal amounts of 1,2,3,5,6,7-hexachloronaphthalene and 1,2,3,4,6,7-

hexachloronaphthalene and a third unidentified hexachloronapthalene) One day after exposure the polychlorinated naphthalene patadministeredtn adipose tissue of animals admin Halowax 1014 was similar to that of the technical product. In 10 days the two hexa-isomers were dominant and after 120 days, they were the only cogeners detected, their concn beings still above 50% of the measured after day 1. In liver samples this selective retention lasted 1 day. Rats dosed with the hexachloronaphthalene mixture showed a strong similar retention of the 1,2,3,5,6,7- and 1,2,3,4,6,7-hexachloronaphthalene (the other unidentified hexachloronaphthalene could not be detected. 1,2,3,4,6,7-Hexachloronaphthalene transfer from dam to offspring has been studied in Wistar rats. Concn of this isomer were noted in the fat of female offspring. Short term exposure to higher chlorinated naphthalenes resulted in mortality, liver damage, degeneration of the kidneys etc in rats, rabbits and cattle. Inhalation of a penta/hexachloronaphthalene mixture for 143 days resulted in a slight to moderate histological liver damage in rats. All chlorinated naphthalenes tested cause skin irritations in laboratory animals. Chlorinated napthalenes appear to be of moderate to high acute toxicity to aquatic organisms. /Chlorinated naphthalenes, Halowaxes, Higher Chlorinated Naphthalenes/

Exposure Routes:

>> The substance can be absorbed into the body by inhalation of fume and through the skin.

>> inhalation, skin absorption, ingestion, skin and/or eye contact

Skin Exposure

>> MAY BE ABSORBED! Redness. Pain.

Eye Exposure

>> Redness. Pain.

>> Acne-form dermatitis, nausea, confusion, jaundice, coma

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:

>> Treatment (Vet): Treatment of hyperkeratosis is purely supportive. Antibiotics can be used to prevent bacterial infection. Vit A and C ...admin, along with B-complex vitamins. Corticosteroids may be of some benefit. Skin should be kept as pliable as possible and free from flies and ectoparasites. /Chlorinated naphthalenes/

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ Causes severe acne-form eruptions and toxic /necrosis/ of the liver.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Hexachloronaphthalene ... was given orally in 3 % solutions in mineral oil over a period of 1 to 10 days /to calves/. Total doses of 5 to 23 mg/kg were administered. Lacrimation, salivation, nasal discharge, red areas in the mouth, depression and anorexia occured by day 5 ...

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. The substance may cause long-term effects in the aquatic environment.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: Hexachloronaphthalene concns of 30-250 ng/kg were detected in surface sediments collected from 10 lakes in central Finland in 1988(1); sediments from eight other lakes had no detectable levels (detection limit not

reported) of hexachloronaphthalene(1). The compound was detected in sediments collected in 1995 from 5 sites selected in the Venice Lagoon, Italy (pg/g, use characteristic): Giudeca Island - 17.20, heavy boat traffic and sewage; Peelestrina - 4.24, undeveloped; Chioggia Harbor - 7.46, harbor activity; Porto Marghera - 102.93, chemical and oil refining plants; and Dese River - 9.45, agricultural impact(2). Water exchange is with the Adriatic Sea(2). Hexachloronaphthalene was also detected in sediments collected in 1995 from 4 sites selected in the Orbetallo Lagoon, Italy, which drains to the Mediterranean Sea(2). Concentrations were as follows (pg/g, use characteristic): Santa Liberata - 5.63, connecting channel; Orbetello - 67.78, sewage treatment plant; fish farm station - 0.90; and Albegua River - 2.13, undeveloped(2). Hexachloronaphthalene was detected in sediment samples from the River Eman, River Dalalven, River Gota and Lake Vanern, Sweden at concns ranging from not detected (detection limit not specified) to 37 ng/g dry weight(3).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> Content of chlorinated fat-sol aromatic hydrocarbons was determined in fish from the Frierfjord and the Eidangerfjord near Oslo, Norway, areas polluted by industrial effluents. The fish species investigated are used for human consumption. Two components of halowax 1014 (pentachloronaphthalene and hexachloronaphthalene) were identified but not quantified.

Animal Concentrations:

Concentrations of this compound in animals.

>> Total hexachloronaphthalene isomer concn ranges of 700-33,000 pg/g lipid weight and 390-2,400 pg/g lipid weight were measured in tissues collected from three Baltic coastal and two in-land white-tailed eagles (Haliaeetus albicilla) recovered in Poland from 1991-1992(1). Hexachloronaphthalene was detected in Swedish marine bird samples, guillemot (Uria aalge), at concns ranging from 1.0 to 170 ng/g lipid weight(2). The compound was detected in seal blubber samples, ranging from 0.08-0.2 ng/g fat in grey seal (Halichoerus grypus) and not detected to 0.04 ng/g fat in ringed seal (Pusa hispida) collected from the Baltic Sea(3).

13. Disposal Considerations

Spillage Disposal

>> Personal protection: chemical protection suit and particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment.

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

Hexachloronaphthalene

IATA

Hexachloronaphthalene

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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. Hexachloronaphthalene is included on this list.

Regulatory Information

California Safe Cosmetics Program (CSCP) Reportable Ingredient

>> Hazard Traits - Bioaccumulation; Environmental Persistence

>> Authoritative List - WA PBTs

>> Report - if used as a fragrance or flavor ingredient

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 hydrogen chloride, phosgene, and carbon monoxide) may be released in a fire involving hexachloronaphthalene.