SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : Isophorone
Catalog Number : io-2538
CAS Number : 78-59-1
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 > 99.9% (2245 of 2246) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for < 0.1% (1 of 2246) of reports.

Pictogram(s)

>> Warning

GHS Hazard Statements

>> H302 (> 99.9%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H312 (> 99.9%): Harmful in contact with skin [Warning Acute toxicity, dermal]

>> H319 (96.1%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

>> H335 (> 99.9%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]

>> H351 (> 99.9%): Suspected of causing cancer [Warning Carcinogenicity]

Precautionary Statement Codes

>> P203, P261, P264, P264+P265, P270, P271, P280, P301+P317, P302+P352, P304+P340, P305+P351+P338, P317, P318, P319, P321, P330, P337+P317, P362+P364, P403+P233, P405, and P501

NFPA 704 Diamond

NFPA Health Rating

>> 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA Fire Rating

>> 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur. Materials would not under normal conditions form hazardous atmospheres with air, but under high ambient temperatures or under moderate heating could release vapor in sufficient quantities to produce hazardous atmospheres with air.

NFPA Instability Rating

>> 0 - Materials that in themselves are normally stable, even under fire conditions.

Health Hazards:

>> LIQUID: Irritating to skin and eyes. Harmful if swallowed. (USCG, 1999)

>> Combustible. (USCG, 1999)

>> Combustible. Above 84 °C explosive vapour/air mixtures may be formed.

3. Composition/Information On Ingredients

Chemical name : Isophorone
CAS Number : 78-59-1
Molecular Formula : C9H14O
Molecular Weight : 138.2100 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. Artificial respiration may be needed. Refer for medical attention.

Skin First Aid

>> Remove contaminated clothes. Rinse and then wash skin with water and soap.

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. Give a slurry of activated charcoal in water to drink. Do NOT induce vomiting.

5. Fire Fighting Measures

>> Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

>> CAUTION: The majority of these products have a very low flash point. Use of water spray when fighting fire may be inefficient. CAUTION: For mixtures containing alcohol or polar solvent, alcohol-resistant foam may be more effective.

>> SMALL FIRE: Dry chemical, CO2, water spray or regular foam. If regular foam is ineffective or unavailable, use alcohol-resistant foam.

>> LARGE FIRE: Water spray, fog or regular foam. If regular foam is ineffective or unavailable, use alcohol-resistant foam. Avoid aiming straight or solid streams directly onto the product. If it can be done safely, move undamaged containers away from the area around the fire.

>> FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. For petroleum crude oil, do not spray water directly into a breached tank car. This can lead to a dangerous boil over. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2024)

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

6. Accidental Release Measures

Isolation and Evacuation:

Isolation and evacuation measures to take when a large amount of this chemical is accidentally released in an emergency.

>> Excerpt from ERG Guide 128 [Flammable Liquids (Water-Immiscible)]:

>> IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area for at least 50 meters (150 feet) in all directions.

>> LARGE SPILL: Consider initial downwind evacuation for at least 300 meters (1000 feet).

>> FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Spillage Disposal:

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

>> Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

7. Handling And Storage

Safe Storage:

>> Separated from strong oxidants, strong bases and amines.

Storage Conditions:

>> store in a cool, dry, well-ventilated location. Outside or detached storage is preferred. Separate from oxidizing materials.

8. Exposure Control/ Personal Protection

REL-TWA (Time Weighted Average)

>> 4 ppm (23 mg/m³)

>> TWA 4 ppm (23 mg/m3)

>> 25.0 [ppm]

PEL-TWA (8-Hour Time Weighted Average)

>> 25 ppm (140 mg/m³)

TLV-Ceiling

>> 5.0 [ppm]

>> Ceiling Limit: 5 ppm.

>> 5 ppm as STEL; A3 (confirmed animal carcinogen with unknown relevance to humans).

TLV-C (Ceiling)

>> 5 ppm [1992]

MAK (Maximale Arbeitsplatz Konzentration)

>> 11 mg/m

Inhalation Risk:

>> A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20 °C.

Effects of Short Term Exposure:

>> The substance and the vapour are irritating to the eyes and respiratory tract. The substance may cause effects on the central nervous system.

Fire Prevention

>> NO open flames. Above 84 °C use a closed system and ventilation.

Exposure Prevention

>> PREVENT GENERATION OF MISTS!

Inhalation Prevention

>> Use ventilation, local exhaust or breathing protection.

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety spectacles.

Ingestion Prevention

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

Exposure Control and Personal Protection

RD50 (Exposure concentration producing a 50% respiratory rate decrease)

>> 27.0 [mmHg]

Maximum Allowable Concentration (MAK)

>> 2.0 [ppm]

9. Physical And Chemical Properties

Molecular Weight:

>> 138.21

Exact Mass:

>> 138.104465066

Physical Description:

>> Isophorone appears as a clear colorless liquid, with a camphor-like odor. Less dense than water and insoluble in water. Boiling point 420 °F. Flash point near 200 °F. Contact irritates skin and eyes. Toxic by ingestion. Used as a solvent and in

pesticides.

>> COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.

Color/Form:

>> Water-white liquid

Odor:

>> Peppermint-like odor

Boiling Point:

>> 419.4 °F at 760 mmHg (NTP, 1992)

>> 215 °C

Melting Point:

>> 18 °F (NTP, 1992)

>> -8 °C

Flash Point:

>> 184 °F (NTP, 1992)

>> 84 °C c.c.

Solubility:

>> 0.1 to 1 mg/mL at 64 °F (NTP, 1992)

>> Solubility in water, g/100ml at 25 °C: 1.2

Density:

>> 0.921 at 77 °F (USCG, 1999) - Less dense than water; will float

>> Relative density (water = 1): 0.92

Vapor Density:

>> 4.77 (NTP, 1992) - Heavier than air; will sink (Relative to Air)

>> Relative vapor density (air = 1): 4.8

Vapor Pressure:

>> 0.2 mmHg at 68 °F ; 1 mmHg at 100 °F (NTP, 1992)

>> Vapor pressure, Pa at 20 °C: 40

LogP:

>> log Kow = 1.70

>> 1.67

Autoignition Temperature:

>> 864 °F (USCG, 1999)

>> 460 °C

Viscosity:

>> 2.62 cP @ 20 °C

Heat of Combustion:

>> -16,170 BTU/lb= -8,980 cal/g= -376x10+5 J/kg

Heat of Vaporization:

>> 43.4 kJ/mol

Surface Tension:

>> 32 dyn/cm @ 20 °C

Ionization Potential:

>> 9.07 eV

Odor Threshold:

>> Odor Threshold Low: 0.19 [mmHg]

>> Odor Threshold High: 0.53 [mmHg]

>> Detection odor threshold from AIHA (mean = 0.19 ppm)

Refractive Index:

>> Index of refraction: 1.4766 @ 18 °C/D

10. Stability And Reactivity

>> Insoluble in water.

>> Peroxidizable Compound

Peroxide Forming Chemical:

Peroxide-forming chemicals (PFCs) are chemicals that can "auto-oxidize" with atmospheric oxygen under ambient conditions to form organic peroxides (contains an -O-O- bond). Peroxide formation can be initiated by exposure to air, self-polymerization, or solvent impurities. Once formed, organic peroxides are sensitive to thermal or mechanical shock and can be violently explosive in concentrated solutions or as solids.

Chemical

>> Isophorone

Class (* = UMN Designation)

>> D: Other compounds that may form peroxides

Reference(s)

>> Kelly, Cameo

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION: Isophorone is a colorless liquid with a peppermint like odor. It is soluble in water and miscible with most organic solvents. HUMAN EXPOSURE: The odor of isophorone can be detected at low concentrations. Eye, nose and throat irritation has been observed along with nausea, headache, dizziness, faintness and inebriation. Dermal and inhalation exposure may occur along with oral exposure from drinking water. ANIMAL STUDIES: Distribution studies in rats using (14)C isophorone showed that 93% of orally administered radioactivity appeared mainly in the urine and expired air within 24 hr. The tissues retaining the highest concentration after this period were the liver, kidney and preputial glands. The metabolites from oral administration of isophorone identified in rabbit urine resulted from the oxidation of the 3-methyl group, reduction of the keto group and hydrogenation of the double bond of the cyclohexene ring, and were eliminated as such or as glucuronide derivatives in the case of the alcohols. In animal studies, data indicate that isophorone is rapidly absorbed through the skin. Acute effects from dermal exposure in rats and rabbits ranged from mild erythema to scabs. Conjunctivitis and corneal damage have been reported following direct application to the eye or exposure to high concentrations of isophorone. In acute and short-term oral studies on rodents at high doses degenerative effects were seen in the liver and CNS depression and some deaths. In a 90 day oral study in beagle dogs (with limited numbers) no effects were seen at doses up to 150 mg/kg body weight per day. Isophorone does not induce gene mutations in bacteria, chromosomal aberrations in vitro, DNA repair in primary rat hepatocytes, or bone marrow micronuclei in mice. Positive effects were observed only in the absence of an exogenous metabolic system in L5178YTK +/- mouse mutagenesis assays as well as in a sister chromatid exchange assay. Isophorone induced morphological transformation in vitro in the absence of an exogenous metabolism system. It did not induce sex linked recessive lethal mutations in Drosophilia. In long term oral toxicity studies in mice and rats, male rats showed several lesions of the kidney, including nephropathy, tubular cell hyperplasia and low incidence of tubular cell adenomas and adenocarcinomas. Isophorone exposure was associated with some neoplastic lesions of the liver, and the integumentary and lymphoreticular systems of male mice, as well non-neoplastic liver and adrenal cortex lesions, but this was not observed in female mice. In /one/ long term inhalation study in rats and rabbits, irritation to eye and nasal mucosa, and lung and liver changes were observed. Very limited studies in rats and mice indicate that isophorone does not affect fertility nor does it cause developmental toxicity in experimental animals. The fact that central nervous system depression occurs in experimental animals could indicate a positive neurotoxic effect. Isophorone also elicited a positive effect in the behavioral despair swimming test. No data on terrestrial animals were available. The available data suggest that isophorone has a low toxicity to aquatic organisms.

USGS Health-Based Screening Levels for Evaluating Water-Quality:

This section provides the USGS Health-Based Screening Levels for Evaluating Water-Quality data.

Chemical

>> Isophorone

USGS Parameter Code

>> 34408

Noncancer HBSL (Health-Based Screening Level)[µg/L]

>> 900

Cancer HBSL [µg/L]

>> 50-5000

Reference

>> Smith, C.D. and Nowell, L.H., 2024. Health-Based Screening Levels for evaluating water-quality data (3rd ed.). DOI:10.5066/F71C1TWP

Evidence for Carcinogenicity:

Evidence that this chemical does or may cause cancer. The information here is collected from various sources by the Hazardous Substances Data Bank (HSDB).

>> Cancer Classification: Group C Possible Human Carcinogen

Carcinogen Classification:

This section provides the International Agency for Research on Cancer (IARC) Carcinogenic Classification and related monograph links. In the IARC Carcinogenic classification, chemicals are categorized into four groups: Group 1 (carcinogenic to humans), Group 2A (probably carcinogenic to humans), Group 2B (possibly carcinogenic to humans), and Group 3 (not classifiable as to its carcinogenicity to humans).

IARC Carcinogenic Agent

>> Isophorone

IARC Carcinogenic Classes

>> Group 2B: Possibly carcinogenic to humans

IARC Monographs

>> Volume 130: (2022) 1,1,1-Trichloroethane and Four Other Industrial Chemicals

Exposure Routes:

>> The substance can be absorbed into the body by inhalation, through the skin and by ingestion.

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

Inhalation Exposure

>> Burning sensation. Sore throat. Cough. Dizziness. Headache. Nausea. Shortness of breath.

Eye Exposure

>> Redness. Pain. Blurred vision.

Ingestion Exposure

>> Abdominal pain. Further see Inhalation.

>> irritation eyes, nose, throat; headache, nausea, dizziness, lassitude (weakness, exhaustion), malaise (vague feeling of discomfort), narcosis; dermatitis; In Animals: kidney, liver damage

Target Organs:

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

>> Dermal (Skin), Hepatic (Liver), Neurological (Nervous System), Ocular (Eyes), Respiratory (From the Nose to the Lungs)

>> Urinary

Cancer Sites:

The site in which cancer develops due to exposure to this compound. Cancers are casually referred to based on their primary sites (e.g., skin, lung, breasts, prostate, colon and rectum).

>> Reproductive

Adverse Effects:

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

>> Neurotoxin - Acute solvent syndrome

>> Dermatotoxin - Skin burns.

>> IARC Carcinogen - Class 3: Chemicals are not classifiable by the International Agency for Research on Cancer.

>> ACGIH Carcinogen - Confirmed Animal.

Toxicity Data:

>> LC50 (rat) = 7,000 mg/m3/4h

Interactions:

>> Joint toxic action of isophorone with 26 industrial liquid chemicals was examined based on acute LD50 data from oral intubations of female albino rats. ... LD50s were determined for each of the cmpds. Based on the assumption of simple similar action, isophorone exhibited >additive toxicity in combination with 9 cmpds & <additive toxicity in combination with 17 cmpds. The significance of the interactions was determined by modifying the interactive ratios (predicted/observed LC50) so that the distribution approximated normality. Significant interaction was then defined as those ratios which were beyond 1.96 standard deviations from the mean ratio. By this criterion none of the mixtures containing isophorone deviated significantly from the assumption of simple similar action. In a subsequent study, equal volume mixtures of isophorone & propylene oxide showed markedly <additive toxicity, but equitoxic mixtures showed slightly >additive toxicity. An equitoxic mixture was defined as a mixture of chemicals in volumes directly proportional to their respective rat oral LD50 values, so that each component contributed the same degree of toxicity to the mixture.

Antidote and Emergency Treatment:

>> Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . For 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. Administer activated charcoal ... . /Ketones and related compounds/

Human Toxicity Excerpts:

>> ... HUMAN VOLUNTEERS EXPOSED AT 40, 85, 200, & 400 PPM ISOPHORONE EXPERIENCED EYE, NOSE, & THROAT IRRITATION. A FEW COMPLAINTS OF NAUSEA, HEADACHE, DIZZINESS, FAINTNESS, INEBRIATION, & A FEELING OF SUFFOCATION RESULTED FROM 200 & 400 PPM. SYMPTOMS OF IRRITATION & ... /CNS DEPRESSION/ ACTION DECREASED @ CONCNS OF 40 & 85 PPM.

Non-Human Toxicity Excerpts:

>> ... /FROM WORK ON/ EXPERIMENTAL ANIMALS ... NO EFFECT WHATEVER RESULTED FROM EXPOSURE AT 25 PPM OF ISOPHORONE OF VAPOR. ... 10 RATS & 10 GUINEA PIGS, WERE EXPOSED 8 HR/DAY FOR 30 DAYS @ CONCN RANGING FROM 25-500 PPM. AT THE HIGHER CONCN THE CHIEF EFFECTS WERE ON THE KIDNEYS.

Non-Human Toxicity Values:

>> LD50 Rat oral 1000-3450 mg/kg.

National Toxicology Program Studies:

Reports from the National Toxicology Program, an interagency program supported by three government agencies (NIH, FDA, and CDC) within the Department of Health and Human Services. This program plays a critical role in generating, interpreting, and sharing toxicological information about chemicals of public health concerns.

>> Toxicology and carcinogenesis studies of isophorone > 94% pure, a widely used solvent and chem intermediate, were conducted by administering 0, 250, or 500 mg isophorone/kg/day by gavage in corn oil to groups of 50 rats and 50 mice of each sex, 5 days/wk for 103 wk. Doses selected for the 2 yr studies were based on 16 day studies in which rats and mice of each sex received doses of 0-2000 mg/kg/day and on 13 wk studies in which rats and mice of each sex received doses ranging from 0 to 1000 mg/kg/day by gavage in corn oil. No chemically related gross or histopathologic effects were observed in the 16 day or 13 wk studied, but 1/5 high-dose male rats, 4/5 high-dose female rats, and all high-dose female mice died. The high dose for the 2 yr studies was set at 500 mg/kg/day for each sex of rats and mice, based mainly on the deaths in the 13 wk studies. Throughout the 2 yr study, the mean body weights of the high-dose male rats averaged 5% lower than those of the vehicle controls. During the second year, the mean body wts of the female high-dose rats averaged 8% lower than those of the vehicle controls, and the high-dose female mice averaged 5% lower. The survival of male mice was also low (16/50; 16/50; 19/50), but there was a significant trend toward increased survival of dosed female mice relative to that of the vehicle controls (26/50; 35/50; 34/50). Dosed male rats showed a variety of proliferative lesions of the kidney ... . Dosed male rats also exhibited increased mineralization of the medullary collecting ducts ... and low-dose male rats showed a more severe nephropathy than is commonly seen in aging rats. Carcinomas of the preputial gland were increased in high-dose male rats ... . With the exception of a

moderate increase in nephropathy, ... female rats did not show chem related increased incidences of neoplastic or nonneoplastic lesions. In high-dose male mice, isophorone exposure was associated with increased incidences of hepatocellular adenomas and carcinomas. An increased incidence of lymphomas or leukemias was noted in low-dose male mice.

TSCA Test Submissions:

Under the Toxic Substances Control Act (TSCA), EPA has broad authority to issue regulations designed to require manufacturers (including importers) or processors to test chemical substances and mixtures for health and environmental effects. This section provides information on test reports submitted for this chemical under TSCA.

>> An inhalation teratology study was conducted with pregnant Fisher 344 rats and CD-1 mice receiving whole body exposure to isophorone at nominal concentrations of 0, 25, 50 or 115ppm in a dynamic air flow chamber. At each concentration, 22 rats and 22 mice were exposed for 6hrs/day on days 6-15 of gestation. There was no effect of treatment for all animals as indicated by mortality, gross necropsy observations and uterine implantation data. Maternal toxicity was evident by statistical differences between dosed groups and controls for: mean body weight and food consumption (115ppm group, rats and mice). No statistically significant differences (ANOVA) among control and treatment groups were found for any of the fetal external, visceral or skeletal parameters.[Bio/dynamics Inc.; Inhalation Teratology Study in Rats and Mice, Final Report. (1984), EPA Document No. 40-8555049, Fiche No. OTS0507224]

12. Ecological Information

Resident Soil (mg/kg)

>> 5.70e+02

Industrial Soil (mg/kg)

>> 2.40e+03

Resident Air (ug/m3)

>> 2.10e+03

Industrial Air (ug/m3)

>> 8.80e+03

Tapwater (ug/L)

>> 7.80e+01

MCL (ug/L)

>> 5.00e+01

Risk-based SSL (mg/kg)

>> 2.60e-02

Oral Slope Factor (mg/kg-day)-1

>> 9.50e-04

Chronic Oral Reference Dose (mg/kg-day)

>> 2.00e-01

Chronic Inhalation Reference Concentration (mg/m3)

>> 2.00e+00

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Fraction of Contaminant Absorbed Dermally from Soil

>> 0.1

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: Isophorone was qualitatively identified in sediment/soil/water samples taken from Love Canal in Niagara Falls, NY during 1980(1). According to the USEPA STORET Data Base, of 318 sediment samples tested, 0% were positive for isophorone(2). The compound was detected in sediments taken from Lake Pontchartrain (LA), concn range 0.98-12 ng/g (ppb) dry wt(3).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> The USEPA STORET Data Base reports that of 123 samples of biota, 0% were positive for isophorone(1). Whole fish samples collected from nearshore tributaries and the Grand Traverse Bay on Lake Michigan in the fall of 1993 tested positive for isophorone, at a mean concn range of not detected to 3.61 mg/kg wet weight(2). Isophorone was not detected in Great Lakes fish collected from the Sheboygen (WI), Milwaukee (WI), Kinninkinnic (WI), Fox (WI), Black (OH), Menominnee (WI), Wolf (WI), Ashtabula (OH) rivers, and Chequamegon Bay (Lake Superior, WI)(3). Bottomfish collected in 1981 from Old Town Dock area, Commencement Bay in Tacoma WA tested positive for isophorone at a max concn of 0.92 ppm(4).

13. Disposal Considerations

Spillage Disposal

>> Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

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.

>> The following wastewater treatment technologies have been investigated for Isophorone. Concentration process: Biological treatment.

>> The following wastewater treatment technologies have been investigated for Isophorone. Concentration process: Solvent extraction.

>> The following wastewater treatment technologies have been investigated for Isophorone. Concentration process: Activated carbon.

>> Spray into incinerator or burn in paper packaging. Additional flammable solvent may be added.

14. Transport Information

DOT

Isophorone

Reportable Quantity of 5000 lb or 2270 kg

IATA

Isophorone

,

15. Regulatory Information

Federal Drinking Water Guidelines:

Federal drinking water guidelines (e.g. maximum containment level (MCL)) for this chemical. In general, these guidelines are recommendations and not legally enforceable.

>> EPA 100 ug/l

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.

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. Isophorone is included on this list.

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: 2-Cyclohexen-1-one, 3,5,5-trimethyl-

REACH Registered Substance

>> Status: Active Update: 24-02-2023 https://echa.europa.eu/registration-dossier/-/registered-dossier/14527

>> Status: Active Update: 09-03-2023 https://echa.europa.eu/registration-dossier/-/registered-dossier/31888

New Zealand EPA Inventory of Chemical Status

>> 2-Cyclohexen-1-one, 3,5,5-trimethyl-: HSNO Approval: HSR001178 Approved with controls

16. Other Information

Other Safety Information

Chemical Assessment

>> IMAP assessments - 2-Cyclohexen-1-one, 3,5,5-trimethyl-: Human health tier II assessment

>> IMAP assessments - 2-Cyclohexen-1-one, 3,5,5-trimethyl-: Environment tier I assessment