SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : 3-Chloro-2-methyl-1-propene
Catalog Number : io-1977
CAS Number : 563-47-3
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

>> H225 (100%): Highly Flammable liquid and vapor [Danger Flammable liquids]

>> H301+H331 (37.7%): Toxic if swallowed or if inhaled [Danger Acute toxicity, oral; acute toxicity, inhalation]

>> H301 (38.1%): Toxic if swallowed [Danger Acute toxicity, oral]

>> H302 (61.9%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H304 (23.8%): May be fatal if swallowed and enters airways [Danger Aspiration hazard]

>> H314 (100%): Causes severe skin burns and eye damage [Danger Skin corrosion/irritation]

>> H317 (100%): May cause an allergic skin reaction [Warning Sensitization, Skin]

>> H318 (62.3%): Causes serious eye damage [Danger Serious eye damage/eye irritation]

>> H331 (65.4%): Toxic if inhaled [Danger Acute toxicity, inhalation]

>> H332 (34.6%): Harmful if inhaled [Warning Acute toxicity, inhalation]

>> H351 (23.8%): Suspected of causing cancer [Warning Carcinogenicity]

>> H411 (100%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P203, P210, P233, P240, P241, P242, P243, P260, P261, P264, P264+P265, P270, P271, P272, P273, P280, P301+P316, P301+P317, P301+P330+P331, P302+P352, P302+P361+P354, P303+P361+P353, P304+P340, P305+P354+P338, P316, P317, P318, P321, P330, P331, P333+P317, P362+P364, P363, P370+P378, P391, P403+P233, P403+P235, 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

>> 3 - Liquids and solids that can be ignited under almost all ambient temperature conditions. Materials produce hazardous atmospheres with air under almost all ambient temperatures or, though unaffected by ambient temperatures, are readily ignited under almost all conditions.

NFPA Instability Rating

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

Health Hazards:

>> Inhalation causes irritation of nose and throat. Contact of vapor or liquid with eyes causes irritation. Liquid irritates skin. Ingestion causes irritation of mouth and stomach. (USCG, 1999)

>> Special Hazards of Combustion Products: Irritating and toxic hydrogen chloride and phosgene vapors may be formed.

>> Behavior in Fire: Vapor is heavier than air and may travel considerable distance to a source of ignition and flash back. (USCG, 1999)

>> Highly flammable. Gives off irritating or toxic fumes (or gases) in a fire. Vapour/air mixtures are explosive. Heating will cause rise in pressure with risk of bursting.

3. Composition/Information On Ingredients

Chemical name : 3-Chloro-2-methyl-1-propene
CAS Number : 563-47-3
Molecular Formula : C4H7Cl
Molecular Weight : 90.5500 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: DO NOT INDUCE VOMITING. Volatile chemicals have a high risk of being aspirated into the victim's lungs during vomiting which increases the medical problems. 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. 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.

>> OTHER: Since this chemical is a known or suspected carcinogen you should contact a physician for advice regarding the possible long term health effects and potential recommendation for medical monitoring. Recommendations from the physician will depend upon the specific compound, its chemical, physical and toxicity properties, the exposure level, length of exposure, and the route of exposure. (NTP, 1992)

First Aid Measures

Inhalation First Aid

>> Fresh air, rest. Half-upright position. 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. Do NOT induce vomiting. Rest. Refer for medical attention .

5. Fire Fighting Measures

>> Excerpt from ERG Guide 130 [Flammable Liquids (Water-Immiscible / Noxious); polymerization hazard]:

>> CAUTION: The majority of these products have a very low flash point. Use of water spray when fighting fire may be inefficient.

>> 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. 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 powder, carbon dioxide, foam. In case of fire: keep drums, etc., cool by spraying with water.

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 130 [Flammable Liquids (Water-Immiscible / Noxious); polymerization hazard]:

>> 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.

>> Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Remove all ignition sources. 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. Do NOT wash away into sewer. Do NOT let this chemical enter the environment.

7. Handling And Storage

Safe Storage:

>> Fireproof. Separated from strong oxidants and strong bases. Cooled. Well closed. Ventilation along the floor. Store in an area without drain or sewer access.

8. Exposure Control/ Personal Protection

MAK (Maximale Arbeitsplatz Konzentration)

>> carcinogen category: 3

Inhalation Risk:

>> A harmful contamination of the air can be reached very quickly on evaporation of this substance at 20 °C.

Effects of Short Term Exposure:

>> Lachrymation. The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the central nervous system. Exposure at high levels could cause lowering of consciousness.

Effects of Long Term Exposure:

>> Repeated or prolonged contact may cause skin sensitization.

Fire Prevention

>> NO open flames, NO sparks and NO smoking. NO contact with hot surfaces. Closed system, ventilation, explosion-proof electrical equipment and lighting. Do NOT use compressed air for filling, discharging, or handling.

Exposure Prevention

>> PREVENT GENERATION OF MISTS! AVOID ALL CONTACT!

Inhalation Prevention

>> Use ventilation, local exhaust or breathing protection.

Skin Prevention

>> Protective gloves.

Eye Prevention

>> Wear safety goggles or eye protection in combination with breathing protection.

Ingestion Prevention

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

9. Physical And Chemical Properties

Molecular Weight:

>> 90.55

Exact Mass:

>> 90.0236279

Physical Description:

>> Methylallyl chloride appears as a colorless to straw-colored liquid with a sharp penetrating odor. Less dense than water and insoluble in water. Flash point below 0 °F. May be toxic by ingestion. Irritating to skin and eyes. Used to make plastics and pharmaceuticals.

>> COLOURLESS-TO-YELLOW LIQUID WITH PUNGENT ODOUR.

Color/Form:

>> COLORLESS TO STRAW-COLORED LIQUID

Odor:

>> SHARP, PENETRATING

Boiling Point:

>> 160 to 162 °F at 760 mmHg (NTP, 1992)

>> 72 °C

Melting Point:

>> less than -112 °F (NTP, 1992)

>> -80 °C

Flash Point:

>> 9 °F (NTP, 1992)

>> -12 °C c.c.

Solubility:

>> less than 1 mg/mL at 70 °F (NTP, 1992)

>> Solubility in water, g/100ml at 25 °C: 0.14 (very poor)

Density:

>> 0.928 at 68 °F (USCG, 1999) - Less dense than water; will float

>> Relative density (water = 1): 0.92

Vapor Density:

>> 3.12 (NTP, 1992) - Heavier than air; will sink (Relative to Air)

>> Relative vapor density (air = 1): 3.1

Vapor Pressure:

>> 101.7 mmHg at 68 °F (NTP, 1992)

>> Vapor pressure, kPa at 20 °C: 14

LogP:

>> 1.98

Stability/Shelf Life:

>> VOLATILE

Autoignition Temperature:

>> 540 °C

Viscosity:

>> 4.2X10-4 Pa.s

Heat of Vaporization:

>> 31.8 kJ/mol

Refractive Index:

>> INDEX OF REFRACTION: 1.4318 AT 15 °C/D; 1.4274 AT 20 °C/D

10. Stability And Reactivity

>> Highly flammable. It may react with water at elevated temperatures. (NTP, 1992). Insoluble in water.

>> Highly Flammable

>> Polymerizable

11. Toxicological Information

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).

>> Evaluation: There is inadequate evidence in humans for the carcinogenicity of 3-chloro-2-methylpropene. There is limited evidence in experimental animals for the carcinogenicity of 3-chloro-2-methylchloropropene. Overall evaluation: 3-Chloro-2-methylpropene is not classifiable as to its carcinogenicity to humans (Group 3).

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

>> 3-Chloro-2-methylpropene, technical grade

IARC Carcinogenic Classes

>> Group 2B: Possibly carcinogenic to humans

IARC Monographs

>> Volume 63: (1995) Dry Cleaning, Some Chlorinated Solvents and Other Industrial Chemicals

>> Volume 115: (2018) Some Industrial Chemicals

Exposure Routes:

>> The substance can be absorbed into the body by inhalation of its vapour and by ingestion.

Inhalation Exposure

>> Cough. Sore throat. Headache. Shortness of breath.

Skin Exposure

>> Redness. Pain.

Eye Exposure

>> Watering of the eyes. Redness. Pain.

Adverse Effects:

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

>> Neurotoxin - Acute solvent syndrome

>> Occupational hepatotoxin - Secondary hepatotoxins: the potential for toxic effect in the occupational setting is based on cases of poisoning by human ingestion or animal experimentation.

>> Dermatotoxin - Skin burns.

>> Lacrimator (Lachrymator) - A substance that irritates the eyes and induces the flow of tears.

>> Skin Sensitizer - An agent that can induce an allergic reaction in the skin.

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

>> NTP Carcinogen - Reasonably anticipated to be a human carcinogen.

Toxicity Data:

>> LC50 (rat) = 34,000 mg/m3/30 min

Human Toxicity Excerpts:

>> SYMPTOMATOLOGY: 1. A. INHALATION, HIGH VAPOR CONCN: GASPING, REFUSAL TO BREATHE, COUGHING, SUBSTERNAL PAIN, & EXTREME RESP DISTRESS @ ... CONCN OVER 1500 PPM. IRRITATION OF EYES & UPPER RESP MUCOSA APPEARS PROMPTLY AFTER EXPOSURE TO CONCENTRATED VAPORS. LACRIMATION AND HEADACHE ARE PROMINENT. COMA MAY OCCUR RAPIDLY. B. INHALATION, LOW VAPOR CONCN: CENTRAL NERVOUS DEPRESSION & MODERATE IRRITATION OF RESP SYSTEM. 2. DERMAL: SEVERE SKIN IRRITATION WITH MARKED INFLAMMATORY RESPONSE OF EPIDERMIS & UNDERLYING TISSUES. /DICHLOROPROPENES/

Non-Human Toxicity Excerpts:

>> LC50 VALUES OF METHALLYL CHLORIDE INHALED BY MICE & RATS WERE 57.0 & 34.5 MG/L, RESPECTIVELY. DECR IN LEVELS OF SULFHYDRYL & DISULFIDE GROUPS IN BLOOD & LIVER WAS OBSERVED IN RATS EXPOSED AT 10 MOLES/L.

Non-Human Toxicity Values:

>> LC50 MOUSE 57.0 MG/L /30 MIN/

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 of technical grade 3-chloro-2-methylpropene (containing 5% dimethylvinyl chloride) ... were performed on F344/N rats and B6C3F1 mice. ... Groups of 50 male and 50 female F344/N rats were admin 3-chloro-2-methylpropene in corn oil by gavage at doses of 0, 75 or 150 mg/kg body wt, 5 days/wk for 103 wk, and groups of 50 male and female B6C3F1 mice received 3-chloro-2-methylpropene at 0, 100 or 200 mg/kg on the same schedule. ... Under the conditions of these two yr gavage studies, there was clear evidence of the carcinogenicity for 3-chloro-2-methylpropene as shown by the incr incidences of squamous cell neoplasms in the forestomach of male and female F344/N rats and of male and female B6C3F1 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.

>> The ability of 3-chloro-2-methylpropene (CMP) to induce morphological transformation in the BALB/3T3 mouse cell line (Cell Transformation Assay) in the presence and absence of added metabolic activation by Aroclor-induced rat liver S9 fraction was evaluated. Based on preliminary clonal toxicity determinations (exposure time=2 hrs), CMP was tested at 0.03, 0.1, 0.3 and 1.0 ul/ml in the absence of activation (cell survival ranging from 100-77% relative to acetone solvent control), and at 0.10, 0.15, 0.20 and 0.25 ul/ml in the presence of added metabolic activation (cell survival ranging from 85% to <1%). Test material did not induce the appearance of a significant number of transformed foci.

12. Ecological Information

ICSC Environmental Data:

>> The substance is harmful to aquatic organisms.

13. Disposal Considerations

Spillage Disposal

>> Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Remove all ignition sources. 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. Do NOT wash away into sewer. Do NOT let this chemical enter the environment.

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.

14. Transport Information

DOT

3-Chloro-2-methyl-1-propene
3
UN Pack Group: II

IATA

3-Chloro-2-methyl-1-propene
3,
UN Pack Group: II

15. Regulatory Information

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: 1-Propene, 3-chloro-2-methyl-

REACH Registered Substance

>> Status: Active Update: 24-09-2020 https://echa.europa.eu/registration-dossier/-/registered-dossier/20647

New Zealand EPA Inventory of Chemical Status

>> 1-Propene, 3-chloro-2-methyl-: Does not have an individual approval but may be used under an appropriate group standard

16. Other Information

Other Safety Information

Chemical Assessment

>> IMAP assessments - 1-Propene, 3-chloro-2-methyl-: Environment tier I assessment

>> IMAP assessments - 1-Propene, 3-chloro-2-methyl-: Human health tier I assessment

>> Evaluation - 1-Propene, 3-chloro-2-methyl-

"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."