

1. Material Identification

Product Name : Cumene

Catalog Number : io-2045

CAS Number : 98-82-8

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% (3175 of 3176) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for < 0.1% (1 of 3176) of reports.

Pictogram(s)



GHS Hazard Statements

>> H226 (> 99.9%): Flammable liquid and vapor [Warning Flammable liquids]

>> H304 (> 99.9%): May be fatal if swallowed and enters airways [Danger Aspiration hazard]

>> H332 (26.4%): Harmful if inhaled [Warning Acute toxicity, inhalation]

>> H335 (97.7%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]

>> H411 (96.9%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P210, P233, P240, P241, P242, P243, P261, P271, P273, P280, P301+P316, P303+P361+P353, P304+P340, P317, P319, P331, 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

- >> 1 – Materials that in themselves are normally stable but that can become unstable at elevated temperatures and pressures.

Health Hazards:

- >> Narcotic action with long-lasting effects; depressant to central nervous system. (USCG, 1999)

ERG 2024, Guide 130 (Isopropylbenzene)

- >> May cause toxic effects if inhaled or absorbed through skin.
- >> Inhalation or contact with material may irritate or burn skin and eyes.
- >> Fire will produce irritating, corrosive and/or toxic gases.
- >> Vapors may cause dizziness or asphyxiation, especially when in closed or confined areas.
- >> Runoff from fire control or dilution water may cause environmental contamination.

ERG 2024, Guide 130 (Cumene)

- >> May cause toxic effects if inhaled or absorbed through skin.
- >> Inhalation or contact with material may irritate or burn skin and eyes.
- >> Fire will produce irritating, corrosive and/or toxic gases.
- >> Vapors may cause dizziness or asphyxiation, especially when in closed or confined areas.
- >> Runoff from fire control or dilution water may cause environmental contamination.

- >> Excerpt from ERG Guide 130 [Flammable Liquids (Water-Immiscible / Noxious)]:
- >> HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along the ground and collect in low or confined areas (sewers, basements, tanks, etc.). Vapor explosion hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids will float on water. (ERG, 2024)

ERG 2024, Guide 130 (Isopropylbenzene)

- >> HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames.
- >> Vapors may form explosive mixtures with air.
- >> Vapors may travel to source of ignition and flash back.
- >> Most vapors are heavier than air. They will spread along the ground and collect in low or confined areas (sewers, basements, tanks, etc.).
- >> Vapor explosion hazard indoors, outdoors or in sewers.
- >> Those substances designated with a (P) may polymerize explosively when heated or involved in a fire.
- >> Runoff to sewer may create fire or explosion hazard.
- >> Containers may explode when heated.
- >> Many liquids will float on water.

ERG 2024, Guide 130 (Cumene)

- >> HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames.
- >> Vapors may form explosive mixtures with air.
- >> Vapors may travel to source of ignition and flash back.
- >> Most vapors are heavier than air. They will spread along the ground and collect in low or confined areas (sewers, basements, tanks, etc.).
- >> Vapor explosion hazard indoors, outdoors or in sewers.
- >> Those substances designated with a (P) may polymerize explosively when heated or involved in a fire.
- >> Runoff to sewer may create fire or explosion hazard.
- >> Containers may explode when heated.

- >> Many liquids will float on water.
- >> Flammable. Above 31 °C explosive vapour/air mixtures may be formed.

3. Composition/Information On Ingredients

Chemical name : Cumene
CAS Number : 98-82-8
Molecular Formula : C₉H₁₂
Molecular Weight : 120.1900 g/mol

4. First Aid Measures

First Aid:

- >> Excerpt from NIOSH Pocket Guide for Cumene:
- >> Eye: IRRIGATE IMMEDIATELY – If this chemical contacts the eyes, immediately wash (irrigate) the eyes with large amounts of water, occasionally lifting the lower and upper lids. Get medical attention immediately.
- >> Skin: WATER FLUSH PROMPTLY – If this chemical contacts the skin, flush the contaminated skin with water promptly. If this chemical penetrates the clothing, immediately remove the clothing and flush the skin with water promptly. If irritation persists after washing, get medical attention.
- >> Breathing: RESPIRATORY SUPPORT – If a person breathes large amounts of this chemical, move the exposed person to fresh air at once. If breathing has stopped, perform artificial respiration. Keep the affected person warm and at rest. Get medical attention as soon as possible.
- >> Swallow: MEDICAL ATTENTION IMMEDIATELY – If this chemical has been swallowed, get medical attention immediately. (NIOSH, 2024)

ERG 2024, Guide 130 (Isopropylbenzene)

- >> General First Aid:
- >> Call 911 or emergency medical service.
- >> Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and avoid contamination.
- >> Move victim to fresh air if it can be done safely.
- >> Administer oxygen if breathing is difficult.
- >> If victim is not breathing:
 - >> DO NOT perform mouth-to-mouth resuscitation; the victim may have ingested or inhaled the substance.
 - >> If equipped and pulse detected, wash face and mouth, then give artificial respiration using a proper respiratory medical device (bag-valve mask, pocket mask equipped with a one-way valve or other device).
 - >> If no pulse detected or no respiratory medical device available, provide continuous compressions. Conduct a pulse check every two minutes or monitor for any signs of spontaneous respirations.
- >> Remove and isolate contaminated clothing and shoes.
- >> For minor skin contact, avoid spreading material on unaffected skin.
- >> In case of contact with substance, remove immediately by flushing skin or eyes with running water for at least 20 minutes.
- >> For severe burns, immediate medical attention is required.
- >> Effects of exposure (inhalation, ingestion, or skin contact) to substance may be delayed.
- >> Keep victim calm and warm.
- >> Keep victim under observation.
- >> For further assistance, contact your local Poison Control Center.
- >> Note: Basic Life Support (BLS) and Advanced Life Support (ALS) should be done by trained professionals.
- >> Specific First Aid:
 - >> Wash skin with soap and water.

- >> In case of burns, immediately cool affected skin for as long as possible with cold water. Do not remove clothing if adhering to skin.

ERG 2024, Guide 130 (Cumene)

- >> General First Aid:
- >> Call 911 or emergency medical service.
- >> Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and avoid contamination.
- >> Move victim to fresh air if it can be done safely.
- >> Administer oxygen if breathing is difficult.
- >> If victim is not breathing:
- >> DO NOT perform mouth-to-mouth resuscitation; the victim may have ingested or inhaled the substance.
- >> If equipped and pulse detected, wash face and mouth, then give artificial respiration using a proper respiratory medical device (bag-valve mask, pocket mask equipped with a one-way valve or other device).
- >> If no pulse detected or no respiratory medical device available, provide continuous compressions. Conduct a pulse check every two minutes or monitor for any signs of spontaneous respirations.
- >> Remove and isolate contaminated clothing and shoes.
- >> For minor skin contact, avoid spreading material on unaffected skin.
- >> In case of contact with substance, remove immediately by flushing skin or eyes with running water for at least 20 minutes.
- >> For severe burns, immediate medical attention is required.
- >> Effects of exposure (inhalation, ingestion, or skin contact) to substance may be delayed.
- >> Keep victim calm and warm.
- >> Keep victim under observation.
- >> For further assistance, contact your local Poison Control Center.
- >> Note: Basic Life Support (BLS) and Advanced Life Support (ALS) should be done by trained professionals.
- >> Specific First Aid:
- >> Wash skin with soap and water.
- >> In case of burns, immediately cool affected skin for as long as possible with cold water. Do not remove clothing if adhering to skin.

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.

Eye First Aid

- >> Rinse with plenty of water (remove contact lenses if easily possible).

Ingestion First Aid

- >> Rinse mouth. Do NOT induce vomiting. Refer immediately for medical attention.

5. Fire Fighting Measures

- >> Excerpt from ERG Guide 130 [Flammable Liquids (Water-Immiscible / Noxious)]:
- >> 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, AFFF, foam, carbon dioxide. 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)]:
- >> 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)

Evacuation: ERG 2024, Guide 130 (Isopropylbenzene)

- >> 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.

Evacuation: ERG 2024, Guide 130 (Cumene)

- >> 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.

Spillage Disposal:

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

- >> Personal protection: chemical protection suit and 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. Do NOT let this chemical enter the environment.

Accidental Release Measures

Public Safety: ERG 2024, Guide 130 (Isopropylbenzene)

- >> CALL 911. Then call emergency response telephone number on shipping paper. If shipping paper not available or no answer, refer to appropriate telephone number listed on the inside back cover.
- >> Keep unauthorized personnel away.
- >> Stay upwind, uphill and/or upstream.
- >> Ventilate closed spaces before entering, but only if properly trained and equipped.

Spill or Leak: ERG 2024, Guide 130 (Isopropylbenzene)

- >> ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area.

- >> All equipment used when handling the product must be grounded.
- >> Do not touch or walk through spilled material.
- >> Stop leak if you can do it without risk.
- >> Prevent entry into waterways, sewers, basements or confined areas.
- >> A vapor-suppressing foam may be used to reduce vapors.
- >> Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers.
- >> Use clean, non-sparking tools to collect absorbed material.
- >> Large Spill
- >> Dike far ahead of liquid spill for later disposal.
- >> Water spray may reduce vapor, but may not prevent ignition in closed spaces.

Public Safety: ERG 2024, Guide 130 (Cumene)

- >> CALL 911. Then call emergency response telephone number on shipping paper. If shipping paper not available or no answer, refer to appropriate telephone number listed on the inside back cover.
- >> Keep unauthorized personnel away.
- >> Stay upwind, uphill and/or upstream.
- >> Ventilate closed spaces before entering, but only if properly trained and equipped.

Spill or Leak: ERG 2024, Guide 130 (Cumene)

- >> ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area.
- >> All equipment used when handling the product must be grounded.
- >> Do not touch or walk through spilled material.
- >> Stop leak if you can do it without risk.
- >> Prevent entry into waterways, sewers, basements or confined areas.
- >> A vapor-suppressing foam may be used to reduce vapors.
- >> Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers.
- >> Use clean, non-sparking tools to collect absorbed material.
- >> Large Spill
- >> Dike far ahead of liquid spill for later disposal.
- >> Water spray may reduce vapor, but may not prevent ignition in closed spaces.

7. Handling And Storage

Safe Storage:

- >> Fireproof. Separated from strong oxidants and acids. Cool. Keep in the dark. Store only if stabilized. Store in an area without drain or sewer access. Provision to contain effluent from fire extinguishing.

Storage Conditions:

- >> ... Precautions ... such as mounds around storage tanks, sills at doorways or especially designed floors /are needed/ to limit spread of escaping liquid. Open flames & other sources of ignition should be excluded where cumene is stored.

8. Exposure Control/ Personal Protection

REL-TWA (Time Weighted Average)

- >> 50 ppm (245 mg/m³)
- >> TWA 50 ppm (245 mg/m³) [skin]
- >> 50.0 [ppm]

PEL-TWA (8-Hour Time Weighted Average)

- >> 50 ppm (245 mg/m³)
- >> 5.0 [ppm]
- >> 5 ppm as TWA; A3 (confirmed animal carcinogen with unknown relevance to humans).

TLV-TWA (Time Weighted Average)

- >> 50 ppm [1997]

EU-OEL

- >> 50 mg/m

MAK (Maximale Arbeitsplatz Konzentration)

- >> 50 mg/m

Emergency Response: ERG 2024, Guide 130 (Isopropylbenzene)

- >> 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.

Emergency Response: ERG 2024, Guide 130 (Cumene)

- >> 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.

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:

- >> If swallowed the substance easily enters the airways and could result in aspiration pneumonitis. The substance may cause effects on the central nervous system. Exposure far above the OEL could cause unconsciousness.

Effects of Long Term Exposure:

- >> Repeated or prolonged contact with skin may cause dermatitis. The substance may have effects on the liver and upper respiratory tract. This substance is possibly carcinogenic to humans.

Fire Prevention

- >> NO open flames, NO sparks and NO smoking. Above 31 °C use a closed system, ventilation and explosion-proof electrical equipment. Prevent build-up of electrostatic charges (e.g., by grounding).

Exposure Prevention

- >> AVOID ALL CONTACT!

Inhalation Prevention

- >> Use ventilation, local exhaust or breathing protection.

Skin Prevention

- >> Protective gloves. Protective clothing.

Eye Prevention

- >> Wear safety spectacles.

Ingestion Prevention

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

Exposure Control and Personal Protection

Protective Clothing: ERG 2024, Guide 130 (Isopropylbenzene)

- >> Wear positive pressure self-contained breathing apparatus (SCBA).
- >> Structural firefighters' protective clothing provides thermal protection but only limited chemical protection.

Protective Clothing: ERG 2024, Guide 130 (Cumene)

- >> Wear positive pressure self-contained breathing apparatus (SCBA).
- >> Structural firefighters' protective clothing provides thermal protection but only limited chemical protection.

Maximum Allowable Concentration (MAK)

- >> 10.0 [ppm]

9. Physical And Chemical Properties

Molecular Weight:

- >> 120.19

Exact Mass:

- >> 120.093900383

Physical Description:

- >> Cumene appears as a clear colorless liquid with an aromatic odor. Less dense than water and insoluble in water. Vapors heavier than air. May be moderately toxic by inhalation, ingestion and skin absorption.
- >> COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.

Color/Form:

- >> Colorless liquid

Odor:

- >> Gasoline-like odor

Boiling Point:

- >> 306.3 °F at 760 mmHg (USCG, 1999)
- >> 152 °C

Melting Point:

- >> -140.9 °F (USCG, 1999)
- >> -96 °C

Flash Point:

- >> 96 °F (USCG, 1999)
- >> 31 °C c.c.

Solubility:

- >> Insoluble (NIOSH, 2024)
- >> Solubility in water, g/l at 20 °C: 0.2 (very poor)

Density:

- >> 0.866 at 59 °F (USCG, 1999) – Less dense than water; will float
- >> Relative density (water = 1): 0.90

Vapor Density:

- >> 4.1 (Air = 1)
- >> Relative vapor density (air = 1): 4.2

Vapor Pressure:

- >> 25.85 mmHg (USCG, 1999)
- >> Vapor pressure, Pa at 20 °C: 427

LogP:

- >> log Kow = 3.66
- >> 3.66

Stability/Shelf Life:

- >> Volatile

Autoignition Temperature:

- >> 797 °F (USCG, 1999)
- >> 420 °C

Decomposition:

- >> Hazardous decomposition products: Toxic gases and vapors (such as carbon monoxide) may be released.

Viscosity:

- >> 0.737 mPa.sec at 25 °C
- >> 0.85 mm²/s at 25 °C

Heat of Vaporization:

- >> 45.13 kJ/mol at 25 °C

Surface Tension:

- >> 27.69 mN/m at 25 °C

Ionization Potential:

- >> 8.75 eV

Dispersion:

In optics, dispersion is defined as the spreading of white light into its full spectrum of wavelengths when it passes through an object. Dispersion occurs whenever the propagation of light depends on wavelength (i.e., when the velocities of different components of a light wave depend on the wavelengths of those components).

- >> Specific dispersion: 166.2

Odor Threshold:

- >> Odor Threshold Low: 0.008 [mmHg]
- >> Odor Threshold High: 0.13 [mmHg]
- >> Detection odor threshold from AIHA (mean = 0.032 ppm)

Refractive Index:

>> Index of refraction: 1.4915

10. Stability And Reactivity

>> Highly flammable. Insoluble in water.

>> Highly Flammable

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

>> Cumene

Class (* = UMN Designation)

>> B: Compounds that form peroxides on concentration (distillation/evaporation)

Peroxide Concentration Over Time

>> 2 samples had 3-30 ppm peroxide; age >9 yrs

Reference(s)

>> Kelly

11. Toxicological Information

Toxicity Summary:

>> IDENTIFICATION: Cumene is a water insoluble petrochemical used in the manufacture of several chemicals, including phenol and acetone. HUMAN EXPOSURE: In humans, cumene is metabolized primarily to the secondary alcohol, 2-phenyl-2-propanol. This alcohol and its conjugates are readily excreted by humans. No data are available with which to quantify human exposure. It is not possible to assess its potential for carcinogenicity in humans, because long term carcinogenicity studies with the chemical have not been performed. ANIMAL/PLANT STUDIES: Cumene is metabolized primarily to the secondary alcohol, 2-phenyl-2-propanol in animals. This alcohol and its conjugates are readily excreted by rodents. Increases in organ weights, primarily the kidney weights are the most prominent effects observed in rodents readily exposed to cumene by either the oral or inhalation route. No adverse effects were observed in rat or rabbit fetuses whose mothers had been exposed to cumene during fetal development. Although no multigenerational reproductive studies have been performed using cumene, the rapid metabolism and excretion, coupled with the lack of effects on sperm morphology in a subchronic study, suggest that it has a low potential for reproductive toxicity. Most genotoxicity test data with cumene are negative. Inadequate data, especially measured exposure information, exist to allow a quantitative evaluation of the risk to populations of aquatic or terrestrial organisms from exposure to cumene. Values indicate a slight potential for bioconcentration in fish. There are no data on the bioaccumulation in fish.

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

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

Chemical

>> Isopropylbenzene

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

>> 600

Benchmark Remarks

>> Last updated 8/1/1997; listed as cumene

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).

- >> Evaluation: No data were available from studies in humans. There is sufficient evidence in experimental animals for the carcinogenicity of cumene. There is sufficient evidence in experimental animals for the carcinogenicity of alpha-methylstyrene. Cumene is possibly carcinogenic to humans (Group 2B). alpha-Methylstyrene is possibly carcinogenic to humans (Group 2B).

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

- >> Cumene

IARC Carcinogenic Classes

- >> Group 2B: Possibly carcinogenic to humans

IARC Monographs

- >> Volume 101: (2012) Some Chemicals Present in Industrial and Consumer Products, Food and Drinking-water
- >> 2B, possibly carcinogenic to humans. (L135)

Health Effects:

- >> Petroleum distillates are aspiration hazards and may cause pulmonary damage, central nervous system depression, and cardiac effects such as cardiac arrhythmias. They may also affect the blood, immune system, liver, and kidney. (A600, L1297)

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

Inhalation Exposure

- >> Dizziness. Incoordination. Drowsiness. Headache.

Skin Exposure

- >> Dry skin.

Eye Exposure

- >> Redness.

Ingestion Exposure

- >> See Inhalation. Aspiration hazard!
- >> irritation eyes, skin, mucous membrane; dermatitis; headache, narcosis, coma

Target Organs:

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

- >> Endocrine
- >> Urinary
- >> Eyes, skin, respiratory system, central nervous system

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.
- >> 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.
- >> ACGIH Carcinogen – Confirmed Animal.

Toxicity Data:

>> LCLo (rat) = 8,000 ppm/4H

Treatment:

Treatment when exposed to toxin

>> Treatment is mainly symptomatic and supportive. Gastric lavage, emesis, and the administration of activated charcoal should be avoided, as vomiting increases the risk of aspiration. (A600)

Antidote and Emergency Treatment:

>> Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Aromatic hydrocarbons and related compounds/

Human Toxicity Excerpts:

>> /SIGNS AND SYMPTOMS/ Cumene appears slightly less toxic than its n-propyl isomer, but more so than benzene or toluene. Like its lower homologs, it may irritate the eyes and skin. It is a CNS depressant characterized by slow induction and long duration of effects.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Cumene has been reported to be slightly irritating in the Draize test for eye irritation. Two drops in the rabbit eye produced slight conjunctival irritation but no corneal injury.

Non-Human Toxicity Values:

>> LC50 Mouse inhalation 2,000 ppm/7 hr

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.

>> Groups of five male and five female F344/N rats were exposed to cumene vapor at concentrations of 0, 250, 500, 1,000, 2,000, or 4,000 ppm, 6 hours plus T90 (12 minutes) per day, 5 days per week for 16 days. All rats exposed to 4,000 ppm died on day 1, and two male and three female rats exposed to 2,000 ppm died by day 4. Mean body weights of 2,000 ppm rats were significantly less than those of the chamber controls. Rats exposed to 2,000 ppm that died early were severely lethargic following daily exposure. Liver and kidney weights of all exposed groups were increased. Accumulation of minimal to mild hyaline droplets was observed in the renal tubular cortex of males exposed to concentrations of 250 to 2,000 ppm.

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 cumene to induce morphological transformation was evaluated in the BALB/3T3 mouse embryo cell line (Cell Transformation Assay). Based on preliminary toxicity determinations (exposure time = 2 days), cumene was tested at concentrations of 5, 20 and 60ug/ml, resulting in colony forming efficiency ranging from 69.0% to 22.0%. Only at the 60ug/ml level was a positive response observed (six - Type III foci). Both positive and negative controls elicited expected results.

Populations at Special Risk:

>> Employees /with kidney, chronic respiratory, liver, or skin disease/ are at increased risk from cumene exposure.

12. Ecological Information

Resident Soil (mg/kg)

>> 1.90e+03

Industrial Soil (mg/kg)

>> 9.90e+03

Resident Air (ug/m3)

>> 4.20e+02

Industrial Air (ug/m3)

>> 1.80e+03

Tapwater (ug/L)

>> 4.50e+02

MCL (ug/L)

>> 1.30e+03

Risk-based SSL (mg/kg)

>> 7.40e-01

Chronic Oral Reference Dose (mg/kg-day)

>> 1.00e-01

Chronic Inhalation Reference Concentration (mg/m3)

>> 4.00e-01

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Soil Saturation Concentration (mg/kg)

>> 2.68e+02

ICSC Environmental Data:

>> The substance is very toxic to aquatic organisms. It is strongly advised not to let the chemical enter into the environment.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: Isopropylbenzene was detected in sediment samples from Puget Sound, WA and Strait of Juan de Fuca, WA; in 23 samples, 16% were positive, with a concentration ranging from 0.02 to 19 ug/g, averaging 2.3 ug/g(1). Isopropylbenzene was detected not quantified in Puget Sound, WA(2). A survey of sediments in the Great Lakes Basin region resulted in 6% isopropylbenzene frequency of detection; 18 samples, median concentration of 12.5 ng/g dry weight(3).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> Approximate concentration causing adverse taste in fish: 0.25 mg/L.

13. Disposal Considerations

Spillage Disposal

>> Personal protection: chemical protection suit and 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. Do NOT let this chemical enter the environment.

Disposal Methods

>> Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U055, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

- >> Cumene is a waste chemical stream constituent which may be subjected to ultimate disposal by controlled incineration.
- >> A good candidate for liquid injection incineration at a temperature range of 650 to 1,600 °C and a residence time of 0.1 to 2 seconds. A good candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids. A good candidate for fluidized bed incineration at a temperature range of 450 to 980 °C and residence times of seconds for liquids and gases, and longer for solids.
- >> ... Large quantities can be collected and atomized in a suitable combustion chamber. Combustion may be improved by mixing with a flammable liquid. Cumene liquid should not be allowed to enter a confined space, such as a sewer, because of the possibility of an explosion.
- >> For more Disposal Methods (Complete) data for Isopropylbenzene (6 total), please visit the HSDB record page.

14. Transport Information

DOT

Cumene

3

UN Pack Group: III

Reportable Quantity of 5000 lb or 2270 kg

IATA

Cumene

3,

UN Pack Group: III

15. Regulatory Information

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. Cumene is included on this list. Effective date: 12/28/84; Sunset date: 12/28/94.

Regulatory Information

The Australian Inventory of Industrial Chemicals

- >> Chemical: Benzene, (1-methylethyl)–

The Australian Inventory of Industrial Chemicals

- >> Chemical: Benzene, (1-methylethyl)–, oxidized cumene residues, .alpha.-methylstyrene fraction, dephenolated

REACH Registered Substance

- >> Status: Active Update: 03-01-2023 <https://echa.europa.eu/registration-dossier/-/registered-dossier/15387>

New Zealand EPA Inventory of Chemical Status

- >> Benzene, (1-methylethyl)–: HSNO Approval: HSR001184 Approved with controls

16. Other Information

Other Safety Information

Chemical Assessment

- >> IMAP assessments – Benzene, (1-methylethyl)–: 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."