SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : 1,2,4-Trimethylbenzene
Catalog Number : io-3166
CAS Number : 95-63-6
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% (3184 of 3186) of reports that indicate hazard statements. This chemical does not meet GHS hazard criteria for < 0.1% (2 of 3186) of reports.

Pictogram(s)

GHS Hazard Statements

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

>> H304 (10.5%): May be fatal if swallowed and enters airways [Danger Aspiration hazard]

>> H315 (99.2%): Causes skin irritation [Warning Skin corrosion/irritation]

>> H319 (> 99.9%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

>> H332 (> 99.9%): Harmful if inhaled [Warning Acute toxicity, inhalation]

>> H335 (99.4%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]

>> H411 (99.2%): 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, P264, P264+P265, P271, P273, P280, P301+P316, P302+P352, P303+P361+P353, P304+P340, P305+P351+P338, P317, P319, P321, P331, P332+P317, P337+P317, P362+P364, P370+P378, P391, P403+P233, P403+P235, P405, and P501

NFPA 704 Diamond

NFPA Health Rating

>> 1 - Materials that, under emergency conditions, can cause significant irritation.

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:

>> Harmful if inhaled or swallowed. Vapor or mist is irritating to the eyes, mucous membrane and upper respiratory tract. Prolonged contact can cause dermatitis, nausea, headache, dizziness, and narcotic effect. (USCG, 1999)

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

>> 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. Substance may be transported hot. For hybrid vehicles, ERG Guide 147 (lithium ion or sodium ion batteries) or ERG Guide 138 (sodium batteries) should also be consulted. If molten aluminum is involved, refer to ERG Guide 169. (ERG, 2024)

>> Flammable. Above 44 °C explosive vapour/air mixtures may be formed.

3. Composition/Information On Ingredients

Chemical name : 1,2,4-Trimethylbenzene
CAS Number : 95-63-6
Molecular Formula : C9H12
Molecular Weight : 120.1900 g/mol

4. First Aid Measures

First Aid:

>> Excerpt from NIOSH Pocket Guide for 1,2,4-Trimethylbenzene:

>> 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: SOAP WASH - If this chemical contacts the skin, wash the contaminated skin with soap and water.

>> 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)

First Aid Measures

Inhalation First Aid

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

Skin First Aid

>> Rinse skin with plenty of water or shower.

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. Refer for medical attention .

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 alcohol-resistant foam, dry powder, 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 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. 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. Well closed. Keep in a well-ventilated room.

Storage Conditions:

>> Prior to working with this chemical you should be trained on its proper handling and storage. Before entering a confined space where this chemical may be present, check to make sure that an explosive concentration does not exist. Trimethylbenzene must be stored to avoid contact with oxidizers (such as perchlorates, peroxides, permanganates, chlorates, and nitrates), and strong oxidizers (such as chlorine, bromine, and fluorine) since violent reactions occur. Store in tightly closed containers in a cool, well-ventilated area away from heat. Sources of ignition such as smoking and

open flames are prohibited where this chemical is used, handled, or stored in a manner that could create a potential fire or explosion hazard. Metal containers involving the transfer of 5 gallons or more of this chemical should be grounded and bonded. Drums must be equipped with self-closing valves, pressure vacuum bungs, and flame arresters. Use only nonsparking tools and equipment, especially when opening and closing containers of this chemical. /Trimethyl benzenes/

8. Exposure Control/ Personal Protection

>> TWA 25 ppm (125 mg/m3)

>> none See Appendix G

>> 10.0 [ppm]

EU-OEL

>> 100 mg/m

MAK (Maximale Arbeitsplatz Konzentration)

>> 100 mg/m

Inhalation Risk:

>> A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20 °C; on spraying or dispersing, however, much faster.

Effects of Short Term Exposure:

>> The substance is irritating to the eyes, skin and respiratory tract. If this liquid is swallowed, aspiration into the lungs may result in chemical pneumonitis. The substance may cause effects on the central nervous system.

Effects of Long Term Exposure:

>> The substance defats the skin, which may cause dryness or cracking. Repeated or prolonged inhalation may cause effects on the lungs. This may result in chronic bronchitis. The substance may have effects on the central nervous system and blood.

Fire Prevention

>> NO open flames, NO sparks and NO smoking. Above 44 °C use a closed system, ventilation and explosion-proof electrical equipment. Prevent build-up of electrostatic charges (e.g., by grounding).

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

Maximum Allowable Concentration (MAK)

>> 20.0 [ppm]

9. Physical And Chemical Properties

Molecular Weight:

>> 120.19

Exact Mass:

>> 120.093900383

Physical Description:

>> 1,2,4-trimethylbenzene appears as a liquid. Flash point near 130 °F. Less dense than water and insoluble in water. Vapors irritate eyes, throat, and nose. Used in dyes and pharmaceuticals.

>> COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.

Color/Form:

>> Clear, colorless liquid

Odor:

>> Distinctive, aromatic odor

Boiling Point:

>> 334.4 °F at 760 mmHg (USCG, 1999)

>> 169 °C

Melting Point:

>> -47.2 °F (USCG, 1999)

>> -44 °C

Flash Point:

>> 111 °F (USCG, 1999)

>> 44 °C c.c.

Solubility:

>> 0.006 % (NIOSH, 2024)

>> Solubility in water: very poor

Density:

>> 0.889 (USCG, 1999) - Less dense than water; will float

>> Relative density (water = 1): 0.88

Vapor Density:

>> 4.15 (Air = 1)

>> Relative vapor density (air = 1): 4.1

Vapor Pressure:

>> 4.9 mmHg (USCG, 1999)

LogP:

>> log Kow = 3.78

>> 3.8

Autoignition Temperature:

>> 932 °F (USCG, 1999)

>> 500 °C

Heat of Combustion:

>> 5194.8 kJ/mol at 25 °C

Heat of Vaporization:

>> 39.2 kJ/mol at boiling point

Surface Tension:

>> 29.71 dyn/cm at 20 °C

Ionization Potential:

>> 8.27 eV

Refractive Index:

>> Index of refraction: 1.5048 at 20 °C/D

10. Stability And Reactivity

>> Insoluble in water.

11. Toxicological Information

EPA Provisional Peer-Reviewed Toxicity Values:

This section provides the EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs) and links of related assessment documents.

Chemical Substance

>> 1,2,4-Trimethylbenzene

PPRTV Assessment

>> PDF Document

Last Revision

>> 2007

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

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

Chemical

>> 1,2,4-Trimethylbenzene

USGS Parameter Code

>> 77222

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

>> 60

Reference

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

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).

>> No indication of carcinogenicity to humans (not listed by IARC).

Exposure Routes:

>> The substance can be absorbed into the body by inhalation.

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

Inhalation Exposure

>> Confusion. Cough. Dizziness. Drowsiness. Headache. Sore throat. Vomiting.

Skin Exposure

>> Redness. Dry skin.

Eye Exposure

>> Redness. Pain.

Ingestion Exposure

>> See Inhalation.

>> irritation eyes, skin, nose, throat, respiratory system; bronchitis; hypochromic anemia; headache, drowsiness, lassitude (weakness, exhaustion), dizziness, nausea, incoordination; vomiting, confusion; chemical pneumonitis (aspiration liquid)

Target Organs:

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

>> Developmental

>> Hematologic

>> Nervous

>> Respiratory

>> Eyes, skin, respiratory system, central nervous system, blood

Adverse Effects:

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

>> Neurotoxin - Acute solvent syndrome

>> ACGIH Carcinogen - Not Classifiable.

Toxicity Data:

>> LC50 (rat) = 18,000 mg/m3/4h

Interactions:

>> ... The toxicokinetics of 124TMB was studied in nine male, healthy volunteers exposed to solvent vapors in an exposure chamber for 2 hr during a work load of 50 W. The subjects were exposed to 2 ppm (11 mg/cu m) of 124TMB during exposure to 300 mg/cu m of white spirit. The 124TMB isomer was analysed in blood, urine and exhaled air by gas chromatography. The DMHA metabolites of all three TMB isomers were analysed in urine by high-performance liquid chromatography. The results were compared with previously published exposures to 2 and 25 ppm (120 mg/cu m) of 124TMB vapor alone. ... Blood levels of 124TMB and excretion rates of 3,4-DMHA in urine were markedly elevated both during and after exposure to white spirit compared to the same exposure level of 124TMB alone. ... It appears that components in white spirit interfere with the metabolic elimination of 124TMB. This should be considered in biological exposure monitoring as well as in risk assessment.

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:

>> /HUMAN EXPOSURE STUDIES/ The objective of this study was to compare the toxicokinetics of inhaled 1,2,4-trimethylbenzene (1,2,4-TMB) in man after exposure to white spirit with that observed after exposure to 1,2,4-TMB alone. ... The toxicokinetics were studied in 9 male, healthy volunteers exposed to solvent vapors in an exposure chamber for 2 hr during a work load of 50 W. The subjects were exposed to 11 mg/cu m of 1,2,4-TMB on two occasions; during exposure to 1,2,4-TMB vapor alone and during exposure to 300 mg/cu m of white spirit. ... Further the occurrence of acute effects was studied by means of a questionnaire. Irritation and central nervous system symptoms were recorded by ratings on a 100-mm visual analogue scale. ... No irritation or central nervous system effects were reported at these conditions.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ Not sensitizing /in/ guinea pig maximization test.

Non-Human Toxicity Values:

>> LD50 Rabbit dermal >3160 mg/kg bw

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.

>> Acute oral toxicity was evaluated in groups of 10 male Wistar rats administered single doses of 98% pseudocumene by oral gavage at levels of 3.51, 5.0, 7.12 and 10.14 g/kg of body weight. Mortality was observed in 3 animals in the 5.0 g/kg

dose group, 7 in the 7.12 g/kg dose group, and all 10 in the highest dose group. The LD50 value was calculated to be 6.0 g/kg of body weight, with confidence limits of 4.92 - 7.32 g/kg, by the Litchfield and Wilcoxon method. Clinical observations included lethargy, ptosis, ataxia, and piloerection. Gross necropsy findings were not reported.

12. Ecological Information

Resident Soil (mg/kg)

>> 3.00e+02

Industrial Soil (mg/kg)

>> 1.80e+03

Resident Air (ug/m3)

>> 6.30e+01

Industrial Air (ug/m3)

>> 2.60e+02

Tapwater (ug/L)

>> 5.60e+01

MCL (ug/L)

>> 5.00e+01

Risk-based SSL (mg/kg)

>> 8.10e-02

Chronic Oral Reference Dose (mg/kg-day)

>> 1.00e-02

Chronic Inhalation Reference Concentration (mg/m3)

>> 6.00e-02

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Soil Saturation Concentration (mg/kg)

>> 2.19e+02

ICSC Environmental Data:

>> The substance is toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish.

Average Daily Intake:

The average amount of the compound taken into the body through eating, drinking, or breathing.

>> The average daily dose of 1,2,4-trimethylbenzene from breathing air in The Netherlands was estimated as 86 ug/day based on average ambient air concentrations of 0.50-1.15 ppb(1).

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. Do NOT wash away into sewer. 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 /SRP: with appropriate emission controls/. /Trimethyl benzenes/

14. Transport Information

DOT

1,2,4-Trimethylbenzene
3
UN Pack Group: III

IATA

1,2,4-Trimethylbenzene
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. 1,2,4-Trimethylbenzene is included on this list. Effective date 4/29/1983; Sunset date 4/29/1993.

Regulatory Information

The Australian Inventory of Industrial Chemicals

>> Chemical: Benzene, 1,2,4-trimethyl-

REACH Registered Substance

>> Status: Active Update: 21-01-2020 https://echa.europa.eu/registration-dossier/-/registered-dossier/13135

New Zealand EPA Inventory of Chemical Status

>> Benzene, 1,2,4-trimethyl-: HSNO Approval: HSR001382 Approved with controls

16. Other Information

Toxic Combustion Products:

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

>> The substance decomposes on burning producing toxic and irritating fumes.

Other Safety Information

Chemical Assessment

>> IMAP assessments - Benzene, 1,2,4-trimethyl-: Human health tier I assessment

>> IMAP assessments - Benzene, 1,2,4-trimethyl-: 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."