

Chemical Safety Data Sheet MSDS / SDS

2,4,4-TRIMETHYL-2-PENTANETHIOL

Revision Date:2024-12-21 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name : 2,4,4-TRIMETHYL-2-PENTANETHIOL
CBnumber : CB4322353
CAS : 141-59-3
EINECS Number : 205-490-1
Synonyms : tert-OCTYL MERCAPTAN,2,4,4-TRIMETHYL-2-PENTANETHIOL

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification**Classification of the substance or mixture**

Flammable liquids, Category 3
Acute toxicity - Category 3, Oral
Acute toxicity - Category 4, Dermal
Acute toxicity - Category 1, Inhalation

Label elements**Pictogram(s)**

☐☐

Signal word : Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H301 Toxic if swallowed
H312 Harmful in contact with skin
H330 Fatal if inhaled

Precautionary statement(s)

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P233 Keep container tightly closed.

P240 Ground and bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

P284 [In case of inadequate ventilation] wear respiratory protection.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P317 Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P320 Specific treatment is urgent (see ... on this label).

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name : 2,4,4-TRIMETHYL-2-PENTANETHIOL

Synonyms : tert-OCTYL MERCAPTAN,2,4,4-TRIMETHYL-2-PENTANETHIOL

CAS : 141-59-3

EC number : 205-490-1
MF : C8H18S
MW : 146.29

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

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

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Excerpt from ERG Guide 131 [Flammable Liquids - Toxic]: TOXIC; may be fatal if inhaled, ingested or absorbed through skin. Inhalation or contact with some of these materials will irritate or burn skin and eyes. Fire will produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

Indication of any immediate medical attention and special treatment needed

Upon ingestion/ rinse mouth, induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention.

SECTION 5: Firefighting measures

Extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped or safely confined. Use water in flooding quantities as fog. Use foam, dry chemical, or carbon dioxide. Keep run-off water out of sewers and water sources. Cool all affected containers with flooding quantities of water.

Specific Hazards Arising from the Chemical

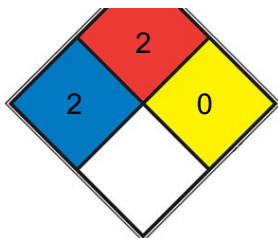
Excerpt from ERG Guide 131 [Flammable Liquids - Toxic]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion and poison 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 are lighter than water. (ERG, 2016)

Advice for firefighters

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

NFPA 704





<input checked="" type="checkbox"/>	HEALTH	2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. diethyl ether , ammonium phosphate, iodine)
<input checked="" type="checkbox"/>	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
<input checked="" type="checkbox"/>	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N₂)
<input type="checkbox"/>	SPEC.		
<input type="checkbox"/>	HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: chemical protection suit including self-contained breathing apparatus. 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.

Environmental precautions

Personal protection: chemical protection suit including self-contained breathing apparatus. 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.

Methods and materials for containment and cleaning up

Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent and remove to safe place. (Extra personal protection: chemical protection suit including self-contained breathing apparatus.)

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 46°C use a closed system, ventilation and explosion-proof electrical equipment. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong bases, strong acids and oxidants. Fireproof. Separated from strong bases, strong acids and oxidants.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

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

Skin protection

Protective gloves.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	No information available.
Colour	Colorless liquid
Odour	no data available
Melting point/freezing point	262°C(lit.)
Boiling point or initial boiling point and boiling range	156°C(lit.)
Flammability	Flammable. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	46°C(lit.)
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water, 31 mg/L at 25 deg C (est)
Partition coefficient n-octanol/water	log Kow = 4.0 (est)
Vapour pressure	4.95mmHg at 25°C
Density and/or relative density	0.837g/cm ³
Relative vapour density	5.0 (Air = 1)

Particle characteristics	no data available
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SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic gases including hydrogen sulfide and sulfur oxides. Reacts violently with oxidants. This generates fire hazard. Reacts with strong acids, strong bases and strong reducing agents. Attacks many metals and rubber.

Chemical stability

no data available

Possibility of hazardous reactions

A flammable liquid when exposed to heat, flame or oxidizers.

Conditions to avoid

no data available

Incompatible materials

Reacts violently with oxidants causing fire hazard. Reacts with strong acids, strong bases and strong reducing agents. Attacks many metals and rubber.

Hazardous decomposition products

When heated to decomposition it emits very toxic fumes of /sulfur oxides/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 52 mg/kg
- Inhalation: LD50 Rat inhalation 33 ppm/4 hr
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is mildly irritating to the eyes. The substance may cause effects on the central nervous system. This may result in convulsions, lowering of consciousness and respiratory depression. Exposure could cause death.

STOT-repeated exposure

no data available

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

An estimated BCF of 240 was calculated for t-octyl mercaptan(SRC), using an estimated log Kow of 4.0(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is high, provided the compound is not metabolized by the organism(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of t-octyl mercaptan can be estimated to be 390(SRC). According to a classification scheme(2), this estimated Koc value suggests that t-octyl mercaptan is expected to have moderate mobility in soil.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN3023 (For reference only, please check.)

IMDG: UN3023 (For reference only, please check.)

IATA: UN3023 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: 2-METHYL-2-HEPTANETHIOL (For reference only, please check.)

IMDG: 2-METHYL-2-HEPTANETHIOL (For reference only, please check.)

IATA: 2-METHYL-2-HEPTANETHIOL (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Not Listed.

IECSC

Not Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

Disclaimer:

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