
SECTION 1: Identification

1.1 GHS Product identifier

Product name 2,4,4-trimethylpentane-2-thiol

1.2 Other means of identification

Product number -

Other names 2,4,4-Trimethyl-2-pentanethiol; 2-Pentanethiol, 2,4,4-trimethyl; tert-Octyl mercaptan

1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research uses.

Uses advised against no data available

SECTION 2: Hazard identification

2.1 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

2.2 GHS label elements, including precautionary statements

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.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

| Chemical name | Common names and synonyms | CAS number | EC number | Concentration |
|--------------------------------|--------------------------------|------------|-----------|---------------|
| 2,4,4-trimethylpentane-2-thiol | 2,4,4-trimethylpentane-2-thiol | 141-59-3 | 205-490-1 | 100% |

SECTION 4: First-aid measures

4.1 Description of necessary 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 .

4.2 Most important symptoms/effects, 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)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

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

SECTION 5: Fire-fighting measures

5.1 Suitable 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.

5.2 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)

5.3 Special protective actions for fire-fighters

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

SECTION 6: Accidental release measures

6.1 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.

6.2 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.

6.3 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

7.1 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.

7.2 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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 Appropriate engineering controls

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

8.3 Individual protection measures, such as personal protective equipment (PPE)

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 and safety characteristics

| | |
|--|--|
| Physical state | No information available. |
| Colour | Colorless liquid |
| Odour | no data available |
| Melting point/freezing point | 262Â°C(lit.) |
| Boiling point or initial boiling point and boiling range | 156Â°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 | 46Â°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 25Â°C |
| Density and/or relative density | 0.837g/cm3 |
| Relative vapour density | 5.0 (Air = 1) |
| Particle characteristics | no data available |

SECTION 10: Stability and reactivity

10.1 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.

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

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

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

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

10.6 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 20Â°C.

SECTION 12: Ecological information

12.1 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

12.2 Persistence and degradability

no data available

12.3 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).

12.4 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.

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 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

14.1 UN Number

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

14.2 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.)

14.3 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.)

14.4 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.)

14.5 Environmental hazards

ADR/RID: No IMDG: No IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

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

| Chemical name | Common names and synonyms | CAS number | EC number |
|--|--------------------------------|------------|-------------|
| 2,4,4-trimethylpentane-2-thiol | 2,4,4-trimethylpentane-2-thiol | 141-59-3 | 205-490-1 |
| 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. |
| Philippines Inventory of Chemicals and Chemical Substances (PICCS) | | | Not Listed. |
| Vietnam National Chemical Inventory | | | Not Listed. |
| Chinese Chemical Inventory of Existing Chemical Substances (China IECSC) | | | Not Listed. |
| Korea Existing Chemicals List (KECL) | | | Not Listed. |

SECTION 16: Other information

Information on revision

Creation Date July 15, 2019
Revision Date July 15, 2019

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>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>