Chemical Safety Data Sheet MSDS / SDS

2-methylpropane-2-thiol SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: 2-methylpropane-2-thiol

CAS: 75-66-1

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.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable liquids, Category 2
Skin sensitization, Sub-category 1B

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H225 Highly flammable liquid and vapour
H317 May cause an allergic skin reaction
H411 Toxic to aquatic life with long lasting effects

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/...
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P273 Avoid release to the environment.

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.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P333+P317 If skin irritation or rash occurs: Get medical help.
P321 Specific treatment (see ... on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.
P391 Collect spillage.

Storage

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

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	2-methylpropane-2-thiol
Common names and synonyms:	2-methylpropane-2-thiol
CAS number:	75-66-1
EC number:	200-890-2
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. 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.

Most important symptoms/effects, acute and delayed

no data available

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

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 m1/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool . Administer activated charcoal . Cover skin burns with dry sterile dressings after decontamination . Sulfur and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

Alcohol foam, dry chemical, mist, fog.

Specific hazards arising from the chemical

Highly flammable. Vapour/air mixtures are explosive.

Special protective actions for fire-fighters

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

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. 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.

Environmental precautions

Evacuate danger area! Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of

the substance. 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.

Methods and materials for containment and cleaning up

Evacuate danger area! Remove all ignition sources. 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. Do NOT wash away into sewer. Carefully collect remainder, then remove to safe place.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Do NOT use compressed air for filling, discharging, or handling. 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 oxidants, strong bases, strong acids, metals and strong reducing agents.Fireproof. Separated from strong oxidants, strong bases, strong acids, metals, strong reducing agents.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

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.

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:	Liquid.
Colour:	Colourless.
Odour:	Heavy skunk odor
Melting point/freezing point:	0 °C. Atm. press.: 1 013 hPa. Remarks: At standard pressure and temperature.
Boiling point or initial boiling point and boiling range:	64 °C. Atm. press.: 1 013 hPa. Remarks: At standard temperature and pressure.
Flammability:	Highly flammable.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	< -25 °C. Atm. press.: 1 013.3 hPa.
Auto-ignition temperature:	255 °C. Atm. press.: 101.3 kPa. Remarks: Standard pressure assumed.

Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 138. Temperature:20°C. Remarks:Reference substance: Standard Oil.;dynamic viscosity (in mPa s) = 45. Temperature:40°C. Remarks:Reference substance: Standard Oil.;dynamic viscosity (in mPa s) = 1.11. Temperature:20°C. Remarks:Constant shear rate of 2000 l/s.
Solubility:	Slightly sol in water; very sol in alcohol, ether, liquid hydrogen sulfide
Partition coefficient n-octanol/water:	log Pow = 2.14. Temperature:20 °C. Remarks:Standard experimental conditions have been assumed.
Vapour pressure:	19 kPa. Temperature:20 °C.
Density and/or relative density:	0.8 g/cm3. Temperature:20 °C.
Relative vapour density:	3.1 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic gases including sulfur oxides. Reacts with strong acids, strong bases, metals, strong oxidants and strong reducing agents. This produces sulfur oxides.

Chemical stability

Remarkably stable to oxidizing agents.

Possibility of hazardous reactions

Dangerous, when exposed to heat or flame.The vapour is heavier than air and may travel along the ground; distant ignition possible.

Conditions to avoid

no data available

Incompatible materials

Reacts with strong acids, strong bases, metals, strong oxidants, strong reducing agents to produce sulfur oxides.

Hazardous decomposition products

The substance decomposes on burning producing toxic gases including sulfur oxides.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male) - 4 729 mg/kg bw.

Inhalation: LC50 - rat (male/female) - 26 643 ppm.

Dermal: LD50 - rabbit - > 2 000 mg/kg bw.

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 irritating to the eyes and respiratory tract. Exposure at high levels could cause lowering of consciousness.

STOT-repeated exposure

no data available

Aspiration hazard

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

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Oncorhynchus mykiss (previous name: Salmo gairdneri) - 34 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 6.7 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 24 mg/L - 72 h.

Toxicity to microorganisms: NOEC - activated sludge of a predominantly domestic sewage - 1 mg/L - 63 d.

Persistence and degradability

AEROBIC: While data specific to t-butyl mercaptan were not available(SRC, 2005), this compound would probably be difficult to biodegrade because of the branching in its structure(1).

Bioaccumulative potential

An estimated BCF of 9 was calculated for t-butyl mercaptan(SRC), using an estimated log Kow of 2.1(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of t-butyl mercaptan can be estimated to be 49(SRC). According to a classification scheme(2), this estimated Koc value suggests that t-butyl mercaptan is expected to have very high mobility in soil. Natural gas containing 0.5 lb of t-butyl mercaptan per million cubic feet was passed through a bed of pulverized, dry, raw montmorillonite clay and then measured for loss of odorant. Within 100 standard cubic feet, over 85% of the average influent concentration of t-butyl mercaptan was present in the effluent(3).

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: UN2347 (For reference only, please check.)
IMDG: UN2347 (For reference only, please check.)
IATA: UN2347 (For reference only, please check.)

UN Proper Shipping Name

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

Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)
IMDG: 3 (For reference only, please check.)
IATA: 3 (For reference only, please check.)

Packing group, if applicable

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

Environmental hazards

ADR/RID: Yes
IMDG: Yes
IATA: Yes

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)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

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

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

Other Information

The auto-ignition temperature is unknown in the literature. Explosive limits are unknown in literature, although the substance is combustible and has a flash point < 61°C. Health effects of exposure to the substance have not been investigated adequately.