

2-Methyl-1-propanethiol

sc-230502



The Power is Question

Material Safety Data Sheet

Hazard Alert Code Key:

EXTREME

HIGH

MODERATE

LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

2-Methyl-1-propanethiol

STATEMENT OF HAZARDOUS NATURE

CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA



SUPPLIER

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EMERGENCY

ChemWatch
Within the US & Canada: 877-715-9305
Outside the US & Canada: +800 2436 2255
(1-800-CHEMCALL) or call +613 9573 3112

SYNONYMS

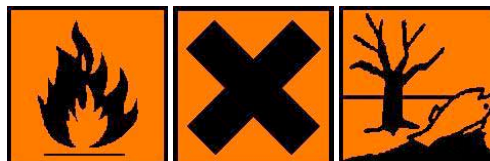
C4-H10-S, (CH3)2CHCH2SH, 2-methyl-1-propanethiol, isobutanethiol

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

	Min	Max
Flammability:	3	
Toxicity:	2	
Body Contact:	2	
Reactivity:	1	
Chronic:	2	

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4



CANADIAN WHMIS SYMBOLS



EMERGENCY OVERVIEW

RISK

May cause SENSITISATION by skin contact.
Irritating to eyes, respiratory system and skin.
Highly flammable.
Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ Although ingestion is not thought to produce harmful effects, the material may still be damaging to the health of the individual following ingestion, especially where pre-existing organ (e.

g.

■ After oral n-butyl mercaptan administration rats and mice, surviving near lethal doses, were found to have kidney and liver damage when autopsied 20 days after exposure.

EYE

■ This material can cause eye irritation and damage in some persons.

SKIN

■ This material can cause inflammation of the skin on contact in some persons.

■ The material may accentuate any pre-existing dermatitis condition.

■ Skin contact with the material may damage the health of the individual; systemic effects may result following absorption.

■ Open cuts, abraded or irritated skin should not be exposed to this material.

■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects.

Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

■ The material can cause respiratory irritation in some persons.

The body's response to such irritation can cause further lung damage.

■ Material is highly volatile and may quickly form a concentrated atmosphere in confined or unventilated areas.

Vapor is heavier than air and may displace and replace air in breathing zone, acting as a simple asphyxiant.

■ In a laboratory engaged in the production of acrylic resins accidental exposure of seven workers at levels believed to be 50-500 ppm n-butyl mercaptan for 1 hour caused symptoms of CNS toxicity; all reported muscular weakness and malaise, flushing of the face, increased rate of breathing and obvious mydriasis; six experiencing sweating, nausea, vomiting and headache; three experienced confusion and one lapsed into coma for 20 minutes.

Six recovered within one day but the most seriously effected worker experienced profound weakness, dizziness, vomiting, drowsiness and depression.

■ Inhalation of aerosols (mists, fumes), generated by the material during the course of normal handling, may be damaging to the health of the individual.

■ Thiols (particularly ethyl mercaptan) produce lethargy or sleepiness.

Exposure to high levels may result in nausea, vomiting, restlessness, muscle incoordination and or paralysis, bluing of skin, depression of breathing, coma and death.

CHRONIC HEALTH EFFECTS

■ Long-term exposure to respiratory irritants may result in disease of the airways involving difficult breathing and related systemic problems.

Skin contact with the material is more likely to cause a sensitization reaction in some persons compared to the general population.

Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or biochemical systems.

Embryotoxic effects were noted in mice exposed at 68 ppm and 152 ppm of n-butyl mercaptan for 6 hours/day on gestation days 6 to 16.

Chronic exposure to mercaptans may result in damage to the lungs, kidneys and liver.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
iso-butyl mercaptan	513-44-0	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

· Immediately give a glass of water. · First aid is not generally required. If in doubt, contact a Poisons Information Center or a doctor.

EYE

■ If this product comes in contact with the eyes: · Wash out immediately with fresh running water. · Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.

SKIN

■ If skin contact occurs: · Immediately remove all contaminated clothing, including footwear · Flush skin and hair with running water (and soap if available).

INHALED

· If fumes or combustion products are inhaled remove from contaminated area. · Lay patient down. Keep warm and rested.

NOTES TO PHYSICIAN

■ For exposures involving sulfides and hydrogen sulfide (including gastric acid decomposition products of alkaline sulfides).

- Hydrogen sulfide anion produces its major toxic effect through inhibition of cytochrome oxidases.
- Symptoms include profuse salivation, nausea, vomiting and diarrhea. Central nervous effects may include giddiness, headache, vertigo, amnesia, confusion and unconsciousness. Tachypnea, palpitation, tachycardia, arrhythmia, sweating, weakness and muscle cramps may also indicate over-exposures.

Section 5 - FIRE FIGHTING MEASURES

Vapor Pressure (mmHg):	123.76 @ 37.8 C.
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	0.831
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA

- Foam.
- Dry chemical powder.

FIRE FIGHTING

- Alert Emergency Responders and tell them location and nature of hazard.
- May be violently or explosively reactive.

When any large container (including road and rail tankers) is involved in a fire, consider evacuation by 1000 metres in all directions.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

- Liquid and vapor are highly flammable.
- Severe fire hazard when exposed to heat, flame and/or oxidizers.

Combustion products include: carbon dioxide (CO₂), sulfur oxides (SO_x), hydrogen sulfide (H₂S), other pyrolysis products typical of burning organic material.

Contains low boiling substance: Closed containers may rupture due to pressure buildup under fire conditions.

FIRE INCOMPATIBILITY

- Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids, chlorine bleaches, pool chlorine etc. as ignition may result.

PERSONAL PROTECTION

Glasses:

Chemical goggles.

Gloves:

Respirator:

Type BAX Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.

WARNING: Never use dry, powdered hypochlorite or other strong oxidizer for mercaptan spills, as autoignition can occur.

MAJOR SPILLS

- Clear area of personnel and move upwind.
- Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Containers, even those that have been emptied, may contain explosive vapours.
- Do NOT cut, drill, grind, weld or perform similar operations on or near containers.

Contains low boiling substance:

Storage in sealed containers may result in pressure buildup causing violent rupture of containers not rated appropriately.

- Check for bulging containers.
- Vent periodically.
- DO NOT allow clothing wet with material to stay in contact with skin.

The careful design and assembly of equipment is paramount to the control of mercaptan odors. Although careful planning reduces the chances for leaks developing in the system, it is important to be prepared to locate and stop small leaks promptly. It is recommended that a leak check be made prior to every run carried out under pressure in metal equipment with a mercaptan or hydrogen sulfide present.

An effective method to obtain a leak-free system involves two steps:

- Charge the system with nitrogen gas or other inert, nontoxic gas to a pressure at least as high as will be used in practice, and check for a drop in pressure with time on a suitable gauge. In some cases, it is advantageous to block off sections of the system to facilitate finding the leak. If any leaks are detected by using a foaming detergent solution, correct them and recheck.
- Recharge the system with hydrogen sulfide gas. Since hydrogen sulfide is very toxic, it is good practice to charge the system in steps of increasing pressure, until it is certain that no large leaks are present. Any remaining small leaks can be located quickly by examining the system with lead acetate paper. Dilution of the hydrogen sulfide with nitrogen can also be considered.

To control odors in mercaptan reactions in the laboratory. All reactions must be carried out in a hood or, in the case of pressure reactions, in a closed in area equipped with an efficient exhaust fan. In the laboratory, the two basic types of reactions used are batch and continuous. Batch-type reactions at atmospheric pressure are generally conducted in glass equipment. If no significant quantity of a volatile mercaptan is

present, the reaction can be carried out in a hood equipped with a charcoal bed in the exhaust line to absorb the mercaptan. In reactions where appreciable quantities of a volatile mercaptan are present, a vent gas line can be connected to two caustic scrubbers in series, with an empty trap inserted between the reaction and scrubbers to avoid reverse flow of caustic into the reaction. Continuous-type reactions often include a continuous flow of volatile C1 to C4 mercaptans. In this case, the vented gases can be fed to an outside gas burner and stack for destruction of the odor by combustion.

A hood, equipped with a charcoal filter in the exhaust line, and a high linear air velocity (100 ft./min., minimum) is necessary for mercaptan reactions carried out in glass and certain small-scale reactions with stainless-steel. In reactions where relatively small amounts of mercaptans can escape, the charcoal bed can absorb the mercaptans and prevent the escape of odor to the outside atmosphere. However, in reactions with hydrogen sulfide or lower molecular weight mercaptans, e.g., C1-C4 mercaptans, the quantity of effluent gases is directed to an outside gas burner to convert the odorous compounds to acceptable combustion products, including CO₂ and SO₂.

A very familiar and successful method for containing the odors of mercaptan (primarily C1 and C6) in laboratory reactions and distillations is to connect the condenser vent to two caustic scrubbers in series with an empty trap between the system and the scrubbers to catch the caustic in the event of reverse flow. Gas bubblers fitted with sintered-glass dip tubes and charged with aqueous sodium hydroxide (5 to 20%) are commonly used. Frequently, a low flow of inert gas, e.g., nitrogen, is used to maintain a steady flow through the bubbler.

Sodium hypochlorite solution (3-10%) destroys the odor by converting the mercaptan predominantly to the corresponding sulfonic acid (sodium salt). A wash bottle with hypochlorite solution is very convenient for quickly eliminating or controlling the odor from small spills or when cleaning up glass equipment. A bath of this solution is also very useful. WARNING! Do not add this solution to a large quantity of concentrated mercaptan, since a violent reaction may occur.

A 30-40% aqueous solution of lead acetate trihydrate serves as a detector for methyl and ethyl mercaptan as well as hydrogen sulfide. A wash bottle of lead acetate solution is used to moisten a piece of filter paper or paper towel which is then held close to (no contact) the suspected leak. With hydrogen sulfide the paper turns black and with the two mercaptans a yellow color is obtained (high sensitivity).

A large plastic bag should be kept in the hood, to store any odorous waste materials. The plastic bags can then be sealed in fiber drums for disposal. Glass bottles containing mercaptans and other odorous compounds can also be packed in fiber drums for odor-containment and properly marked for disposal.

A box of disposable gloves should be available, and the gloves should be discarded (in plastic bag in hood) after each use. Disposable aprons or lab coats are recommended, since clothing contacted with mercaptan is often difficult to deodorise.

Types of tubing found useful with mercaptans include: Teflon, TFE, FEP, and PFA, Bev-a-line (IV or V), and 316 stainless steel. Bev-a-line tubing has a polyethylene liner cross-linked to an ethylene vinyl acetate shell, a useful temperature range of -60 C to +250 C, and is heat bondable. It is less expensive than TFE tubing and is convenient for flexible connections between glass and metal tubing lines. It is available from most laboratory supply houses. Copper and brass are unacceptable materials for handling mercaptans, because mercaptans are H₂S are highly corrosive to copper and brass. Care should be taken not to use valves and gauges with brass components.

Atofina Chemicals.

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.

RECOMMENDED STORAGE METHODS

- Packing as supplied by manufacturer. Plastic containers may only be used if approved for flammable liquid.
- For low viscosity materials (i): Drums and jerricans must be of the non-removable head type. (ii): Where a can is to be used as an inner package, the can must have a screwed enclosure.
- For materials with a viscosity of at least 2680 cSt. (23 deg. C).

STORAGE REQUIREMENTS

- Store in original containers in approved flame-proof area.
- No smoking, naked lights, heat or ignition sources.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m ³	STEL ppm	STEL mg/m ³	Peak ppm	Peak mg/m ³	TWA F/CC	Notes
Canada - Alberta Occupational Exposure Limits	iso-butyl mercaptan (Butyl mercaptan (Butanethiol))	0.5	1.8						
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	iso-butyl mercaptan (Butyl mercaptan)	0.5	1.5						
US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants	iso-butyl mercaptan (Butyl mercaptan)	10	35						
Canada - Quebec Permissible Exposure Values for Airborne Contaminants	iso-butyl mercaptan (Butyl mercaptan)	0.5	1.8						

(English)

ENDOELTABLE

PERSONAL PROTECTION



RESPIRATOR

Type BAX Filter of sufficient capacity
Consult your EHS staff for recommendations

EYE

- Safety glasses with side shields.
- Chemical goggles.

HANDS/FEET

■ Wear chemical protective gloves, eg. PVC.

NOTE: The material may produce skin sensitization in predisposed individuals. Care must be taken, when removing gloves and other protective equipment, to avoid all possible skin contact.

Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:

- frequency and duration of contact,
- chemical resistance of glove material,
- glove thickness and
- dexterity

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).

- When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
- When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
- Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

OTHER

- Overalls.
- PVC Apron.
- Some plastic personal protective equipment (PPE) (e.g. gloves, aprons, overshoes) are not recommended as they may produce static electricity.
- For large scale or continuous use wear tight-weave non-static clothing (no metallic fasteners, cuffs or pockets), non sparking safety footwear.

ENGINEERING CONTROLS

■ For flammable liquids and flammable gases, local exhaust ventilation or a process enclosure ventilation system may be required. Ventilation equipment should be explosion-resistant.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Liquid.

Does not mix with water.

Floats on water.

State	Liquid	Molecular Weight	90.2
Melting Range (°F)	Not available	Viscosity	Not Available
Boiling Range (°F)	189- 192	Solubility in water (g/L)	Immiscible
Flash Point (°F)	15	pH (1% solution)	Not applicable
Decomposition Temp (°F)	Not Available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapor Pressure (mmHg)	123.76 @ 37.8 C.
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	0.831
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	3.1
Volatile Component (%vol)	100	Evaporation Rate	Fast

APPEARANCE

Colourless, flammable liquid with strong obnoxious, garlic-like odour; does not mix with water. Soluble in alcohol, ether and liquid hydrogen sulfide.

Terrestrial fate An estimated Koc value of 410, determined from a log Kow of 2.28 indicates that n-butyl mercaptan is expected to have moderate mobility in soil. Volatilisation of n-butyl mercaptan from moist soil surfaces is expected to be an important fate process given a Henry's Law constant of 4.54×10^{-3} atm-cu m/mole. n-Butyl mercaptan is expected to volatilize from dry soil surfaces based upon a vapor pressure of 45.5 mm Hg.

Material	Value
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Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.

STORAGE INCOMPATIBILITY

- n-Butyl mercaptan
 - may react with water, steam or acids to produce toxic or flammable vapours
 - reacts violently with ignition or explosion with strong oxidisers, calcium hypochlorite, strong acids, alkalis, alkali metals
 - is incompatible with aliphatic amines, ethylene oxide, isocyanates, nitric acid, sulfuric acid
 - attacks some forms of plastics, coatings and rubber
 - may generate electrostatic charges.
 - Contact with acids produces toxic fumes.

Avoid reaction with oxidizing agents, bases and strong reducing agents.

Avoid alkali metals.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

iso-butyl mercaptan

TOXICITY AND IRRITATION

ISO-BUTYL MERCAPTAN:

- unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

TOXICITY	IRRITATION
Oral (rat) LD50: 7168 mg/kg	Eye (rabbit): 84 mg
Intraperitoneal (rat) LD50: 917 mg/kg	

- Contact allergies quickly manifest themselves as contact eczema, more rarely as urticaria or Quincke's edema. The pathogenesis of contact eczema involves a cell-mediated (T lymphocytes) immune reaction of the delayed type.

Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.

Spastic paralysis, excitement and cyanosis recorded.

Section 12 - ECOLOGICAL INFORMATION

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

This material and its container must be disposed of as hazardous waste.

Avoid release to the environment.

Refer to special instructions/ safety data sheets.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
iso-butyl mercaptan	HIGH		LOW	HIGH

Section 13 - DISPOSAL CONSIDERATIONS

US EPA Waste Number & Descriptions

A. General Product Information

Ignitability characteristic: use EPA hazardous waste number D001 (waste code I)

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.

‡ Puncture containers to prevent re-use and bury at an authorized landfill.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in

their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- Reduction
- Reuse
- Recycling
- Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.

DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.

· Recycle wherever possible.

· Consult manufacturer for recycling options or consult Waste Management Authority for disposal if no suitable treatment or disposal facility can be identified.

Section 14 - TRANSPORTATION INFORMATION



DOT:

Symbols: None Hazard class or Division: 3

Identification Numbers: UN2347 PG: II

Label Codes: 3 Special provisions: A3, A6, IB2, T4,

TP1

Packaging: Exceptions: 150 Packaging: Non- bulk: 202

Packaging: Exceptions: 150 Quantity limitations: 5 L

Passenger aircraft/rail:

Quantity Limitations: Cargo 60 L Vessel stowage: Location: D aircraft only:

Vessel stowage: Other: 52, 95

Hazardous materials descriptions and proper shipping names:

Butyl mercaptans

Air Transport IATA:

ICAO/IATA Class: 3 ICAO/IATA Subrisk: None

UN/ID Number: 2347 Packing Group: II

Special provisions: None

Cargo Only

Packing Instructions: 60 L Maximum Qty/Pack: 5 L

Passenger and Cargo Passenger and Cargo

Packing Instructions: 364 Maximum Qty/Pack: 353

Passenger and Cargo Limited Quantity Passenger and Cargo Limited Quantity

Packing Instructions: 1 L Maximum Qty/Pack: Y341

Shipping Name: BUTYL MERCAPTAN

Maritime Transport IMDG:

IMDG Class: 3 IMDG Subrisk: None

UN Number: 2347 Packing Group: II

EMS Number: F-E , S-D Special provisions: None

Limited Quantities: 1 L Marine Pollutant: Yes

Shipping Name: BUTYL MERCAPTANS

Section 15 - REGULATORY INFORMATION

iso-butyl mercaptan (CAS: 513-44-0) is found on the following regulatory lists;

"Canada Domestic Substances List (DSL)", "Canada Toxicological Index Service - Workplace Hazardous Materials Information System - WHMIS (English)", "US Food Additive Database", "US Toxic Substances Control Act (TSCA) - Inventory"

Section 16 - OTHER INFORMATION

ND

Substance CAS Suggested codes iso- butyl mercaptan 513- 44- 0 R43

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representations and assumes no liability for any direct, incidental or consequential damages resulting from its use. For additional technical information please call our toxicology department on +800 CHEMCALL.

■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

A list of reference resources used to assist the committee may be found at:

www.chemwatch.net/references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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