Safety Data Sheet

1-Butane-d_9-thiol

Section 1. Chemical product and company identifications

Product code: D-5311
Chemical formula: C_4HD_9S
CAS: 352431-09-5
CAS (unlabelled): 109-79-5
Synonyms: *n*-Butyl Mercaptan

Supplier / Manufacturer:

C/D/N Isotopes Inc.
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In case of emergency:

TOXYSCAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

Physical state: Liquid
Warning: Highly flammable liquid and vapour. Causes skin irritation. Causes serious eye irritation.
Routes of entry: Inhalation, skin and eyes

GHS (Globally Harmonized System of Classification and Labelling of Chemicals):

GHS Classification:
- Flammable liquids (Category 2)
- Acute toxicity, Oral (Category 4)
- Acute toxicity, Inhalation (Category 4)
- Skin corrosion/irritation (Category 2)
- Serious eye damage/eye irritation (Category 2A)
- Skin sensitisation (Category 1)
- Specific target organ toxicity - single exposure (Category 3), Respiratory system

GHS Label elements:
- Pictograms:
- Signal word: Danger

Hazards statement:
- H225 Highly flammable liquid and vapour.
- H302 + H332 Harmful if swallowed or if inhaled
- H315 Causes skin irritation.
- H319 Causes serious eye irritation.
- H335 May cause respiratory irritation.

Precautionary statement:
- P210 Keep away from heat/ hot surfaces/ sparks/ open flames/ ignition sources. No smoking.
- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Section 3. Composition and information on ingredients

Name	CAS	Concentration %
1-Butane-d_9-thiol	352431-09-5	> 98

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Section 4. First aid measures

Eye contact: Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.
Skin contact: Wash off with soap and plenty of water. Consult a physician.
Inhalation: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
Ingestion: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.
General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

Section 5. Firefighting measures

Flammability of the product: Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.
Lower explosion limit: 1.4 Vol%
Upper explosion limit: 11.3 Vol%
Auto-ignition temperature: 272 °C (522 °F)
Flash point: 2 °C (36 °F)
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, sulphur oxides.
Firefighting media and instructions: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
Special protective equipment for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Section 6. Accidental release measures

Personal precautions: Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains.
Methods for cleaning up: Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build-up of electrostatic charge.
Storage: Store at room temperature. Adequate ventilation. Protect from heat and ignition sources.

Section 8. Exposure Controls, Personal Protections

Engineering controls: Use mechanical exhaust or laboratory fumehood to avoid exposure.
Eyes: Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).
Respiratory: Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US).
Hands: Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.
Skin/body: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Section 9. Physical and chemical properties (unlabelled)

Molecular weight: 90.19 g/mol
Physical status: Liquid
Color: Colorless
Odour: Stench
Density: 0.842 g/cm^3 at 25 °C (77 °F)
Melting point: -116 °C (-177 °F) - lit.
Boiling point: 98 °C (208 °F) - lit.
Vapour tension: 61 hPa (46 mmHg) at 25 °C (77 °F)
Density of vapour: 3.11 (Air = 1)
Coefficient of division (water/oil): log Pow: 2.28
Solubility in water: 0.6 g/L

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Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
Incompatibility: Bases, oxidizing agents, alkali metals.
Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, sulphur oxides.
Reactivity conditions: Heat, flames and sparks. Vapours may form explosive mixture with air.

Section 11. Toxicological information (unlabelled)

Toxicological data: 1-Butanethiol

Information on ingredients:

Name	CAS	LD_{50}	LC_{50}
1-Butanethiol	109-79-5	Oral - Rat - 1,500 mg/kg	Inhalation - Rat - 4 h - 4020 ppm

Potential acute effects

- **Eyes:** Causes eye irritation.
- **Skin:** Harmful if absorbed through skin. Causes skin irritation.
- **Inhalation:** May be harmful if inhaled. Causes respiratory tract irritation.
- **Ingestion:** Harmful if swallowed.

Potential chronic effects

- **Carcinogenic effects:** IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** No data available.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

Name	Results	Species	Period
1-Butanethiol	1,100 mg/l LC50	Ictalurus punctatus	96 h

Effects on environment: No data available.
Mobility: No data available.
Environmental precautions: No data available.
Persistence and degradability: No data available.
Bioaccumulative potential: No data available.

Section 13. Disposal considerations

Waste disposal: Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Butyl mercaptan
UN number: UN2347
Class: 3
Packaging group: II

Additional information: None

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Section 15. Regulatory information

UNITED STATES:
NFPA classification

Health: 2
Flammable: 3
Reactivity: 1
Specials conditions: None

Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous

U.S. Federal regulations:

TSCA 8(b) inventory: 1-Butanethiol
SARA 302/304/311/312 extremely hazardous substances: Not Listed
SARA 302/304 emergency planning and notification: Not Listed
SARA 302/304/311/312 hazardous chemicals: Not Listed
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Listed
CWA (Clean Water Act) 307: Not Listed
CWA (Clean Water Act) 311: Not Listed
CAA (Clean Air Act) 112 accidental release prevention: Not Listed
CAA (Clean Air Act) 112 regulated flammable substances: Not Listed
CAA (Clean Air Act) 112 regulated toxic substances: Not Listed

State regulations:

DEA List I Chemicals (Precursor Chemicals): Not Listed
DEA List II Chemicals (Essential Chemicals): Not Listed
Substances in Massachusetts: Listed
Dangerous substances in New Jersey: Listed
New York – Dangerous substances with acute effects: Not Listed
Dangerous substances in Pennsylvania – right to know: Listed

WHMIS (Canada):

B2 - Flammable liquid

D2B - Toxic material causing other toxic effects

Section 16. Additional information

References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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Elaborated by: **Toxyscan Inc., 1-866-780-0599**
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