

1-Hexane-d₁₃-thiol

Section 1. Chemical product and company identifications

Product code: D-6419
Chemical formula: C₆HD₁₃S
CAS: 1142922-50-6
CAS (unlabelled): 111-31-9
Synonyms: *n*-Hexyl Mercaptan

Supplier / Manufacturer:

C/D/N Isotopes Inc.
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Pointe-Claire (Québec) H9R 1H1
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In case of emergency:

TOXYSKAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications




Physical state: Liquid
Warning: Flammable liquid and vapour. Harmful if swallowed. Toxic if inhaled.
Routes of entry: Inhalation, ingestion, skin and eyes

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

GHS Classification:

- Flammable liquids (Category 3)
- Acute toxicity, Oral (Category 4)
- Acute toxicity, Inhalation (Category 3)

GHS Label elements:

- Pictograms:   
- Signal word: Danger

Hazards statement:

- H226 Flammable liquid and vapour.
- H302 Harmful if swallowed.
- H331 Toxic if inhaled.

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.
- P301 + P 330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- P316 Get emergency medical help immediately.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
1-Hexane-d ₁₃ -thiol	1142922-50-6	> 98

Section 4. First aid measures

Eye contact: Flush eyes with water as a precaution.
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: 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: 0.7 Vol%

Upper explosion limit: 5.5 Vol%

Auto-ignition temperature: No data available.

Flash point: 30 °C (86 °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.

Environmental precautions: Do not let product enter drains.

Methods for cleaning up: Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Provide appropriate exhaust ventilation. Keep away from sources of ignition - No smoking.

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: Safety glasses with side-shields conforming to 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: 118.24 g/mol

Physical status: Liquid

Color: Colorless to yellow

Odour: Stench

Density: 0.838 g/cm³

Melting point: -81 °C (-114 °F)

Boiling point: 150 - 154 °C (302 - 309 °F)

Vapour pressure: No data available

Vapour density: 5.04 (Air = 1)

Partition coefficient (octanol/water): No data available

Water solubility: No data available

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.

Incompatibility: Bases, oxidizing agents.

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides, sulphur oxides.

Reactivity conditions: Heat, flames and sparks.

Section 11. Toxicological information (unlabelled)

Toxicological data: 1-Hexanethiol

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
1-Hexanethiol	111-31-9	Oral - Rat - 1,254 mg/kg	Inhalation - Rat - 4 h - 1,080 ppm

Potential acute effects

- **Eyes:** May cause eye irritation.
- **Skin:** May be harmful if absorbed through skin. May cause skin irritation.
- **Inhalation:** Toxic if inhaled. May cause 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:

<u>Name</u>	<u>Results</u>	<u>Species</u>	<u>Period</u>
1-Hexanethiol	No data available		

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: Contact a licensed professional waste disposal service to dispose of this material.

Section 14. Transportation information

Classification DOT/ IMDG/IATA label:

Shipping name: Mercaptans, liquid, flammable, toxic, n.o.s. (1-Hexanethiol)

UN number: UN1228

Class: 3 (6.1)

Packaging group: III

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 3
Flammable: 3
Reactivity: 0
Special conditions: None

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

U.S. Federal regulations:

TSCA 8(b) inventory: 1-Hexanethiol

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: Not Listed

Dangerous substances in New Jersey: Listed

New York – Dangerous substances with acute effects: Not Listed

Dangerous substances in Pennsylvania – right to know: Not Listed

WHMIS (Canada):



B3 - Combustible liquid



D1B - Toxic material causing immediate and serious toxic effects

Section 16. Additional information

References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part 1910.1200 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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