

3-(Methyl-d₃-thio)propionaldehyde

Section 1. Chemical product and company identifications

Product code: D-7844

Chemical formula: C₄H₅D₃OS

CAS: 136430-27-8

CAS (unlabelled): 3268-49-3

Synonyms: Methional, 3-(Methylmercapto)propionaldehyde, 4-Thiapentanal

Supplier / Manufacturer:

C/D/N Isotopes Inc.

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In case of emergency:

TOXYSKAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications

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

- GHS Classification:**
- Flammable liquids (Category 4)
 - Acute toxicity, Oral (Category 4)
 - Acute toxicity, Dermal (Category 3)
 - Acute toxicity, Inhalation (Category 4)
 - Skin irritation (Category 2)
 - Serious eye damage (Category 1)
 - Skin sensitization (Category 1)

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

- Hazards statement:**
- H227 Combustible liquid.
 - H302 + H332 Harmful if swallowed or inhaled.
 - H311 Toxic in contact with skin.
 - H315 Causes skin irritation.
 - H317 May cause an allergic skin reaction.
 - H318 Causes serious eye damage.

- Precautionary statement:**
- P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
 - P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
 - P264 Wash hands thoroughly after handling.
 - P270 Do not eat, drink or smoke when using this product.
 - P271 Use only outdoors or in a well-ventilated area.
 - P272 Contaminated work clothing should not be allowed out of the workplace.
 - P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
 - P301+P312 IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
 - P302 + P352 IF ON SKIN: wash with plenty of soap and water.
 - P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 - P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
 - P310 Immediately call a POISON CENTER or doctor/physician.
 - P312 Call a POISON CENTER or doctor/physician if you feel unwell.
 - P333+P313 IF SKIN irritation or rash occurs: Get medical advice/attention.
 - P361 Remove/Take off immediately all contaminated clothing..
 - P363 Wash contaminated clothing before reuse.
 - P370 +P378 In case of fire: Use dry chemical or carbon dioxide for extinction.
 - P403+P235 Store in a well-ventilated place. Keep cool.
 - P405 Store locked up.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
3-(Methyl-d ₃ -thio)propionaldehyde	136430-27-8	> 96

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: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

General advice: Move out of dangerous area. Consult a physician. Show this safety data sheet to the doctor in attendance.

Indication of immediate medical attention and special treatment needed, if necessary: No data available

Most important symptoms and effects, both acute and delayed: No data available.

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.

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. Discharge into the environment must be avoided.

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 FROZEN. Adequate ventilation. Protect from air.

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: 104.17 g/mol

Physical status: Liquid

Color: Colorless to yellow

Odour: Stench

Density: 1.052 g/cm³

Melting point: -58 °C (-72 °F)

Boiling point: 165 - 166 °C (329 - 331 °F)

Vapour pressure: 0.53 hPa (0.4 mmHg) at 20 °C (68 °F)

Vapour density: 3.59 (Air = 1)

Partition coefficient (octanol/water): No data available

Water solubility: Soluble

Lower explosion limit: No data available.

Upper explosion limit: No data available.
Auto-ignition temperature: No data available.
Flash point: 64 °C (147 °F)

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.
Incompatibility: Strong oxidizing agents, strong bases.
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: 3-(Methylthio)propionaldehyde

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
3-(Methylthio)propionaldehyde	3268-49-3	Oral - Rat - 700 mg/kg Dermal - Rat - 747 mg/kg	Inhalation - Rat - 4 h - 5,820 mg/m ³

Potential acute effects

- **Eyes:** Causes serious eye damage.
- **Skin:** Toxic if absorbed through skin. Causes skin irritation. May cause an allergic skin reaction.
- **Inhalation:** Harmful 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>
3-(Methylthio)propionaldehyde	14 mg/l LC50	Danio rerio	24 h
	4.5 mg/l EC50	Daphnia magna	48 h
	2.45 mg/l EC50	Desmodesmus subspicatus	72 h

Effects on environment: An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Mobility: No data available.
Environmental precautions: No data available.
Persistence and degradability: Readily biodegradable.
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: 4-Thiapentanal
UN number: 2785
Class: 6.1
Packaging group: III

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 3
Flammable: 2
Reactivity: 0
Special conditions: None

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

U.S. Federal regulations:

California proposition 65 requirements : Not Listed
SARA section 313 (specific toxic chemical listings) : Not Listed
CERCLA reportable quantity : Not listed
Sections 302-304 reportable quantity : Not listed
Community Right-to-Know (Sections 311 and 312) : Not Listed

Section 16. Additional information

Date of issue: September 15th, 20212

Version: 4

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

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This safety data sheet has been prepared in accordance with the OSHA (USA), WHMIS (Canada) / GHS classification rules in effect at the time of writing.