

SAFETY DATA SHEET

Version 8.6
Revision Date 08/14/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 3-(Methylthio)butanal

Product Number : W337404
Brand : Aldrich
CAS-No. : 16630-52-7

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids : Category 3

Acute toxicity
(Inhalation) : Category 3

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Serious eye damage : Category 1

Germ cell mutagenicity : Category 2

Carcinogenicity : Category 2

Specific target organ toxicity - repeated exposure : Category 2

Short-term (acute) aquatic hazard : Category 1

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal Word : Danger

Hazard Statements :

- H226 Flammable liquid and vapour.
- H318 Causes serious eye damage.
- H331 Toxic if inhaled.
- H341 Suspected of causing genetic defects.
- H351 Suspected of causing cancer.
- H373 May cause damage to organs through prolonged or repeated exposure.
- H400 Very toxic to aquatic life.

Precautionary statements :

Prevention:

- P201 Obtain special instructions before use.
- P202 Do not handle until all safety precautions have been read and understood.
- P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
- P233 Keep container tightly closed.
- P240 Ground/bond container and receiving equipment.
- P241 Use explosion-proof electrical/ ventilating/ lighting equipment.
- P242 Use only non-sparking tools.
- P243 Take precautionary measures against static discharge.
- P260 Do not breathe mist or vapours.
- P271 Use only outdoors or in a well-ventilated area.
- P273 Avoid release to the environment.
- P280 Wear protective gloves/ protective clothing/ eye

protection/ face protection.

Response:

P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.

P304 + P340 + P311 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor.

P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391 Collect spillage.

Storage:

P403 + P233 Store in a well-ventilated place. Keep container tightly closed.

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

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
(2E)-2-Butenal	123-73-9*	>= 1 - < 5	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Immediately call in physician.
If breathing stops: immediately apply artificial

respiration, if necessary also oxygen.

In case of skin contact	: In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.
In case of eye contact	: After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.
If swallowed	: After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
Most important symptoms and effects, both acute and delayed	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible. Forms explosive mixtures with air at elevated temperatures. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Carbon oxides Sulphur oxides

Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	: Do not let product enter drains. Risk of explosion.
Methods and materials for containment and cleaning up	: Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	: Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	: Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Further information on	: Keep container tightly closed in a dry and well-

Tightly fitting safety goggles

Skin and body protection : Flame retardant antistatic protective clothing.

Hygiene measures : Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid

Color : colourless

Odor : No data available

Odor Threshold : No data available

pH : No data available

Melting point : No data available

Boiling point/boiling range : 144 - 147 °F / 62 - 64 °C (13 hPa)
Method: lit.

Flash point : No data available

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Upper explosion limit /
Upper flammability limit : No data available

Lower explosion limit /
Lower flammability limit : No data available

Vapor pressure : 60 mmHg (68 °F / 20 °C)

Relative vapour density : 4.08
(Air = 1.0)

Relative density : No data available

Density : 1.001 g/cm³ (77 °F / 25 °C)
Method: lit.

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Water solubility	: No data available
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 118.20 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Vapour/air-mixtures are explosive at intense warming.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Heating.
Incompatible materials	: Strong oxidizing agents Strong bases
Hazardous decomposition products	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - > 5,000 mg/kg

(Calculation method)

Oral: No data available

Acute toxicity estimate Inhalation - 4 h - 10 mg/l - vapour (Calculation method)

Inhalation: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg

(Calculation method)

Dermal: No data available

No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: 2B - Group 2B: Possibly carcinogenic to humans ((2E)-2-Butenal)

NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available (3-(Methylthio)butyraldehyde)

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Nausea, Headache, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (3-(Methylthio)butyraldehyde)

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

(2E)-2-Butenal:

Toxicity to fish : Remarks: No data available

M-Factor (Acute aquatic toxicity) : 10

Persistence and degradability

Components:

(2E)-2-Butenal:

Biodegradability : Remarks: No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Other adverse effects

Components:

(2E)-2-Butenal:

Additional ecological information : No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 1989
Proper shipping name : Aldehydes, n.o.s.
(3-(Methylthio)butyraldehyde)

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Class : 3
Packing group : III
Labels : Class 3 - Flammable liquids
Packing instruction (cargo aircraft) : 366
Packing instruction (passenger aircraft) : 355

IMDG-Code

UN number : UN 1989
Proper shipping name : ALDEHYDES, N.O.S.

Class : 3
Packing group : III
Labels : 3
EmS Code : F-E, S-D
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 1989
Proper shipping name : Aldehydes, n.o.s.
(3-(Methylthio)butyraldehyde)

Class : 3
Packing group : III
Labels : Class 3 - Flammable liquids
ERG Code : 129P
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
(2E)-2-Butenal	123-73-9	100	3333

SARA 304 Extremely Hazardous Substances Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
(2E)-2-Butenal	123-73-9	100	3333

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
(2E)-2-Butenal	123-73-9	1000

SARA 311/312 Hazards : Fire Hazard
Acute Health Hazard
Chronic Health Hazard

SARA 313 : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

US State Regulations

Massachusetts Right To Know

(2E)-2-Butenal 123-73-9

Pennsylvania Right To Know

(2E)-2-Butenal 123-73-9

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

OSHA Z-1 : USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants

OSHA Z-1 / TWA : 8-hour time weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response;

EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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