



# MATERIAL SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Date of issue: 02/13/2013

Version 1.0

## SECTION 1. Identification

### Product identifier

Product number	841168
Product name	3-(Methylthio)-propionaldehyde for synthesis

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

Identified uses	Chemical for synthesis
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### Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation   290 Concord Road, Billerica, MA 01821, United States of America   SDS Phone Support: +1-978-715-1335   General Inquiries: +1-978-715-4321   Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)  e-mail: mm_sds@merckgroup.com
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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## SECTION 2. Hazards identification

### GHS Classification

Acute toxicity, Category 4, Inhalation, H332  
Acute toxicity, Category 4, Dermal, H312  
Skin sensitization, Category 1, H317  
Eye irritation, Category 2, H319  
Acute toxicity, Category 4, Oral, H302  
Skin irritation, Category 2, H315

For the full text of the H-Statements mentioned in this Section, see Section 16.

### GHS-Labeling

*Hazard pictograms*



*Signal Word*  
Warning

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## *Hazard Statements*

H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.

H315 Causes skin irritation.

H317 May cause an allergic skin reaction.

H319 Causes serious eye irritation.

## *Precautionary Statements*

P280 Wear protective gloves.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

## **Other hazards**

None known.

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## **SECTION 3. Composition/information on ingredients**

Formula C<sub>4</sub>H<sub>8</sub>OS (Hill)

CAS-No. 3268-49-3

Molar mass 104.17 g/mol

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## **SECTION 4. First aid measures**

### **Description of first-aid measures**

#### *Inhalation*

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

#### *Skin contact*

After skin contact: wash off with plenty of water. Remove contaminated clothing. Get medical attention.

#### *Eye contact*

After eye contact: rinse out with plenty of water. Call in ophthalmologist.

#### *Ingestion*

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

Never give anything by mouth to an unconscious person.

### **Most important symptoms and effects, both acute and delayed**

Allergic reactions, irritant effects

### **Indication of any immediate medical attention and special treatment needed**

No information available.

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## **SECTION 5. Fire-fighting measures**

### **Extinguishing media**

#### *Suitable extinguishing media*

Water, Carbon dioxide (CO<sub>2</sub>), Foam, Dry powder

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### *Unsuitable extinguishing media*

For this substance/mixture no limitations of extinguishing agents are given.

### **Special hazards arising from the substance or mixture**

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapors possible in the event of fire.

Fire may cause evolution of:

Sulfur oxides

### **Advice for firefighters**

#### *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.

#### *Further information*

Prevent fire extinguishing water from contaminating surface water or the ground water system.

Suppress (knock down) gases/vapors/mists with a water spray jet.

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## **SECTION 6. Accidental release measures**

### **Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapors, aerosols. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

### **Environmental precautions**

Do not empty into drains.

### **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 with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

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## **SECTION 7. Handling and storage**

### **Precautions for safe handling**

Observe label precautions.

Work under hood. Do not inhale substance/mixture. Avoid generation of vapors/aerosols.

### **Conditions for safe storage, including any incompatibilities**

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Store below +15°C (+59°F).

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## SECTION 8. Exposure controls/personal protection

### Exposure limit(s)

#### Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

#### Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

#### Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

#### Eye/face protection

Safety glasses

#### Hand protection

Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary.

#### Other protective equipment:

protective clothing

#### Respiratory protection

required when vapors/aerosols are generated.

Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

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## SECTION 9. Physical and chemical properties

Physical state	liquid
Color	colorless
Odor	malodorous
Odor Threshold	No information available.
pH	No information available.
Melting point	-58 °C
Boiling point/boiling range	329 - 331 °F ( 165 - 166 °C) at 1,013 hPa
Flash point	145 °F ( 63 °C) Method: DIN 51758

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Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1.3 %(V)
Upper explosion limit	26.1 %(V)
Vapor pressure	0.53 hPa at 68 °F ( 20 °C)
Relative vapor density	3.6
Relative density	1.052 g/cm <sup>3</sup> at 68 °F ( 20 °C)
Water solubility	<= 75 g/l at 68 °F ( 20 °C)
Partition coefficient: n-octanol/water	log Pow: 0.34 ( 20 °C) Bioaccumulation is not expected (log Pow <1). (IUCLID)
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	1.7 mPa.s at 50 °F ( 10 °C)
Explosive properties	Not classified as explosive.

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### SECTION 10. Stability and reactivity

#### Reactivity

Vapor/air-mixtures are explosive at intense warming.

#### Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

#### Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents

#### Conditions to avoid

Heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

#### Incompatible materials

no information available

#### Hazardous decomposition products

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in the event of fire: See section 5.

## SECTION 11. Toxicological information

### Information on toxicological effects

#### *Acute oral toxicity*

LD50 rat: 755 mg/kg

OECD Test Guideline 401

absorption

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

#### *Acute inhalation toxicity*

LC50 rat:  $\geq 4.84$  mg/l; 4 h

OECD Test Guideline 403

absorption

Symptoms: Possible damages:, mucosal irritations

#### *Acute dermal toxicity*

LD50 rat: 1,650 mg/kg

(IUCLID)

absorption

#### *Skin irritation*

rabbit

Result: Irritations

OECD Test Guideline 404

Causes skin irritation.

#### *Eye irritation*

rabbit

Result: Eye irritation

(IUCLID)

Causes serious eye irritation.

#### *Sensitization*

Sensitization test (Magnusson and Kligman):

Result: positive

(IUCLID)

May cause an allergic skin reaction.

#### *Genotoxicity in vitro*

Ames test

Result: negative

(IUCLID)

#### *Specific target organ systemic toxicity - single exposure*

The substance or mixture is not classified as specific target organ toxicant, single exposure.

#### *Specific target organ systemic toxicity - repeated exposure*

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

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### *Aspiration hazard*

Regarding the available data the classification criteria are not fulfilled.

### **Further information**

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## **SECTION 12. Ecological information**

### **Ecotoxicity**

#### *Toxicity to fish*

LC50 Danio rerio (zebra fish): 14 mg/l; 24 h

ISO 7346 (IUCLID)

#### *Toxicity to daphnia and other aquatic invertebrates*

EC50 Daphnia magna (Water flea): 25 mg/l; 24 h (IUCLID)

#### *Toxicity to algae*

IC50 Desmodesmus subspicatus (green algae): 7.4 mg/l; 72 h

OECD Test Guideline 201

### **Persistence and degradability**

#### *Biodegradability*

100 %; 18 d

(IUCLID)

Readily biodegradable.

### **Bioaccumulative potential**

#### *Partition coefficient: n-octanol/water*

log Pow: 0.34 ( 20 °C)

Bioaccumulation is not expected (log Pow <1). (IUCLID)

### **Mobility in soil**

No information available.

### **Other adverse effects**

#### *Additional ecological information*

Discharge into the environment must be avoided.

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## **SECTION 13. Disposal considerations**

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

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## SECTION 14. Transport information

### Land transport (DOT)

UN number	UN 2785
Proper shipping name	4-THIAPENTANAL
Class	6.1
Packing group	III
Environmentally hazardous	--

### Air transport (IATA)

UN number	UN 2785
Proper shipping name	4-THIAPENTANAL
Class	6.1
Packing group	III
Environmentally hazardous	--
Special precautions for user	no

### Sea transport (IMDG)

UN number	UN 2785
Proper shipping name	4-THIAPENTANAL
Class	6.1
Packing group	III
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-A S-A

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## SECTION 15. Regulatory information

### United States of America

#### OSHA Hazards

Combustible Liquid  
Toxic by inhalation.  
Harmful if swallowed.  
Harmful by skin absorption.  
Skin irritant  
Eye irritant  
Skin sensitizer

This information is based on 29 CFR 1910.1200 criteria prior to adoption of the GHS, and may deviate from the GHS information on the label and in section 2.

#### SARA 311/312 Hazards

Fire Hazard  
Acute Health Hazard



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### Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

### DEA List I

Not listed

### DEA List II

Not listed

## US State Regulations

### Massachusetts Right To Know

Remarks

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know

*Ingredients*

3-(Methylthio)propionaldehyde

### New Jersey Right To Know

*Ingredients*

3-(Methylthio)propionaldehyde

### Notification status

TSCA:

On TSCA Inventory

DSL:

All components of this product are on the Canadian DSL.

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## SECTION 16. Other information

### Training advice

Provide adequate information, instruction and training for operators.

### Full text of H-Statements referred to under sections 2 and 3.

H302

Harmful if swallowed.

H312

Harmful in contact with skin.

H315

Causes skin irritation.

H317

May cause an allergic skin reaction.

H319

Causes serious eye irritation.

H332

Harmful if inhaled.

### Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

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The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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