



SAFETY DATA SHEET

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

Revision Date 02/05/2015

Version 1.1

SECTION 1. Identification

Product identifier

Product number	814674
Product name	2-Mercaptobenzothiazole for synthesis
CAS-No.	149-30-4

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 General Inquiries: +1-978-715-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
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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

Skin sensitization, Category 1, H317

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

GHS-Labeling

Hazard pictograms



Signal Word
Warning

Hazard Statements

H317 May cause an allergic skin reaction.

Precautionary Statements

P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

P280 Wear protective gloves.

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

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P321 Specific treatment (see supplemental first aid instructions on this label).
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P363 Wash contaminated clothing before reuse.
P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula $C_7H_5NS_2$ (Hill)
Molar mass 167.25 g/mol

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

benzothiazole-2-thiol ($\geq 90\%$ - $\leq 100\%$)

149-30-4

Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air.

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. Immediately 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

irritant effects, Allergic reactions, Cough, Shortness of breath, Nausea, Vomiting, Headache

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Water, Carbon dioxide (CO₂), Foam, Dry powder

Unsuitable extinguishing media

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

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Special hazards arising from the substance or mixture

Combustible material, Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapors possible in the event of fire.
Fire may cause evolution of:
nitrogen oxides, 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

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid generation of dusts; do not inhale dusts. Avoid substance contact. 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Conditions for safe storage, including any incompatibilities

Tightly closed. Dry.

Store at +15°C to +25°C (+59°F to +77°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Contains no substances with occupational exposure limit values.

Engineering measures

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

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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.

Respiratory protection

required when dusts 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.

SECTION 9. Physical and chemical properties

Physical state	solid
Color	light yellow
Odor	characteristic
Odor Threshold	No information available.
pH	7 at 0.12 g/l 77 °F (25 °C)
Melting point	180 - 183 °C
Boiling point/boiling range	> 500 °F (> 260 °C) decomposes
Flash point	469 °F (243 °C) Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	15 %(V)
Upper explosion limit	No information available.

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Vapor pressure	< 0.000003 hPa at 77 °F (25 °C)
Relative vapor density	No information available.
Density	1.42 g/cm ³ at 68 °F (20 °C)
Relative density	No information available.
Water solubility	0.12 g/l at 77 °F (25 °C)
Partition coefficient: n-octanol/water	log Pow: 2.42 (experimental) (Lit.) Bioaccumulation is not expected.
Autoignition temperature	No information available.
Decomposition temperature	> 500 °F (> 260 °C)
Viscosity, dynamic	No information available.
Explosive properties	No information available.
Oxidizing properties	No information available.
Ignition temperature	869 °F (465 °C)
Bulk density	ca. 390 kg/m ³

SECTION 10. Stability and reactivity

Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

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

Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents

Conditions to avoid

Strong heating.

Incompatible materials

no information available

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Hazardous decomposition products

in the event of fire: See section 5.

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Eye contact, Skin contact, Ingestion

Acute oral toxicity

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

LD50 Rat: 3,800 mg/kg (ECHA) (Lit.)

Acute inhalation toxicity

LC50 Rat: > 1,270 mg/m³ (RTECS)

Symptoms: Irritation symptoms in the respiratory tract., Cough, Shortness of breath, After a latency period., Inhalation may lead to the formation of oedemas in the respiratory tract.

Acute dermal toxicity

LD50 Rabbit: > 7,940 mg/kg
(IUCLID)

Eye irritation

slight irritation

Sensitization

Sensitization test: Guinea pig

Result: positive

(IUCLID) May cause sensitization by skin contact.

May cause an allergic skin reaction.

Genotoxicity in vivo

Micronucleus test

Result: negative

(National Toxicology Program)

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.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

Carcinogenicity

IARC

No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

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

Further information

After absorption:

Headache, Nausea, Vomiting

Further data:

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

Ecotoxicity

Toxicity to fish

LC50 Pimephales promelas (fathead minnow): 11 mg/l; 96 h

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 0.025 mg/l; 48 h (External MSDS)

EC50 Tetrahymen pyriformis: 10 mg/l; 24 h (IUCLID)

Toxicity to algae

IC50 Pseudokirchneriella subcapitata (green algae): 0.25 mg/l; 96 h

OECD Test Guideline 201

Persistence and degradability

Biodegradability

2.5 %; 14 d

OECD Test Guideline 301C

Not readily biodegradable.

Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2.42

(experimental)

(Lit.) Bioaccumulation is not expected.

Mobility in soil

No information available.

Additional ecological information

Further information on ecology

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.

SECTION 14. Transport information

Land transport (DOT)

UN number	UN 3077
Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2-MERCAPTOBENZOTHIAZOLE)
Class	9
Packing group	III
Environmentally hazardous	--

Air transport (IATA)

UN number	UN 3077
Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2-MERCAPTOBENZOTHIAZOLE)
Class	9
Packing group	III
Environmentally hazardous	--
Special precautions for user	no

Sea transport (IMDG)

UN number	UN 3077
Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2-MERCAPTOBENZOTHIAZOLE)
Class	9
Packing group	III
Environmentally hazardous	--
Special precautions for user	yes
EmS	F-A S-F

SECTION 15. Regulatory information

United States of America

SARA 313

The following components are subject to reporting levels established by SARA Title III, Section 313:

Ingredients

benzothiazole-2-thiol	149-30-4	100 %
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No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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.

New Jersey Right To Know

Ingredients

benzothiazole-2-thiol

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA: All components of the product are listed in the TSCA-inventory.

DSL: All components of this product are on the Canadian DSL.

KOREA: Not in compliance with the inventory

SECTION 16. Other information

Training advice

Provide adequate information, instruction and training for operators.

Labeling

Hazard pictograms



Signal Word

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Hazard Statements

H317 May cause an allergic skin reaction.

H410 Very toxic to aquatic life with long lasting effects.

Precautionary Statements

Prevention

P273 Avoid release to the environment.

P280 Wear protective gloves.

Response

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

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

H317 May cause an allergic skin reaction.

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.

Revision Date 02/05/2015

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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