

SAFETY DATA SHEET

Version 6.4 Revision Date 07/16/2020 Print Date 06/01/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : 1,3-Benzenedithiol

Product Number : 269093 Brand : Aldrich CAS-No. : 626-04-0

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

Identified uses : Laboratory chemicals, Synthesis of substances

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

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-

527-3887 CHEMTREC (International) 24

Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 2), H300

Acute toxicity, Inhalation (Category 1), H330

Acute toxicity, Dermal (Category 2), H310

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Reproductive toxicity (Category 2), H361

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Specific target organ toxicity - repeated exposure, Oral (Category 1), Kidney, H372

Short-term (acute) aquatic hazard (Category 1), H400 Long-term (chronic) aquatic hazard (Category 1), H410

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

2.2 GHS Label elements, including precautionary statements

Aldrich - 269093 Page 1 of 9



Pictogram



Signal	l word	Danger
--------	--------	--------

Signal word	Danger
Hazard statement(s) H300 + H310 + H330 H315 H319 H335 H361 H372	Fatal if swallowed, in contact with skin or if inhaled. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation. Suspected of damaging fertility or the unborn child. Causes damage to organs (Kidney) through prolonged or repeated exposure if swallowed.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement P201 P202	Obtain special instructions before use. Do not handle until all safety precautions have been read and understood.
P260 P262 P264 P270	Do not breathe dust/ fume/ gas/ mist/ vapors/ spray. Do not get in eyes, on skin, or on clothing. Wash skin thoroughly after handling. Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P273 P280	Avoid release to the environment. Wear protective gloves/ protective clothing/ eye protection/ face protection.
P284	Wear respiratory protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P302 + P350 + P310	IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362 P391	Take off contaminated clothing and wash before reuse. Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405 + P255	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS Stench.

SECTION 3: Composition/information on ingredients

3.1 Substances

Aldrich - 269093 Page 2 of 9



Synonyms : 1,3-Dimercaptobenzene

Formula : $C_6H_6S_2$ Molecular weight : 142.24 g/mol CAS-No. : 626-04-0 EC-No. : 210-925-3

Component	Classification	Concentration		
Benzene-1,3-dithiol				
	Acute Tox. 2; Acute Tox.	<= 100 %		
	1; Acute Tox. 2; Skin Irrit.			
	2; Eye Irrit. 2A; Repr. 2;			
	STOT SE 3; STOT RE 1;			
	Aquatic Acute 1; Aquatic			
	Chronic 1; H300, H330,			
	H310, H315, H319, H361,			
	H335, H372, H400, H410			

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

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

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

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

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed No data available

Aldrich - 269093 Page 3 of 9



SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Sulfur oxides Combustible.

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

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

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Storage class (TRGS 510): 6.1A: Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

Millipore SigMa

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a fullface 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) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

Information on basic physical and chemical properties

Form: liquid a) Appearance

Color: colorless

No data available b) Odor c) Odor Threshold No data available No data available d) pH

Melting point/range: 24 - 25 °C (75 - 77 °F) - lit. e) Melting

point/freezing point

No data available f)

Initial boiling point and boiling range



g) Flash point 113 °C (235 °F) - closed cup h) Evaporation rate No data available Flammability (solid, No data available gas) Upper/lower No data available j) flammability or explosive limits

No data available k) Vapor pressure Vapor density No data available m) Relative density No data available n) Water solubility No data available o) Partition coefficient: No data available

n-octanol/water

p) Autoignition No data available temperature

q) Decomposition No data available temperature

r) Viscosity No data available s) Explosive properties No data available No data available Oxidizing properties

Other safety information 9.2

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

No data available

10.5 Incompatible materials

Strong basesStrong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Sulfur oxides

Other decomposition products - No data available

In the event of fire: see section 5

Aldrich - 269093 Page 6 of 9

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

No data available

Inhalation: No data available Dermal: No data available

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

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.

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.

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

Some evidence of adverse effects on sexual function and fertility, and/or on development, based on animal experiments.

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

Oral - The substance or mixture is classified as specific target organ toxicant, repeated exposure, category 1. - Kidney

Aspiration hazard

No data available

Additional Information

RTECS: Not available

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

12.1 Toxicity

No data available

Aldrich - 269093 Page 7 of 9

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting effects.

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 3382 Class: 6.1I Packing group: I

Proper shipping name: Toxic by inhalation liquid, n.o.s. (Benzene-1,3-dithiol)

Reportable Quantity (RQ):

Poison Inhalation Hazard: Hazard Zone B

IMDG

UN number: 3382 Class: 6.1 Packing group: I EMS-No: F-A, S-A Proper shipping name: TOXIC BY INHALATION LIQUID, N.O.S. (Benzene-1,3-dithiol)

Marine pollutant : yes

IATA

UN number: 3382 Class: 6.1

Proper shipping name: Toxic by inhalation liquid, n.o.s. (Benzene-1,3-dithiol)

IATA Passenger: Not permitted for transport IATA Cargo: Not permitted for transport

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

Aldrich - 269093 Page 8 of 9

SARA 313 Components

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.

SARA 311/312 Hazards

Acute Health Hazard

Massachusetts Right To Know Components

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

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

Pennsylvania Right To Know Components

Benzene-1,3-dithiol CAS-No. Revision Date

626-04-0

New Jersey Right To Know Components

Benzene-1,3-dithiol CAS-No. Revision Date

626-04-0

SECTION 16: Other information

Further information

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.4 Revision Date: 07/16/2020 Print Date: 06/01/2022

Aldrich - 269093 Page 9 of 9

