

MATERIAL SAFETY DATA SHEET

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Version 1.7

Section 1 - Product and Company Information

Product Name 1,4-PHENYLENE DIISOTHIOCYANATE, 98%
Product Number 258555
Brand ALDRICH

Company Sigma-Aldrich
Address 3050 Spruce Street
SAINT LOUIS MO 63103 US

Technical Phone: 800-325-5832
Fax: 800-325-5052
Emergency Phone: 314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
1,4-PHENYLENE DIISOTHIOCYANATE	4044-65-9	Yes

Formula C8H4N2S2
Synonyms Biscomate * Bitoscanate *
1,4-Diisothiocyanatobenzene * Isothiocyanic acid
p-phenylene ester * Jonit *
Phenylene-1,4-diisothiocyanate * Phenylene
thiocyanate * PDITC * p-Phenylene diisothiocyanate

RTECS Number: NX9150000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Toxic (USA) Harmful (EU).

Harmful if swallowed. Irritating to eyes, respiratory system and skin. May cause sensitization by inhalation.

Lachrymator.

HMIS RATING

HEALTH: 2

FLAMMABILITY: 0

REACTIVITY: 1

NFPA RATING

HEALTH: 2

FLAMMABILITY: 0

REACTIVITY: 1

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician.

INHALATION EXPOSURE

If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE

In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

EYE EXPOSURE

In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

Section 5 - Fire Fighting Measures

FLASH POINT

N/A

AUTOIGNITION TEMP

N/A

FLAMMABILITY

N/A

EXTINGUISHING MEDIA

Suitable: Water spray. Carbon dioxide, dry chemical powder, or appropriate foam.

FIREFIGHTING

Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Emits toxic fumes under fire conditions.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL

Evacuate area.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)

Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP

Sweep up, place in a bag and hold for waste disposal. Avoid raising dust. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Do not breathe dust. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep tightly closed. Store in a cool dry place. Store under nitrogen.

SPECIAL REQUIREMENTS

Moisture sensitive. Store under inert gas.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Mechanical exhaust required. Safety shower and eye bath.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N99 (US) or type P2 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator.

Hand: Compatible chemical-resistant gloves.

Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance	Physical State: Solid Color: Faintly beige	
Property	Value	At Temperature or Pressure
Molecular Weight	192.26 AMU	
pH	N/A	
BP/BP Range	N/A	
MP/MP Range	129 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	N/A	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	
Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	N/A	
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	N/A	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Stable: Stable.

Conditions of Instability: May decompose on exposure to moist air or water.

Materials to Avoid: Strong oxidizing agents, Strong acids, Strong

bases.

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide, Nitrogen oxides, Sulfur oxides, Hydrogen cyanide.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: Causes skin irritation.

Skin Absorption: May be harmful if absorbed through the skin.

Eye Contact: Causes eye irritation. Lachrymator.

Inhalation: Material is irritating to mucous membranes and upper respiratory tract. May be harmful if inhaled.

Ingestion: Harmful if swallowed.

SENSITIZATION

Respiratory: May cause allergic respiratory reaction.

SIGNS AND SYMPTOMS OF EXPOSURE

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

TOXICITY DATA

Intraperitoneal

Rat

21 MG/KG

LD50

Oral

Mouse

230 mg/kg

LD50

Intraperitoneal

Mouse

21 MG/KG

LD50

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT

Proper Shipping Name: Toxic solids, organic, n.o.s.

UN#: 2811

Class: 6.1

Packing Group: Packing Group III
Hazard Label: Toxic substances.
PIH: Not PIH

IATA

Proper Shipping Name: Toxic solid, organic, n.o.s.
IATA UN Number: 2811
Hazard Class: 6.1
Packing Group: III

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION

Symbol of Danger: Xn
Indication of Danger: Harmful.
R: 22-36/37/38-42
Risk Statements: Harmful if swallowed. Irritating to eyes, respiratory system and skin. May cause sensitization by inhalation.
S: 22-26-36/37
Safety Statements: Do not breathe dust. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing and gloves.

US CLASSIFICATION AND LABEL TEXT

Indication of Danger: Toxic (USA) Harmful (EU).
Risk Statements: Harmful if swallowed. Irritating to eyes, respiratory system and skin. May cause sensitization by inhalation.
Safety Statements: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing.
US Statements: Lachrymator.

UNITED STATES REGULATORY INFORMATION

SARA LISTED: Yes
NOTES: This product is subject to SARA section 313 reporting requirements.
TSCA INVENTORY ITEM: Yes

CANADA REGULATORY INFORMATION

WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: No
NDSL: Yes

Section 16 - Other Information

DISCLAIMER

For R&D use only. Not for drug, household or other uses.

WARRANTY

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 Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.

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