

## SAFETY DATA SHEET

Version 6.1

Revision Date 11/06/2017

Print Date 11/14/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : Benzyl isothiocyanate

Product Number : 252492

Brand : Aldrich

CAS-No. : 622-78-6

## 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 Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

## 1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

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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 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Respiratory sensitisation (Category 1), H334

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

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

## 2.2 GHS Label elements, including precautionary statements

Pictogram { error: file not found: C:\WWI\graphics\CUST-N15.00931430 } { error: file not found: C:\WWI\graphics\CUST-N15.00931410 }

Signal word CUST-N15.00700525

Hazard statement(s)

H302 + H312 + H332

H315

H319

H334

Harmful if swallowed, in contact with skin or if inhaled.

Causes skin irritation.

Causes serious eye irritation.

May cause allergy or asthma symptoms or breathing difficulties if inhaled.

H335	May cause respiratory irritation.
Precautionary statement(s)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear eye protection/ face protection.
P280	Wear protective gloves/ protective clothing.
P285	In case of inadequate ventilation wear respiratory protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell.
P304 + P340 + P312	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/ physician if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P342 + P311	If experiencing respiratory symptoms: Call a POISON CENTER/doctor.
P362	Take off contaminated clothing and wash before reuse.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	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

Lachrymator.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms : Isothiocyanatoamethylbenzene  
Benzyl mustard oil

Formula : C<sub>8</sub>H<sub>7</sub>NS  
Molecular weight : 149.21 g/mol  
CAS-No. : 622-78-6  
EC-No. : 210-753-9

#### Hazardous components

Component	Classification	Concentration
<b>Benzyl isothiocyanate</b>		
	Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; Resp. Sens. 1; STOT SE 3; H302 + H312 + H332, H315, H319, H334, H335	<= 100 %

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this 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. 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

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**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, Nitrogen oxides (NO<sub>x</sub>), Sulphur oxides

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

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**6. ACCIDENTAL RELEASE MEASURES****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

For personal protection see section 8.

**6.2 Environmental precautions**

Do not let product enter drains.

**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.

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**7. HANDLING AND STORAGE****7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour 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.

Recommended storage temperature 2 - 8 °C

Light sensitive. Moisture sensitive. Handle and store under inert gas.

Storage class (TRGS 510): 10: Combustible liquids

**7.3 Specific end use(s)**

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

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### 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 full-face 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

Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Appearance                                   | Form: liquid<br>Colour: dark brown       |
| b) Odour  | No data available                        |
| c) Odour Threshold                              | No data available                        |
| d) pH   | No data available                        |
| e) Melting point/freezing point                 | No data available                        |
| f) Initial boiling point and boiling range      | 242 - 243 °C (468 - 469 °F) - lit.       |
| g) Flash point                                  | > 110 °C (> 230 °F) - closed cup         |
| h) Evaporation rate                             | No data available                        |
| i) Flammability (solid, gas)                    | No data available                        |
| j) Upper/lower flammability or explosive limits | No data available                        |
| k) Vapour pressure                              | No data available                        |
| l) Vapour density                               | No data available                        |
| m) Relative density                             | 1.125 g/cm <sup>3</sup> at 25 °C (77 °F) |
| n) Water solubility                             | No data available                        |
| o) Partition coefficient: n-octanol/water       | No data available                        |

- |    |                           |                   |
|----|---------------------------|-------------------|
| p) | Auto-ignition temperature | No data available |
| q) | Decomposition temperature | No data available |
| r) | Viscosity                 | No data available |
| s) | Explosive properties      | No data available |
| t) | Oxidizing properties      | No data available |

## 9.2 Other safety information

No data available

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## 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

Heat

### 10.5 Incompatible materials

Strong oxidizing agents, Alcohols, Strong bases, Amines, acids

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Sulphur oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

Hamster

ovary

Cytogenetic analysis

Hamster

ovary

DNA damage

Hamster

ovary

Sister chromatid exchange

Mammal

Cytogenetic analysis

Mammal

Other mutation test systems

#### **Carcinogenicity**

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

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

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 identified as a carcinogen or potential carcinogen by OSHA.

#### **Reproductive toxicity**

No data available

No data available

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

Inhalation - May cause respiratory irritation.

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

No data available

#### **Aspiration hazard**

No data available

#### **Additional Information**

RTECS: NX8250000

Cough, Shortness of breath, Headache, Nausea, Vomiting

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

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## **12. ECOLOGICAL INFORMATION**

### **12.1 Toxicity**

No data available

Toxicity to daphnia and other aquatic invertebrates LC50 - Daphnia magna (Water flea) - 0.043 mg/l - 48 h(Benzyl isothiocyanate)

### **12.2 Persistence and degradability**

No data available

### **12.3 Bioaccumulative potential**

No data available

### **12.4 Mobility in soil**

No data available(Benzyl isothiocyanate)

### **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**

No data available

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## 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. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

#### DOT (US)

Not dangerous goods

#### IMDG

Not dangerous goods

#### IATA

UN number: 3334

Class: 9

Packing group: III

Proper shipping name: Aviation regulated liquid, n.o.s. (Benzyl isothiocyanate)

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## 15. REGULATORY INFORMATION

#### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### 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.

#### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Benzyl isothiocyanate	622-78-6	

#### New Jersey Right To Know Components

	CAS-No.	Revision Date
Benzyl isothiocyanate	622-78-6	

#### California Prop. 65 Components

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

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## 16. OTHER INFORMATION

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

H302	Harmful if swallowed.
H302 + H312 +	Harmful if swallowed, in contact with skin or if inhaled.
H332	
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.

H335 May cause respiratory irritation.

**HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	*
Flammability:	1
Physical Hazard	0

**NFPA Rating**

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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