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

1.1 Product identifiers

- Product name: Benzyl isothiocyanate
- Product Number: W442800
- 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 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 4), H302
- Skin irritation (Category 2), H315
- Eye irritation (Category 2A), H319
- Respiratory sensitization (Category 1), H334
- Skin sensitization (Category 1), H317
- 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
- Signal word: Danger
Hazard statement(s)
H302 Harmful if swallowed.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H319 Causes serious eye irritation.
H334 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/ vapors/ 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.
P272 Contaminated work clothing must not be allowed out of the workplace.
P280 Wear protective gloves/ eye protection/ face protection.
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.
P304 + P340 + P312 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor 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.
P333 + P313 If skin irritation or rash 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.

SECTION 3: Composition/information on ingredients

3.1 Substances
Synonyms: Isothiocyanotaomethylbenzene
Benzyl mustard oil

Formula: C₈H₇NS
Molecular weight: 149.21 g/mol
CAS-No.: 622-78-6
EC-No.: 210-753-9

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>benzyl isothiocyanate</td>
<td>Acute Tox. 4; Skin Irrit. 2;</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Aldrich - W442800
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Call in physician.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Water Foam Carbon dioxide (CO2) Dry powder

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

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Sulfur oxides
Combustible.
Vapors are heavier than air and may spread along floors.
Risk of dust explosion.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapours possible in the event of fire.

Eye Irrit. 2A; Resp. Sens. 1; Skin Sens. 1; STOT SE 3; H302, H315, H319, H334, H317, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.
5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 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

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
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
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Work under hood. Do not inhale substance/mixture.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Storage conditions
Tightly closed. Dry. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability
Recommended storage temperature
2 - 8 °C
Moisture sensitive. Handle and store under inert gas.

Storage class
Storage class (TRGS 510): 11: Combustible Solids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated
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**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

**Skin protection**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

**Body Protection**
protective clothing

**Respiratory protection**
required when dusts are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: solid
   Color: yellow

b) Odor
   like mustard, pungent

c) Odor Threshold
   No data available

d) pH
   No data available

e) Melting point/freezing point
   Melting point: 41 °C (106 °F)

f) Initial boiling point and boiling range
   242 - 243 °C 468 - 469 °F - lit.

g) Flash point
   106 °C (223 °F)

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   No data available

k) Vapor pressure
   ca.0.02 hPa at 25 °C (77 °F)

l) Vapor density
   No data available

m) Density
   1.125 g/cm3 at 25 °C (77 °F) - lit.
   Relative density
   No data available

n) Water solubility
   0.1 g/l at 25 °C (77 °F)

o) Partition coefficient: n-octanol/water
   log Pow: 3.16 at 25 °C (77 °F) - Bioaccumulation is not expected., (Lit.)

p) Autoignition temperature
   No data available

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   none

9.2 Other safety information
   No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
   Forms explosive mixtures with air on intense heating.
   A range from approx. 15 Kelvin below the flash point is to be rated as critical.
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.

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

10.3 Possibility of hazardous reactions
Violent reactions possible with:
- Strong oxidizing agents
- Strong acids

10.4 Conditions to avoid
- Heat.
- Strong heating.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
Symptoms: After swallowing: irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.
Acute toxicity estimate Oral - 500.1 mg/kg
(Expert judgment)
Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages: damage of respiratory tract
Dermal: 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
No data available
Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 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.
Other dangerous properties can not be excluded.
Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity
No data available

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 Endocrine disrupting properties
No data available

12.7 Other adverse effects
No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned
SECTION 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)

SECTION 15: Regulatory information

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

**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**
benzyl isothiocyanate  CAS-No.  622-78-6  Revision Date

**New Jersey Right To Know Components**
benzyl isothiocyanate  CAS-No.  622-78-6  Revision Date

SECTION 16: Other information

**Further information**
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.

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Version: 6.5 Revision Date: 10/08/2021 Print Date: 12/31/2023