

## SAFETY DATA SHEET

Version 8.2  
Revision Date 09/17/2021  
Print Date 05/28/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Allyl isothiocyanate

Product Number : W203408

Brand : Aldrich

CAS-No. : 57-06-7

**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)**

Flammable liquids (Category 3), H226

Acute toxicity, Oral (Category 4), H302

Acute toxicity, Inhalation (Category 2), H330

Acute toxicity, Dermal (Category 2), H310

Skin corrosion (Category 1B), H314

Serious eye damage (Category 1), H318

Skin sensitization (Category 1), H317

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**

Pictogram



Signal word

Danger

Hazard statement(s)

H226 Flammable liquid and vapor.  
H302 Harmful if swallowed.  
H310 + H330 Fatal in contact with skin or if inhaled.  
H314 Causes severe skin burns and eye damage.  
H317 May cause an allergic skin reaction.  
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.  
P233 Keep container tightly closed.  
P240 Ground/bond container and receiving equipment.  
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.  
P242 Use only non-sparking tools.  
P243 Take precautionary measures against static discharge.  
P260 Do not breathe dust/ fume/ gas/ mist/ vapors/ spray.  
P262 Do not get in eyes, on skin, or on clothing.  
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.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.  
P284 Wear respiratory protection.  
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.  
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
P302 + P350 + P310 IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.  
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.  
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.  
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.  
P362 Take off contaminated clothing and wash before reuse.  
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.  
P391 Collect spillage.  
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P403 + P235 Store in a well-ventilated place. Keep cool.  
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

Vesicant., Lachrymator.

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms : Oil of mustard  
AITC

Formula : C<sub>4</sub>H<sub>5</sub>NS  
Molecular weight : 99.15 g/mol  
CAS-No. : 57-06-7  
EC-No. : 200-309-2

Component	Classification	Concentration
<b>3-isothiocyanato-1-propene</b>		
	Flam. Liq. 3; Acute Tox. 4; Acute Tox. 2; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H226, H302, H330, H310, H314, H318, H317, H400, H410 M-Factor - Aquatic Acute: 10 - Aquatic Chronic: 10	<= 100 %

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

Take off contaminated clothing and shoes immediately. 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. Continue rinsing eyes during transport to hospital.

##### If swallowed

Do NOT induce vomiting. 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

---

### **SECTION 5: Firefighting measures**

#### **5.1 Extinguishing media**

##### **Suitable extinguishing media**

Dry powder Dry sand

##### **Unsuitable extinguishing media**

Do NOT use water jet.

#### **5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Sulfur oxides

#### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

#### **5.4 Further information**

Use water spray to cool unopened containers.

---

### **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. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low 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**

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

#### **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**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

**Advice on protection against fire and explosion**

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

**Hygiene measures**

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

For precautions see section 2.2.

**7.2 Conditions for safe storage, including any incompatibilities****Storage conditions**

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 stability**

Recommended storage temperature

2 - 8 °C

Handle and open container with care. Store under inert gas.

**Storage class**

Storage class (TRGS 510): 3: Flammable liquids

**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**

Component	CAS-No.	Value	Control parameters	Basis
3-isothiocyanato-1-propene	57-06-7	STEL	1 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
	Remarks	Skin Dermal Sensitization Notation		

**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**

Tightly fitting safety goggles. Faceshield (8-inch minimum). 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.

Full contact

Material: Fluorinated rubber  
Minimum layer thickness: 0.7 mm  
Break through time: 480 min  
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact  
Material: butyl-rubber  
Minimum layer thickness: 0.3 mm  
Break through time: 60 min  
Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### **Body Protection**

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., 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**

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**

### **9.1 Information on basic physical and chemical properties**

- |  |  |
|--|--|
| a) Appearance                              | Form: clear, liquid<br>Color: light orange                             |
| b) Odor                                    | mustard-like   |
| c) Odor Threshold                          | No data available  |
| d) pH                                      | No data available  |
| e) Melting point/freezing point            | Melting point/range: -80 °C (-112 °F) - lit.                           |
| f) Initial boiling point and boiling range | 150 °C 302 °F - lit.   |
| g) Flash point                             | 45 °C (113 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9 |
| h) Evaporation rate                        | No data available  |
| i) Flammability (solid, gas)               | No data available  |

Aldrich - W203408

Page 6 of 11

	gas)	
j)	Upper/lower flammability or explosive limits	No data available
k)	Vapor pressure	4.5 hPa at 23 °C (73 °F) 4.930 hPa at 20 °C (68 °F) 4.9 hPa at 30 °C (86 °F)
l)	Vapor density	No data available
m)	Density	1.013 g/cm <sup>3</sup> at 25 °C (77 °F) - lit.
	Relative density	No data available
n)	Water solubility	2,000 g/l at 20 °C (68 °F)
o)	Partition coefficient: n-octanol/water	log Pow: 1.83 at 20 °C (68 °F) - (ECHA), Bioaccumulation is not expected.
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

Surface tension	53.4 mN/m at 20 °C (68 °F) - OECD Test Guideline 115
-----------------	--

---

## 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

Heat, flames and sparks.

### 10.5 Incompatible materials

Water, Alcohols, Strong bases, Amines, Acids, Strong oxidizing agents

### 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

LD50 Oral - Rat - female - 425.4 mg/kg

(OPPTS 870.1100)

LC50 Inhalation - Rat - male and female - 4 h - 0.206 - 0.508 mg/l

(OPPTS 870.1300)

Inhalation: Irritating to respiratory system.

Acute toxicity estimate Inhalation - 4 h - 0.51 mg/l

(Expert judgment)

LD50 Dermal - Rat - male and female - 200 - 2,000 mg/kg

(OPPTS 870.1200)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive

Remarks: (ECHA)

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: Causes sensitization.

(OPPTS 870.2600)

#### Germ cell mutagenicity

Test Type: reverse mutation assay

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: reverse mutation assay

Species: Mouse

Method: OECD Test Guideline 474

Result: negative

#### 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

No data available



**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

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

---

**SECTION 12: Ecological information****12.1 Toxicity**

Toxicity to fish                      LC50 - *Oryzias latipes* (Orange-red killifish) - 0.07 mg/l - 96 h  
Remarks: (ECHA)

Toxicity to daphnia                  Remarks: (ECHA)  
and other aquatic                  (3-isothiocyanato-1-propene)  
invertebrates

**12.2 Persistence and degradability**

Biodegradability                  aerobic - Exposure time 29 d  
Result: 0 % - Not readily biodegradable.

**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.

Discharge into the environment must be avoided.

---

**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. 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: 1545 Class: 6.1 (3) Packing group: II  
Proper shipping name: Allyl isothiocyanate, stabilized  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 1545 Class: 6.1 (3) Packing group: II EMS-No: F-E, S-D  
Proper shipping name: ALLYL ISOTHIOCYANATE, STABILIZED  
Marine pollutant : yes

### IATA

UN number: 1545 Class: 6.1 (3) Packing group: II  
Proper shipping name: Allyl isothiocyanate, stabilized  
IATA Passenger: Not permitted for transport

---

## SECTION 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

Fire Hazard, Acute Health Hazard

### Massachusetts Right To Know Components

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

### Pennsylvania Right To Know Components

3-isothiocyanato-1-propene

CAS-No.  
57-06-7

Revision Date  
2007-03-01

---

## 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](http://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](mailto:mlsbranding@sial.com).

Version: 8.2

Revision Date: 09/17/2021

Print Date: 05/28/2022