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Safety & Environmental  
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SIGMA-ALDRICH

## Material Safety Data Sheet

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Version 1.30

## Section 1 - Product and Company Information

**Product Name** Allyl isothiocyanate, 95%  
**Product Number** 377430  
**Brand** Aldrich Chemical

**Company Address** Sigma-Aldrich  
 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	EC no	Annex I Index Number
ALLYL ISOTHIOCYANATE	57-06-7	No	200-309-2	

Ingredient Name	CAS #	Percent	SARA 313
Stabilized with: BUTYLATED HYDROXYTOLUENE	128-37-0	0.100%	No

**Formula** C4H5NS  
**Synonyms** Allyl isorhodanide, Allyl isosulfocyanate, Allyl isosulphocyanate, Allyl isothiocyanate, Allyl isothiokyanat (Czech), Allyl mustard oil, Allylsenevol, Allylseoel (German), Allyl sevenclom, Allyl thiocarbonimide, Artificial mustard oil, Artificial oil of mustard, Carbospol, FEMA No. 2034, Isothiocyanate d'allyle (French), 3-Isothiocyanato-1-propene, Mustard oil, NCIC50464, Oil of mustard, artificial, Oil of mustard BPC 1949, Oleum sinapis volatile, Propene, 2-isothiocyanato-, 2-Propenyl isothiocyanate, Redskin, Senf oil (German), Synthetic mustard oil, Volatile oil of mustard

## Section 3 - Hazards Identification

## Emergency Overview

Combustible (USA) Flammable (EU). Toxic.  
 Toxic in contact with skin and if swallowed. Causes burns. May cause sensitization by inhalation and skin contact.  
 Vesicant. Lachrymator.

**HMS Rating**  
 Health: 3+ Flammability: 2 Reactivity: 0

**NFPA Rating**  
 Health: 3 Flammability: 2 Reactivity: 0

\*additional chronic hazards present.

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. Do not induce vomiting.

## 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

## Explosion Hazards

Vapor may travel considerable distance to source of ignition and flash back.

**Flash Point:** 114.8 °F 46 °C

**Autoignition Temp:** N/A

## Extinguishing Media

## Suitable

For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be effective. Cool all affected containers with flooding quantities of water.

## Firefighting

## Protective Equipment

Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

## Specific Hazard(s)

Combustible liquid. Vapor may travel considerable distance to source of ignition and flash back. Emits toxic fumes under fire conditions.

## Section 6 - Accidental Release Measures

## Procedure to be Followed in Case of Leak or Spill

Evacuate area. Shut off all sources of ignition.

## Procedure(s) of Personal Precaution(s)

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

## Methods for Cleaning Up

Cover with an activated carbon adsorbent, take up and place in closed containers. Transport outdoor/ventilate area and wash spill site after material pickup is complete.

## Section 7 - Handling and Storage

## Handling

## User Exposure

Do not breathe vapor. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

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Page 2

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**Storage**  
**Suitable**  
Keep tightly closed. Store at 2-8°C

**Special Requirements**  
May develop pressure. Open carefully.

### Section 8 - Exposure Controls / PPE

**Engineering Controls**  
Safety shower and eye bath. Use only in a chemical fume hood.

#### 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 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 fullface supplied air respirator.

##### Hand

Compatible chemical-resistant gloves.

##### Eye

Chemical safety goggles.

##### Other

Face shield (8-inch minimum).

#### General Hygiene Measures

Wash contaminated clothing before reuse. Discard contaminated shoes. Wash thoroughly after handling.

### Section 9 - Physical/Chemical Properties

Appearance	Color	Form
<b>Physical State</b> Liquid	Faintly yellow-green	Clear liquid

**Molecular Weight** 99.16 AMU

<b>pH</b>	N/A
<b>BP/BP Range</b>	151 - 153 °C
<b>MP/MP Range</b>	-80 °C
<b>Freezing Point</b>	N/A
<b>Vapor Pressure</b>	N/A
<b>Vapor Density</b>	N/A
<b>Saturated Vapor Conc.</b>	N/A
<b>SG/Density</b>	1.02 g/cm <sup>3</sup>
<b>Bulk Density</b>	N/A
<b>Odor Threshold</b>	N/A
<b>Volatile%</b>	N/A
<b>VOC Content</b>	N/A
<b>Water Content</b>	N/A
<b>Solvent Content</b>	N/A
<b>Evaporation Rate</b>	N/A
<b>Viscosity</b>	N/A
<b>Partition Coefficient</b>	Log Kow: 2.092
<b>Decomposition Temp.</b>	N/A
<b>Flash Point °F</b>	114.8 °F
<b>Flash Point °C</b>	46 °C

Method: closed cup  
Method: closed cup

**Explosion Limits** N/A

**Flammability** N/A

<b>Autoignition Temp</b>	N/A
<b>Refractive Index</b>	1.532
<b>Solubility</b>	N/A

N/A = not available

### Section 10 - Stability and Reactivity

#### Stability

**Stable**  
Stable.

#### Conditions to Avoid

Heat

#### Materials to Avoid

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

#### Hazardous Decomposition Products

##### Hazardous Decomposition Products

Carbon monoxide, carbon dioxide, and nitrogen oxides, Hydrogen cyanide, Sulfur oxides

#### Stabilizers Present

Inhibited with 100 ppm BHT.

#### Hazardous Polymerization

##### Hazardous Polymerization

Will not occur.

### Section 11 - Toxicological Information

#### Route of Exposure

##### Skin Contact

Vesicant. Causes blisters on contact with skin. Causes burns.

##### Skin Absorption

Toxic if absorbed through skin.

##### Eye Contact

Causes burns. Lachrymator.

##### Inhalation

May be harmful if inhaled. Material is extremely destructive to the tissue of the mucous membranes and upper respiratory tract.

##### Ingestion

Toxic if swallowed.

#### Sensitization

##### Sensitization

Sensitizer.

##### Respiratory

May cause allergic respiratory reaction.

##### Skin

May cause allergic skin reaction.

#### Signs and Symptoms of Exposure

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin. Inhalation may result in spasm, inflammation and edema of the larynx and bronchi, chemical pneumonitis, and pulmonary edema. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting.

**RTECS Number:** NX8225000

#### Toxicity Data

Oral - Rat: 112 mg/kg (LD50)

Remarks: Lungs, Thorax, or Respiration: Other changes.

Gastrointestinal: Other changes.

Subcutaneous - Rat: 92 MG/KG (LD50)

Remarks: Behavioral:Coma,  
Skin and Appendages:Skin: After systemic exposure: Dermatitis, other

Oral - Mouse: 308 mg/kg (LD50)

Subcutaneous - Mouse: 80 MG/KG (LD50)

Remarks: Behavioral:Convulsions or effect on seizure threshold.

Skin - Rabbit: 88 mg/kg (LD50)

#### Irritation Data

Eyes - Rabbit: 2 mg

#### Chronic Exposure - Carcinogen

Result: This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

Rat - Oral: 12875 MG/KG 2Y 1

Result: Tumorigenic:Neoplastic by RTECS criteria. Kidney, Ureter, Bladder:Tumors.

Mouse - Skin: 12 GM/KG 12W 1

Result: Tumorigenic:Equivocal tumorigenic agent by RTECS criteria.Tumorigenic:Increased incidence of tumors in susceptible strains. Tumorigenic:Facilitates action of known carcinogens.

#### IARC Carcinogen List

Rating

Group 3

#### NTP Carcinogen List

Rating

Clear evidence.

No evidence.

Species

Rat

Mouse

Route

Gavage

Gavage

#### Chronic Exposure - Teratogen

Species

Dose

Route of Application

Exposure Time

Rat

100 MG/KG

Subcutaneous

(8-9D PREG)

Result:Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

#### Chronic Exposure - Mutagen

Species

Dose

Cell Type

Mutation test

Mouse

400 UG/L

lymphocyte

Mutation in mammalian somatic cells.

Hamster

5 NMOL/L

fibroblast

Morphological transformation.

Hamster

4 MG/L

fibroblast

Cytogenetic analysis

Hamster

5 MG/L

ovary

Cytogenetic analysis

Hamster

160 UG/L

ovary

Sister chromatid exchange

Mammal

800 UG/L

Skin

Other mutation test systems

#### Chronic Exposure - Reproductive Hazard

Species

Dose

Route of Application

Exposure Time

Rat

200 MG/KG

Subcutaneous

(8-9D PREG)

Result: Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants).

### Section 12 - Ecological Information

N/A

### 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.

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Page 5

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### Section 14 - Transport Information

#### DOT

**Proper Shipping Name:** Allyl isothiocyanate, stabilized

**UN#:** 1545

**Class:** 6.1

**Packing Group:** Packing Group II

**Hazard Label:** Toxic substances.

**Hazard Label:** Flammable liquid

**PIH:** Not PIH

#### IATA

**Proper Shipping Name:** Allyl isothiocyanate, stabilized

**IATA UN Number:** 1545

**Hazard Class:** 6.1

**Packing Group:** II

**Not Allowed - Aircraft:** Cargo aircraft only. Not permitted on passenger aircraft.

### Section 15 - Regulatory Information

#### EU Additional Classification

**Symbol of Danger:** T

**Indication of Danger**

Toxic.

**Risk Statements** R: 10 24/25 34 42/43

Flammable. Toxic in contact with skin and if swallowed. Causes burns. May cause sensitization by inhalation and skin contact.

**Safety Statements** S: 23 26 36/37/39 45

Do not breathe vapor. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves, and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

#### US Classification and Label Text

**Indication of Danger**

Combustible (USA) Flammable (EU), Toxic.

**Risk Statements**

Toxic in contact with skin and if swallowed. Causes burns. May cause sensitization by inhalation and skin contact.

**Safety Statements**

Do not breathe vapor. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves, and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

**US Statements**

Vesicant. Lachrymator.

#### United States Regulatory Information

**SARA Listed:** No

**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:** Yes

**NDSL:** No

### Section 16 - Other Information

#### Disclaimer

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

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Page 6

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**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. SigmaAldrich 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. Copyright 2009 Sigma-Aldrich Co. License granted to make unlimited paper copies for internal use only.