

## SECTION 1: CHEMICAL PRODUCT and COMPANY IDENTIFICATION

Product Name: Allyl isothiocyanate

Product Code: A14740

Supplier: Pfaltz & Bauer, Inc.  
172 E. Aurora Street  
Waterbury, CT 06708 USA

Phone: 203-574-0075

FAX: 203-574-3181

Emergency Phone: INFOTRAC, US: 1-800-535-5053  
INFOTRAC, INTERNATIONAL: +1-352-323-3500

## SECTION 2: HAZARDS IDENTIFICATION

Statement of Hazard: Environmentally hazardous, Flammable liquid, Irritant, Respiratory sensitizer, Toxic

Acute Health Hazard: Irritant to eyes, skin, mucous membranes and respiratory system. May be harmful by ingestion, fatal by skin absorption and toxic by inhalation.

Chronic Health Hazard: Not Available

HMIS Rating: H: 3 F: 2 P: 0

NFPA Rating: H: 3 F: 2 R: 0

To the best of our knowledge, the toxicological properties of this chemical have not been thoroughly investigated. Use appropriate procedures and precautions to prevent or minimize exposure.

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS):

GHS Classification in accordance with Regulation (EC) No 1272/2008:

Acute toxicity, dermal (Category 1), H310  
Acute toxicity, inhalation (Category 3), H331  
Acute toxicity, oral (Category 4), H302  
Flammable liquids (Category 3), H226  
Hazardous to the aquatic environment, chronic toxicity (Category 1), H410  
Sensitization, respiratory (Category 1), H334  
Serious eye damage/eye irritation (Category 2A), H319  
Skin corrosion/irritation (Category 2), H315

Pictogram:



Signal Word:

Danger

Hazard Statement(s):

H226 Flammable liquid and vapor.  
H302 Harmful if swallowed.  
H310 Fatal in contact with skin.  
H315 Causes skin irritation.  
H319 Causes serious eye irritation.  
H331 Toxic if inhaled.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
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.  
P260 Do not breathe dust/fume/gas/mist/vapors/spray.  
P262 Do not get in eyes, on skin, or on clothing.  
P271 Use only outdoors or in a well-ventilated area.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P285 In case of inadequate ventilation wear respiratory protection.  
P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.  
P302+P352 IF ON SKIN: wash with plenty of soap and water.  
P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.  
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.

### **SECTION 3: COMPOSITION/INFORMATION on INGREDIENTS**

Chemical Name:

Allyl isothiocyanate

Synonyms:

Allyl mustard oil; 2-Propenyl isothiocyanate; Isothiocyanic acid allyl ester; AITC; Oil of mustard

CAS Number:

57-06-7

MDL Number: MFCD00004822  
EINECS Number: 200-309-2  
Beilstein Registry Number: 773748  
Molecular Formula: C<sub>4</sub>H<sub>5</sub>NS  
Molecular Weight: 99.15  
Content: As specified in product name.

#### **SECTION 4: FIRST AID MEASURES**

Eye Contact: Flush eyes with large amounts of water for fifteen minutes. Separate eyelids with fingers. If irritation persists, seek medical attention.

Skin Contact: Wash skin with soap and water. If irritation persists, seek medical attention.

Ingestion: Do not induce vomiting. Seek medical attention.

Inhalation: Move to a fresh air environment. Contact a physician if breathing becomes difficult.

#### **SECTION 5: FIRE FIGHTING MEASURES**

Flash Point (°C): 46

Explosion Limits: Not Available

Auto Ignition Temperature (°C): Not Available

Extinguishing Media: Carbon dioxide, dry chemical powder, alcohol-resistant foam, or water spray

Protective Equipment: Wear self-contained respirator and fully protective impervious suit.

Specific Hazards: May emit hazardous fumes under fire conditions.

#### **SECTION 6: ACCIDENTAL RELEASE MEASURES**

Personal Protection: Wear a self-contained breathing apparatus, rubber boots and gloves, and disposable coveralls. Dispose of coveralls after use. Remove from ignition sources if safe to do so. Follow emergency response plan and contact proper authorities if needed. Keep unprotected persons away.

Environmental Protection: Keep spills out of sewers and bodies of water. Dike and contain the spill with inert material. Absorb on sand, vermiculite or diatomite. Transfer material to a container for disposal or recovery. Ventilate area and wash spill site after material pickup is complete.

## **SECTION 7: HANDLING and STORAGE**

Handling and Storage: Avoid breathing dust, vapor, mist or gas. Avoid contact with skin and eyes. Avoid prolonged or repeated exposure. Use only in a chemical fume hood. Open and handle container with care. Keep ignition sources away.  
Store in a tightly closed container in a dry, well-ventilated place.

Sensitivities: Moisture

Storage Temperature (°C): 2 to 8

## **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

Engineering Controls: Use product in a well ventilated area or under a fume hood. Use proper lab equipment while handling this product. Keep away from incompatible materials for possible risk of hazardous reaction.

Eye Protection: Wear appropriate protective eyeglass or chemical safety goggles. Make sure that there is an eyewash station in your vicinity.

Skin Protection: Wear impervious gloves and protective clothing.

Respiratory Protection: Use a NIOSH approved respirator when exposure limits are exceeded or if irritation or other symptoms are experienced.

<u>Exposure Limits:</u>	<u>Country</u>	<u>Source</u>	<u>Type</u>	<u>Value</u>
	USA	ACGIH	TWA	Not Available
	USA	OSHA	STEL	Not Available
	USA	OSHA	PEL	Not Available

## **SECTION 9: PHYSICAL and CHEMICAL PROPERTIES**

Appearance: Light yellow liquid

Odor: Not Available

Odor Threshold: Not Available

Flash Point (°C): 46

Auto Ignition Temperature (°C): Not Available

<u>UEL % by Volume:</u>	Not Available
<u>LEL % by Volume:</u>	Not Available
<u>Melting Point (°C):</u>	-80
<u>Boiling Point (°C):</u>	150
<u>Evaporation Rate:</u>	Not Available
<u>pH Value:</u>	Not Available
<u>Density (g/cm<sup>3</sup>):</u>	1.013
<u>Refractive Index (n<sup>20</sup><sub>D</sub>):</u>	1.529
<u>Viscosity:</u>	Not Available
<u>Solubility in Water:</u>	Slightly soluble, 2 g/lL at 20 C
<u>Solubility in Other:</u>	Not Available
<u>Vapor Pressure (mmHg):</u>	Not Available
<u>Vapor Density (Air=1):</u>	Not Available

## **SECTION 10: STABILITY and REACTIVITY**

<u>Stability:</u>	Stable under normal temperatures and pressures.
<u>Incompatibility:</u>	Water, Alcohols, Strong bases, Amines, Acids, Strong oxidizing agents
<u>Reactivity:</u>	Product may react with incompatible materials to release other hazardous substances.
<u>Conditions to Avoid:</u>	Heat, flame, sparks, other ignition sources.
<u>Hazardous Decomposition Products:</u>	Carbon oxides, Nitrogen oxides, Sulfur oxides

## **SECTION 11: TOXICOLOGICAL INFORMATION**

<u>RTECS Reference:</u>	NX8225000
<u>Target Organs:</u>	Not Available

Toxicity Data: Oral Rat LD<sub>50</sub> mg/kg: 112.00  
Dermal Rabbit LD<sub>50</sub> mg/kg: 88.00

Carcinogenicity: National Toxicology Program (NTP) listed:  
Not Available  
International Agency for Research on Cancer (IARC) listed: Not Available

Potential Symptoms: Not Available

## **SECTION 12: ECOLOGICAL INFORMATION**

Toxicity: Flathead minnow LC<sub>50</sub>: 85.60 mg/l - 85.60 hrs.

## **SECTION 13: DISPOSAL CONSIDERATIONS**

Contact a licensed professional waste disposal service. Dispose in a manner consistent with federal, state and local environmental regulations.

## **SECTION 14: TRANSPORT INFORMATION**

DOT Shipping Name: Allyl Isothiocyanate, Stabilized

DOT UN Number: UN1545

DOT Hazard Class: Class 6.1, 3

DOT Packing Group: PGII

IMDG Shipping Name: Allyl Isothiocyanate, Stabilized

IMDG UN Number: UN1545

IMDG Hazard Class: Class 6.1, 3

IMDG Packing Group: PG II

Marine Pollutant: No

IATA Shipping Name: Allyl Isothiocyanate, Stabilized

IATA UN Number: UN1545

IATA Hazard Class: Class 6.1, 3

## **SECTION 15: REGULATORY INFORMATION**

### United States

Toxic Substance Control Act (TSCA) listed: Yes

Superfund Amendments and Reauthorization Act (SARA 302) listed: No

Superfund Amendments and Reauthorization Act (SARA 311/312) listed: No

Superfund Amendments and Reauthorization Act (SARA 313) listed: No

### European Union

European Inventory of Existing Chemical Substances (EINECS): 200-309-2

GHS Classification in accordance with Regulation (EC) No 1272/2008: Yes

### Canada

Canadian Domestic Substances List (DSL) listed: Yes

Canadian Non-Domestic Substances List (NDSL) listed: No

## **SECTION 16: OTHER INFORMATION**

Date Prepared: 1/4/2023

The information above is presented in good faith. It is believed to be accurate and represents the best information currently available to us. However, we make no warranty with respect to such information and we assume no liability resulting from its use. The user should consider this information as a supplement to other information that may be available and make independent judgement to ensure proper use to protect the health and safety of employees and the environment. Pfaltz and Bauer shall not be held liable for any damage resulting from handling or from contact with the above product.