

Material Safety Data Sheet

Version 4.3

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1. PRODUCT AND COMPANY IDENTIFICATION

Product name : Allyl isothiocyanate

Product Number : 377430

Brand : Aldrich

Supplier : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

Emergency Phone # (For both supplier and manufacturer) : (314) 776-6555

Preparation Information : Sigma-Aldrich Corporation
Product Safety - Americas Region
1-800-521-8956

2. HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards

Combustible Liquid, Toxic by ingestion, Highly toxic by skin absorption, Skin and respiratory sensitizer, Irritant

Target Organs

Eyes, Skin

Other hazards which do not result in classification

Vesicant., Lachrymator.

GHS Classification

Flammable liquids (Category 3)

Acute toxicity, Oral (Category 3)

Acute toxicity, Inhalation (Category 3)

Acute toxicity, Dermal (Category 2)

Skin irritation (Category 2)

Eye irritation (Category 2A)

Respiratory sensitization (Category 1)

Skin sensitization (Category 1)

Acute aquatic toxicity (Category 1)

Chronic aquatic toxicity (Category 1)

GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H226

Flammable liquid and vapour.

H301 + H331

Toxic if swallowed or if inhaled

H310

Fatal in contact with skin.

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.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing.
P302 + P350 IF ON SKIN: Gently wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310 Immediately call a POISON CENTER or doctor/ physician.
P501 Dispose of contents/ container to an approved waste disposal plant.

HMIS Classification

Health hazard: 3
Chronic Health Hazard: *
Flammability: 2
Physical hazards: 0

NFPA Rating

Health hazard: 3
Fire: 2
Reactivity Hazard: 0

Potential Health Effects

Inhalation May be harmful if inhaled. Causes respiratory tract irritation.
Skin May be fatal if absorbed through skin. Causes skin irritation.
Eyes Causes eye irritation.
Ingestion Toxic if swallowed.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Synonyms : Oil of mustard
AITC

Formula : C₄H₅NS
Molecular Weight : 99.15 g/mol

Component		Concentration
Allyl isothiocyanate		
CAS-No.	57-06-7	-
EC-No.	200-309-2	

4. 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. 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.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

5. FIREFIGHTING MEASURES

Conditions of flammability

Flammable in the presence of a source of ignition when the temperature is above the flash point. Keep away from heat/sparks/open flame/hot surface. No smoking.

Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

Hazardous combustion products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO_x), Sulphur oxides

Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions

Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

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.

Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

7. HANDLING AND STORAGE

Precautions for safe handling

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

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

Conditions for safe storage

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

Handle and open container with care.

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Components with workplace control parameters

Components	CAS-No.	Value	Control parameters	Basis
Allyl isothiocyanate	57-06-7	STEL	1 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
Remarks	Skin Dermal Sensitization Notation			

Personal protective equipment

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).

Hand 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.

Eye 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 and 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.

Hygiene measures

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

9. PHYSICAL AND CHEMICAL PROPERTIES**Appearance**

Form	clear, liquid
Colour	light yellow

Safety data

pH	no data available
Melting point/freezing point	Melting point/range: -80 °C (-112 °F) - lit.
Boiling point	150 °C (302 °F) - lit.
Flash point	46 °C (115 °F) - closed cup
Ignition temperature	no data available
Autoignition temperature	no data available
Lower explosion limit	no data available
Upper explosion limit	no data available
Vapour pressure	4.9 hPa (3.7 mmHg) at 30 °C (86 °F) 4.930 hPa (3.698 mmHg) at 20 °C (68 °F)
Density	1.013 g/cm ³ at 25 °C (77 °F)
Water solubility	2 g/l at 20 °C (68 °F)
Partition coefficient: n-octanol/water	no data available
Relative vapour density	3.4 - (Air = 1.0)
Odour	pungent
Odour Threshold	no data available
Evaporation rate	no data available

10. STABILITY AND REACTIVITY**Chemical stability**

Stable under recommended storage conditions.

Possibility of hazardous reactions

no data available

Conditions to avoid

Heat, flames and sparks.

Materials to avoid

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

Hazardous decomposition products

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

Other decomposition products - no data available

11. TOXICOLOGICAL INFORMATION**Acute toxicity****Oral LD50**

LD50 Oral - rat - 112 mg/kg

Inhalation LC50

Irritating to respiratory system.

Dermal LD50

LD50 Dermal - rabbit - 88 mg/kg

Other information on acute toxicity

no data available

Skin corrosion/irritation

no data available

Serious eye damage/eye irritation

no data available

Respiratory or skin sensitization

May cause allergic respiratory and skin reactions

Germ cell mutagenicity

no data available

Carcinogenicity

Carcinogenicity - rat - Oral

Tumorigenic:Neoplastic by RTECS criteria. Kidney, Ureter, Bladder:Kidney tumors.

IARC: 3 - Group 3: Not classifiable as to its carcinogenicity to humans (Allyl isothiocyanate)

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

Teratogenicity

Developmental Toxicity - rat - Subcutaneous

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

no data available

Specific target organ toxicity - single exposure (Globally Harmonized System)

no data available

Specific target organ toxicity - repeated exposure (Globally Harmonized System)

no data available

Aspiration hazard

no data available

Potential health effects

Inhalation	May be harmful if inhaled. Causes respiratory tract irritation.
Ingestion	Toxic if swallowed.
Skin	May be fatal if absorbed through skin. Causes skin irritation.
Eyes	Causes eye irritation.

Signs and Symptoms of Exposure

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

Synergistic effects

no data available

Additional Information

RTECS: Not available

12. ECOLOGICAL INFORMATION

Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 85.6 µg/l - 96.0 h
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Persistence and degradability

Biodegradability	aerobic
	Result: 0 % - Not readily biodegradable.

Bioaccumulative potential

no data available

Mobility in soil

no data available

PBT and vPvB assessment

no data available

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.

no data available

13. DISPOSAL CONSIDERATIONS

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

UN number: 1545 Class: 6.1 (3) Packing group: II
Proper shipping name: Allyl isothiocyanate, stabilized
Reportable Quantity (RQ):
Marine pollutant: No
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: No

IATA

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

15. REGULATORY INFORMATION

OSHA Hazards

Combustible Liquid, Toxic by ingestion, Highly toxic by skin absorption, Skin and respiratory sensitizer, Irritant

SARA 302 Components

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

SARA 313 Components

SARA 313: 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

	CAS-No.	Revision Date
Allyl isothiocyanate	57-06-7	1993-04-24

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Allyl isothiocyanate	57-06-7	1993-04-24

New Jersey Right To Know Components

	CAS-No.	Revision Date
Allyl isothiocyanate	57-06-7	1993-04-24

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.

16. OTHER INFORMATION

Further information

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