

# Material Safety Data Sheet

## Allyl isothiocyanate, 94%

ACC# 52810

### Section 1 - Chemical Product and Company Identification

**MSDS Name:** Allyl isothiocyanate, 94%

**Catalog Numbers:** AC102950050, AC102951000, AC102955000

**Synonyms:** Isothiocyanic acid, allyl ester; Allyl isorhodanide; Allyl isosulfocyanate; Allyl isosulphocyanate; Allyl mustard oil; Allyl thiocarbonimide; Artificial mustard oil; Artificial oil of mustard; Carbospol; Isothiocyanate d'allyle; 3-Isothiocyanato-1-propene; Mustard oil; Propene, 3-isothiocyanato-; 2-Propenyl isothiocyanate

**Company Identification:**

Acros Organics N.V.  
One Reagent Lane  
Fair Lawn, NJ 07410

**For information in North America, call:** 800-ACROS-01

**For emergencies in the US, call CHEMTREC:** 800-424-9300

### Section 2 - Composition, Information on Ingredients

CAS#	Chemical Name	Percent	EINECS/ELINCS
57-06-7	Allyl isothiocyanate	94	200-309-2

### Section 3 - Hazards Identification

#### EMERGENCY OVERVIEW

Appearance: clear colorless to pale yellow liquid. Flash Point: 46 deg C.

**Warning!** May be fatal if absorbed through the skin. **Flammable liquid and vapor.** Vesicant (agent that induces blistering). Harmful if swallowed. Causes eye, skin, and respiratory tract irritation. May cause allergic respiratory and skin reaction. This substance has caused adverse reproductive and fetal effects in animals. Moisture sensitive.

**Target Organs:** Respiratory system, eyes, skin.

#### Potential Health Effects

**Eye:** Causes eye irritation. Lachrymator (substance which increases the flow of tears).

**Skin:** May be fatal if absorbed through the skin. May cause skin sensitization, an allergic reaction, which becomes evident upon re-exposure to this material. This material is a vesicant, that is, it will induce blistering. Causes skin irritation and possible burns. Prolonged exposure may produce blisters.

**Ingestion:** Harmful if swallowed. May cause gastrointestinal irritation with nausea, vomiting and diarrhea. Effects may be delayed.

**Inhalation:** Causes respiratory tract irritation. May cause asthmatic attacks due to allergic sensitization of the respiratory tract. Vapors may cause dizziness or suffocation.

**Chronic:** May cause reproductive and fetal effects. Laboratory experiments have resulted in mutagenic effects.

### Section 4 - First Aid Measures

**Eyes:** Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid. Do NOT allow victim to rub eyes or keep eyes closed.

**Skin:** Get medical aid immediately. Immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse.

**Ingestion:** Do not induce vomiting. If victim is conscious and alert, give 2-4 cupfuls of milk or water. Never give anything by mouth to an unconscious person. Get medical aid immediately.

**Inhalation:** Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.

**Notes to Physician:** Treat symptomatically and supportively. Effects may be delayed.

### Section 5 - Fire Fighting Measures

**General Information:** As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Will burn if involved in a fire. Use water spray to keep fire-exposed containers cool. Containers may explode in the heat of a fire. Flammable liquid and vapor.

**Extinguishing Media:** For small fires, use dry chemical, carbon dioxide, water spray or alcohol-resistant foam. For large fires, use water spray, fog, or alcohol-resistant foam. Use water spray to cool fire-exposed containers. Water may be ineffective. Do NOT get water inside containers. Do NOT use straight streams of water.

**Flash Point:** 46 deg C ( 114.80 deg F)

**Autoignition Temperature:** Not applicable.

**Explosion Limits, Lower:** Not available.

**Upper:** Not available.

**NFPA Rating:** (estimated) Health: 3; Flammability: 2; Instability: 0

### Section 6 - Accidental Release Measures

**General Information:** Use proper personal protective equipment as indicated in Section 8.

**Spills/Leaks:** Absorb spill with inert material (e.g. vermiculite, sand or earth), then place in suitable container. Clean up spills immediately, observing precautions in the Protective Equipment section. Remove all sources of ignition. Use a spark-proof tool. Provide ventilation. Do not get water inside containers. A vapor suppressing foam may be used to reduce vapors.

## Section 7 - Handling and Storage

**Handling:** Remove contaminated clothing and wash before reuse. Ground and bond containers when transferring material. Use spark-proof tools and explosion proof equipment. Contents may develop pressure upon prolonged storage. Do not breathe dust, vapor, mist, or gas. Do not get in eyes, on skin, or on clothing. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep container tightly closed. Keep away from heat, sparks and flame. Do not ingest or inhale. Do not allow contact with water. Use only in a chemical fume hood. Do not pressurize, cut, weld, braze, solder, drill, grind, or expose empty containers to heat, sparks or open flames. Keep from contact with moist air and steam.

**Storage:** Keep away from heat, sparks, and flame. Keep away from sources of ignition. Keep refrigerated. (Store below 4°C/39°F.) Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances. Flammables-area. Store protected from moisture.

## Section 8 - Exposure Controls, Personal Protection

**Engineering Controls:** Use explosion-proof ventilation equipment. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use only under a chemical fume hood.

### Exposure Limits

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
Allyl isothiocyanate	none listed	none listed	none listed

**OSHA Vacated PELs:** Allyl isothiocyanate: No OSHA Vacated PELs are listed for this chemical.

### Personal Protective Equipment

**Eyes:** Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

**Skin:** Wear appropriate protective gloves to prevent skin exposure.

**Clothing:** Wear appropriate protective clothing to prevent skin exposure.

**Respirators:** A respiratory protection program that meets OSHA's 29 CFR 1910.134 and ANSI Z88.2 requirements or European Standard EN 149 must be followed whenever workplace conditions warrant respirator use.

## Section 9 - Physical and Chemical Properties

**Physical State:** Liquid

**Appearance:** clear colorless to pale yellow

**Odor:** mustard-like - pungent odor

**pH:** Not available.

**Vapor Pressure:** 4 mm Hg @ 20 C

**Vapor Density:** 3.41

**Evaporation Rate:** Not available.

**Viscosity:** Not available.

**Boiling Point:** 150 deg C @ 760.00mm Hg

**Freezing/Melting Point:** -80 deg C

**Decomposition Temperature:** > 250 deg C

**Solubility:** Slightly soluble.

**Specific Gravity/Density:** 1.0150g/cm<sup>3</sup>

**Molecular Formula:** H<sub>2</sub>C=CHCH<sub>2</sub>NCS

**Molecular Weight:** 99.15

## Section 10 - Stability and Reactivity

**Chemical Stability:** Stable under normal temperatures and pressures. Moisture sensitive.

**Conditions to Avoid:** Incompatible materials, ignition sources, moisture, excess heat.

**Incompatibilities with Other Materials:** Moisture, amines, acids, strong oxidizing agents, strong bases, alcohols.

**Hazardous Decomposition Products:** Hydrogen cyanide, nitrogen oxides, carbon monoxide, oxides of sulfur, irritating and toxic fumes and gases, carbon dioxide, nitrogen.

**Hazardous Polymerization:** Will not occur.

## Section 11 - Toxicological Information

### RTECS#:

**CAS#** 57-06-7: NX8225000

### LD50/LC50:

**CAS#** 57-06-7:

Draize test, rabbit, eye: 2 mg;

Oral, mouse: LD50 = 308 mg/kg;

Oral, rat: LD50 = 112 mg/kg;

Skin, rabbit: LD50 = 88 mg/kg;

**Carcinogenicity:**

CAS# 57-06-7: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

**Epidemiology:** Oral, rat: TDLo = 12875 mg/kg/2Y-I (Tumorigenic - neoplastic by RTECS criteria - Kidney, Ureter, Bladder - tumors).; Administration onto the skin, mouse: TDLo = 12 gm/kg/12W-I (Tumorigenic - equivocal tumorigenic agent by RTECS criteria - increased incidence of tumors in susceptible strains and facilitates action of known carcinogen).;

**Teratogenicity:** Subcutaneous, rat: TDLo = 100 mg/kg (female 8-9 day(s) after conception) Effects on Embryo or Fetus - fetotoxicity (except death, e.g., stunted fetus).

**Reproductive Effects:** Subcutaneous, rat: TDLo = 200 mg/kg (female 8-9 day(s) after conception) Fertility - post-implantation mortality (e.g. dead and/or resorbed implants per total number of implants).

**Mutagenicity:** Mutation in Mammalian Somatic Cells: Mouse, Lymphocyte = 400 ug/L.; Morphological Transformation: Hamster, Fibroblast = 5 nmol/L.; Cytogenetic Analysis: Hamster, Fibroblast = 4 mg/L.; Sister Chromatid Exchange: Hamster, Ovary = 160 ug/L.

**Neurotoxicity:** No information found

**Other Studies:**

## Section 12 - Ecological Information

**Ecotoxicity:** Bacteria: Phytobacterium phosphoreum: EC50 = 0.099-0.11 mg/L; 5,15,30 min; Microtox test at 15C

Fish: Fathead Minnow: LC50 = 0.0856 mg/L; Unspecified; Flow-through at 25.1C (pH 7.8)

## Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

**RCRA P-Series:** None listed.

**RCRA U-Series:** None listed.

## Section 14 - Transport Information

	US DOT	Canada TDG
<b>Shipping Name:</b>	ALLYL ISOTHIOCYANATE, STABILIZED	ALLYL ISOTHIOCYANATE, STABILIZED
<b>Hazard Class:</b>	6.1	6.1(3)
<b>UN Number:</b>	UN1545	UN1545
<b>Packing Group:</b>	II	II

## Section 15 - Regulatory Information

### US FEDERAL

**TSCA**

CAS# 57-06-7 is listed on the TSCA inventory.

**Health & Safety Reporting List**

None of the chemicals are on the Health & Safety Reporting List.

**Chemical Test Rules**

None of the chemicals in this product are under a Chemical Test Rule.

**Section 12b**

None of the chemicals are listed under TSCA Section 12b.

**TSCA Significant New Use Rule**

None of the chemicals in this material have a SNUR under TSCA.

**CERCLA Hazardous Substances and corresponding RQs**

None of the chemicals in this material have an RQ.

**SARA Section 302 Extremely Hazardous Substances**

None of the chemicals in this product have a TPQ.

**Section 313** No chemicals are reportable under Section 313.**Clean Air Act:**

This material does not contain any hazardous air pollutants.

This material does not contain any Class 1 Ozone depleters.

This material does not contain any Class 2 Ozone depleters.

**Clean Water Act:**

None of the chemicals in this product are listed as Hazardous Substances under the CWA.

None of the chemicals in this product are listed as Priority Pollutants under the CWA.

None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

**OSHA:**

None of the chemicals in this product are considered highly hazardous by OSHA.

**STATE**

CAS# 57-06-7 can be found on the following state right to know lists: California, New Jersey, Pennsylvania, Minnesota, Massachusetts.

**California Prop 65**

California No Significant Risk Level: None of the chemicals in this product are listed.

**European/International Regulations****European Labeling in Accordance with EC Directives**

**Hazard Symbols:**

T

**Risk Phrases:**

R 10 Flammable.

R 23/24/25 Toxic by inhalation, in contact with skin and if swallowed.

R 36/37/38 Irritating to eyes, respiratory system and skin.

**Safety Phrases:**

S 16 Keep away from sources of ignition - No smoking.

S 26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S 36/37/39 Wear suitable protective clothing, gloves and eye/face protection.

S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

S 28B After contact with skin, wash immediately with plenty of water and soap.

**WGK (Water Danger/Protection)**

CAS# 57-06-7: No information available.

**Canada - DSL/NDSL**

CAS# 57-06-7 is listed on Canada's DSL List.

**Canada - WHMIS**

not available.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

**Canadian Ingredient Disclosure List**

CAS# 57-06-7 is listed on the Canadian Ingredient Disclosure List.

## Section 16 - Additional Information

**MSDS Creation Date:** 5/26/1999**Revision #3 Date:** 10/03/2005

*The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall Fisher be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if Fisher has been advised of the possibility of such damages.*