

Material Safety Data Sheet

Allyl isothiocyanate, 94%

MSDS# 52810

Section 1 - Chemical Product and Company Identification

MSDS Name: Allyl isothiocyanate, 94%

Catalog Numbers: AC102950000, 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 BVBA
Janssen Pharmaceuticaaan 3a
2440 Geel, Belgium

Company Identification: (USA) Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

For information in the US, call: 800-ACROS-01

For information in Europe, call: +32 14 57 52 11

Emergency Number, Europe: +32 14 57 52 99

Emergency Number US: 201-796-7100

CHEMTREC Phone Number, US: 800-424-9300

CHEMTREC Phone Number, Europe: 703-527-3887

Section 2 - Composition, Information on Ingredients

CAS#: 57-06-7

Chemical Name: Allyl isothiocyanate

%: 94

EINECS#: 200-309-2

Hazard Symbols: T



Risk Phrases: 10 23/24/25 36/37/38

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

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

Autoignition Temperature: Not applicable.

Flash Point: 46 deg C (114.80 deg F)

Explosion Limits: Lower: Not available

Explosion Limits: Upper: Not available

NFPA Rating: 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, mist, or vapor. 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 sources of ignition. Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances. Refrigerator/flammables. Store protected from moisture.

Section 8 - Exposure Controls, Personal Protection

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

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

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

Color: 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 (302.00°F)

Freezing/Melting Point: -80 deg C (-112.00°F)

Decomposition Temperature:

Solubility in water: Slightly soluble

Specific Gravity/Density: 1.0150g/cm3

Molecular Formula: H2C=CHCH2NCS

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: Strong oxidizing agents, acids, strong bases, alcohols, amines, moisture.
- Hazardous Decomposition Products: Hydrogen cyanide, nitrogen oxides, carbon monoxide, oxides of sulfur, carbon dioxide, nitrogen gas.
- Hazardous Polymerization: Will not occur.

Section 11 - Toxicological Information

- RTECS#: CAS# 57-06-7: NX8225000
- RTECS: CAS# 57-06-7: Draize test, rabbit, eye: 2 mg;
- LD50/LC50: Oral, mouse: LD50 = 308 mg/kg;
- Oral, rat: LD50 = 112 mg/kg;
- Skin, rabbit: LD50 = 88 mg/kg;
- Carcinogenicity: Allyl isothiocyanate - IARC: Group 3 (not classifiable)
- Other: See actual entry in RTECS for complete information.

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

Dispose of in a manner consistent with federal, state, and local regulations.

Section 14 - Transport Information

US DOT

Shipping Name: ALLYL ISOTHIOCYANATE, STABILIZED

Hazard Class: 6.1

UN Number: UN1545

Packing Group: II

Canada TDG

Shipping Name: Not available

Hazard Class:

UN Number:

Packing Group:

Section 15 - Regulatory Information

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

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).

WGK (Water Danger/Protection)

CAS# 57-06-7: Not available

Canada

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

Canadian WHMIS Classifications: 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.

CAS# 57-06-7 is listed on Canada's Ingredient Disclosure List

US Federal

TSCA

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

Section 16 - Other Information

MSDS Creation Date: 5/26/1999

Revision #5 Date 7/20/2009

REVIEWED

DATE: April 13/2012

Butterford

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 the company 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 the company has been advised of the possibility of such damages.
