

Section 1 - Product and Company Information

Product Name ALLYL ISO-THIOCYANATE STABILIZED, PESTA&
Product Number 36682
Brand FLUKA
Company Sigma-Aldrich Canada, Ltd
Address 2149 Winston Park Drive
Oakville ON L6H 6J8 CA
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Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313	
ALLYL ISOTHIOCYANATE, STABILIZED	57-06-7	No	
WITH BHT			
Ingredient Name	CAS #	Percent	SARA 313
Stabilized with:	None		
BUTYLATED HYDROXYTOLUENE	128-37-0	0.1	No

Formula C4H5NS
Synonyms Allyl isorhodanide * Allyl isosulfocyanate * Allyl isosulphocyanate * Allyl isothiocyanate * Allyl isothioxyanat (Czech) * Allyl mustard oil * Allylsevenol * Allylisenfoel (German) * Allyl sevenolum * Allyl thiocarbonyl * Artificial mustard oil * Artificial oil of mustard * Carbospol * FEMA No. 2034 * Isothiocyanate d'allyle (French) * 3-Isothiocyanato-1-propene * Mustard oil * NCI-C50464 * Oil of mustard, artificial * Oil of mustard BPC 1949 * Oleum sinapis volatile * Propene, 3-isothiocyanato- * 2-Propenyl isothiocyanate * Redskin * Senf oel (German) * Synthetic mustard oil * Volatile oil of mustard

RTECS Number: NX8225000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Combustible (USA) Flammable (EU). Toxic. Dangerous for the environment.
Toxic in contact with skin and if swallowed. Irritating to eyes, respiratory system and skin. May cause sensitization by inhalation and skin contact. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.
Vesicant. Lachrymator.

HMIS 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 immediately.

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.

EYES 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

FLAMMABLE HAZARDS

Flammable Hazards: Yes

EXPLOSION HAZARDS

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

FLASH POINT

114.8 °F 46 °C Method: closed cup

AUTOIGNITION TEMP

N/A

FLAMMABILITY

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 ineffective. 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

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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 outdoors. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Do not breathe vapor. Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep container closed. Keep away from heat, sparks, and open flame.

SPECIAL REQUIREMENTS

May develop pressure. Open carefully.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Safety shower and eye bath. Use nonsparking tools. 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 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. Hand: Compatible chemical-resistant gloves. Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash thoroughly after handling. Remove and wash contaminated clothing promptly.

Section 9 - Physical/Chemical Properties

Appearance Physical State: Liquid
Color: Faintly yellow-green
Form: clear liquid

Property Value At Temperature or Pressure

Molecular Weight 99.16 AMU

pH N/A

BP/BP Range 151.0 - 153.0 °C

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MP/MP Range - 80.0 °C

Freezing Point N/A

Vapor Pressure N/A

Vapor Density N/A

Saturated Vapor Conc. N/A

SG/Density 1.02 g/cm3

Bulk Density N/A

Odor Threshold N/A

Volatile% N/A

VOC Content N/A

Water Content N/A

Solvent Content N/A

Evaporation Rate N/A

Viscosity N/A

Surface Tension N/A

Partition Coefficient Log Kow: 2.092

Decomposition Temp. N/A

Flash Point 114.8 °F 46 °C Method: closed cup

Explosion Limits N/A

Flammability N/A

Autoignition Temp N/A

Refractive Index 1.532

Optical Rotation N/A

Miscellaneous Data N/A

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

SENSITIZATION

Sensitization: Sensitizer.
Respiratory: May cause allergic respiratory reaction.
Skin: May cause allergic skin reaction.

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TOXICITY DATA

Oral

Rat

112 mg/kg

LD50

Skin

Rabbit

88 mg/kg

LD50

Oral

Rat

112 mg/kg

LD50

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

Subcutaneous

Rat

92 MG/KG

LD50

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

Oral

Mouse

308 mg/kg

LD50

Subcutaneous

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.

Species: Rat

Route of Application: Oral

Dose: 12875 MG/KG

Exposure Time: 2Y

Frequency: 1

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

Species: Mouse

Route of Application: Skin

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Dose: 12 GM/KG

Exposure Time: 12W

Frequency: 1

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

IARC CARCINOGEN LIST

Rating: Group 3

NTP CARCINOGEN LIST

Rating: Clear evidence.

Species: Rat

Route: Gavage

CHRONIC EXPOSURE - TERATOGEN

Species: Rat

Dose: 100 MG/KG

Route of Application: Subcutaneous

Exposure Time: (8-9D PREG)

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

CHRONIC EXPOSURE - MUTAGEN

Species: Mouse

Dose: 400 UG/L

Cell Type: lymphocyte

Mutation test: Mutation in mammalian somatic cells.

Species: Hamster

Dose: 5 NMOL/L

Cell Type: fibroblast

Mutation test: Morphological transformation.

Species: Hamster

Dose: 4 MG/L

Cell Type: fibroblast

Mutation test: Cytogenetic analysis

Species: Hamster

Dose: 5 MG/L

Cell Type: ovary

Mutation test: Cytogenetic analysis

Species: Hamster

Dose: 160 UG/L

Cell Type: ovary

Mutation test: Sister chromatid exchange

Species: Mammal

Route: Skin

Dose: 800 UG/L

Mutation test: Other mutation test systems

CHRONIC EXPOSURE - REPRODUCTIVE HAZARD

Species: Rat

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Dose: 200 MG/KG

Route of Application: Subcutaneous

Exposure Time: (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

ACCUMULATION

Bioaccumulation Potential: Indication of bioaccumulation.

ACUTE ECOTOXICITY TESTS

Test Type: LC50 Fish

Species: Brachydanio rerio

Time: 96 h

Value: 0.1 mg/l

ELIMINATION

Elimination: 0 %

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION

Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Observe all federal, state, and local environmental regulations.

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-N

Indication of Danger: Toxic. Dangerous for the environment.

R: 10-24/25-36/37/38-42/43-50/53

Risk Statements: Flammable. Toxic in contact with skin and if swallowed. Irritating to eyes, respiratory system and skin. May cause sensitization by inhalation and skin contact. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Safety Statements: Do not breathe vapor. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). This material and its container must be disposed of as hazardous waste. Avoid release to the environment. Refer to special instructions/safety data sheets. 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.

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. Sigma-Aldrich 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.

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