

**SECTION 1: Identification****1.1. Identification**

Product form	: Substance
Substance name	: Allyl isothiocyanate
CAS-No.	: 57-06-7
Product code	: (US) W01333
Formula	: C4H5NS
Synonyms	: Allyl isosulfofyanate / Allyl isosulphocyanate / Allyl isothiocyanate, stabilized / Allyl mustard oil / Allyl thiocarbonimide / Artificial mustard oil / Artificial oil of mustard / FEMA No. 2034 / 3-Isothiocyanato-1-propene / Isothiocyanic acid, allyl ester / Mustard oil / NCI-C50464 / Oil of mustard, artificial / 1-Propene, 3-isothiocyanato- / Propene, 3-isothiocyanato- / 2-Propenyl isothiocyanate / Synthetic mustard oil / Volatile oil of mustard / Allylisothiocyanate / 1-Propene,3-isothiocyanato / Allyl thiocyanate / Allyl isothiocyanate as a component of food grade oil of mustard / Mustered oil / Allyl isothiocyanate, unstabilized / 3-Isothiocyanato-prop-1-ene / Mustard and oil of mustard (brown and yellow) / Oils, mustard / 3-Isothiocyanatoprop-1-ene

**1.2. Recommended use and restrictions on use**

No additional information available

**1.3. Supplier**

Synerzine  
5340 Hwy 42 S  
Ellenwood, Georgia 30294 - USA  
T 404-524-6744 - F 404-577-1651  
[info@synerzine.com](mailto:info@synerzine.com) - [www.synerzine.com](http://www.synerzine.com)

**1.4. Emergency telephone number**

Emergency number : Infotrac 1-800-535-5053 (Contract# 102471) Dial +1-352-323-3500 when outside the US

**SECTION 2: Hazard(s) identification****2.1. Classification of the substance or mixture****GHS-US classification**

Flammable liquids Category 3	H226	Flammable liquid and vapour
Acute toxicity (oral) Category 3	H301	Toxic if swallowed
Acute toxicity (dermal) Category 2	H310	Fatal in contact with skin
Acute toxicity (inhalation) Category 3	H331	Toxic if inhaled
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Respiratory sensitization, Category 1	H334	May cause an allergy or asthma symptoms or breathing difficulties if inhaled
Skin sensitization, Category 1	H317	May cause an allergic skin reaction
Hazardous to the aquatic environment - Acute Hazard Category 1	H400	Very toxic to aquatic life
Hazardous to the aquatic environment - Chronic Hazard Category 1	H410	Very toxic to aquatic life with long lasting effects
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation

Full text of H statements : see section 16

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### 2.2. GHS Label elements, including precautionary statements

#### GHS-US labeling

Hazard pictograms (GHS-US)



Signal word (GHS-US)

: Danger

Hazard statements (GHS-US)

: 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 an allergy or asthma symptoms or breathing difficulties if inhaled  
H400 - Very toxic to aquatic life  
H410 - Very toxic to aquatic life with long lasting effects

Precautionary statements (GHS-US)

: P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking, heat, hot surfaces, open flames, sparks  
P233 - Keep container tightly closed.  
P240 - Ground/Bond container and receiving equipment  
P241 - Use explosion-proof electrical, ventilating, lighting equipment  
P242 - Use only non-sparking tools.  
P243 - Take precautionary measures against static discharge.  
P261 - Avoid breathing dust, fume, gas, mist, vapors, spray.  
P262 - Do not get in eyes, on skin, or on clothing.  
P264 - Wash hands, forearms and face thoroughly after handling.  
P270 - Do not eat, drink or smoke when using this product.  
P271 - Use only outdoors or in a well-ventilated area.  
P272 - Contaminated work clothing must not be allowed out of the workplace  
P273 - Avoid release to the environment.  
P280 - Wear eye protection, face protection, protective clothing, protective gloves.  
P284 - [In case of inadequate ventilation] wear respiratory protection..  
P301+P310 - If swallowed: Immediately call a doctor, a POISON CENTER  
P302+P352 - If on skin: Wash with plenty of soap and water  
P303+P361+P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower  
P304+P340 - If inhaled: Remove person to fresh air and keep 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  
P310 - Immediately call a doctor, a POISON CENTER  
P311 - Call a doctor, a POISON CENTER  
P321 - Specific treatment (see supplemental first aid instructions on this label)  
P330 - Rinse mouth.  
P332+P313 - If skin irritation occurs: Get medical advice/attention.  
P333+P313 - If skin irritation or rash occurs: Get medical advice/attention.  
P337+P313 - If eye irritation persists: Get medical advice/attention.  
P342+P311 - If experiencing respiratory symptoms: Call a doctor, a POISON CENTER  
P361 - Take off immediately all contaminated clothing.  
P362 - Take off contaminated clothing and wash before reuse.  
P362+P364 - Take off contaminated clothing and wash it before reuse.  
P363 - Wash contaminated clothing before reuse.  
P370+P378 - In case of fire: Use alcohol resistant foam, carbon dioxide (CO2), dry sand to extinguish.  
P391 - Collect spillage.  
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.  
P403+P235 - Store in a well-ventilated place. Keep cool.  
P405 - Store locked up.  
P501 - Dispose of contents/container to an approved waste disposal plant

### 2.3. Other hazards which do not result in classification

No additional information available

### 2.4. Unknown acute toxicity (GHS US)

Not applicable

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### SECTION 3: Composition/Information on ingredients

#### 3.1. Substances

Name	Product identifier	%	GHS-US classification
Allyl isothiocyanate (Main constituent)	(CAS-No.) 57-06-7	95 - 100	Flam. Liq. 3, H226 Acute Tox. 3 (Oral), H301 Acute Tox. 2 (Dermal), H310 Acute Tox. 3 (Inhalation), H331 Skin Irrit. 2, H315 Resp. Sens. 1, H334 Skin Sens. 1, H317 Aquatic Acute 1, H400 Aquatic Chronic 1, H410 Eye Irrit. 2A, H319

Full text of hazard classes and H-statements : see section 16

#### 3.2. Mixtures

Not applicable

### SECTION 4: First-aid measures

#### 4.1. Description of first aid measures

- First-aid measures general : Call a physician immediately.
- First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. Call a doctor.
- First-aid measures after skin contact : Rinse skin with water/shower. Remove/Take off immediately all contaminated clothing. Call a physician immediately.
- First-aid measures after eye contact : Rinse eyes with water as a precaution.
- First-aid measures after ingestion : Rinse mouth. Call a physician immediately.

#### 4.2. Most important symptoms and effects (acute and delayed)

- Symptoms/effects after inhalation : May cause an allergy or asthma symptoms or breathing difficulties if inhaled.
- Symptoms/effects after skin contact : Irritation. May cause an allergic skin reaction.

#### 4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

### SECTION 5: Fire-fighting measures

#### 5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Water spray. Dry powder. Foam. Carbon dioxide.

#### 5.2. Specific hazards arising from the chemical

- Fire hazard : Flammable liquid and vapour.
- Reactivity : Flammable liquid and vapour.

#### 5.3. Special protective equipment and precautions for fire-fighters

Protection during firefighting : Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

### SECTION 6: Accidental release measures

#### 6.1. Personal precautions, protective equipment and emergency procedures

##### 6.1.1. For non-emergency personnel

Emergency procedures : No open flames, no sparks, and no smoking. Only qualified personnel equipped with suitable protective equipment may intervene. Avoid breathing dust, fume, gas, mist, spray, vapors.

##### 6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

#### 6.2. Environmental precautions

Avoid release to the environment.

#### 6.3. Methods and material for containment and cleaning up

- For containment : Collect spillage.
- Methods for cleaning up : Take up liquid spill into absorbent material. Notify authorities if product enters sewers or public waters.

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Other information : Dispose of materials or solid residues at an authorized site.

### 6.4. Reference to other sections

For further information refer to section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Precautions for safe handling : Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Ground/bond container and receiving equipment. Use only non-sparking tools. Take precautionary measures against static discharge. Flammable vapors may accumulate in the container. Use explosion-proof equipment. Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Use only outdoors or in a well-ventilated area. Avoid breathing dust, fume, gas, mist, spray, vapors.

Hygiene measures : Wash contaminated clothing before reuse. Contaminated work clothing should not be allowed out of the workplace. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Ground/bond container and receiving equipment.

Storage conditions : Store in a well-ventilated place. Keep cool. Keep container tightly closed. Store locked up.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

#### Allyl isothiocyanate (57-06-7)

AIHA	WEEL STEL (ppm)	1 ppm (15-min. STEL)
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### 8.2. Appropriate engineering controls

Appropriate engineering controls : Ensure good ventilation of the work station.

Environmental exposure controls : Avoid release to the environment.

### 8.3. Individual protection measures/Personal protective equipment

#### Hand protection:

Protective gloves

#### Eye protection:

Safety glasses

#### Skin and body protection:

Wear suitable protective clothing

#### Respiratory protection:

Wear respiratory protection.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state : Liquid

Appearance : A colorless liquid.

Color : Colorless

Odor : Pungent Irritating

Odor threshold : No data available

pH : No data available

Melting point : Not applicable

Freezing point : No data available

Boiling point : 152 °C

Flash point : 115 °F TCC

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Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: Not applicable.
Vapor pressure	: 4.93 hPa (at 20 °C)
Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Specific gravity / density	: 1.0126 g/cm <sup>3</sup> (at 20 °C)
Molecular mass	: 99.16 g/mol
Solubility	: No data available
Log Pow	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Flammable liquid and vapour.

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

### 10.4. Conditions to avoid

Avoid contact with hot surfaces. Heat. No flames, no sparks. Eliminate all sources of ignition.

### 10.5. Incompatible materials

No additional information available

### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity : Not classified

Allyl isothiocyanate (57-06-7)	
LD50 oral rat	112 mg/kg
LD50 dermal rabbit	88 mg/kg
ATE US (oral)	112 mg/kg body weight
ATE US (dermal)	50 mg/kg body weight
ATE US (gases)	700 ppmV/4h
ATE US (vapors)	3 mg/l/4h
ATE US (dust, mist)	0.5 mg/l/4h

Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: May cause an allergy or asthma symptoms or breathing difficulties if inhaled. May cause an allergic skin reaction.
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified

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Allyl isothiocyanate (57-06-7)	
IARC group	3 - Not classifiable
National Toxicology Program (NTP) Status	Evidence of Carcinogenicity
Reproductive toxicity	: Not classified
Specific target organ toxicity – single exposure	: Not classified
Specific target organ toxicity – repeated exposure	: Not classified
Aspiration hazard	: Not classified
Symptoms/effects after inhalation	: May cause an allergy or asthma symptoms or breathing difficulties if inhaled.
Symptoms/effects after skin contact	: Irritation. May cause an allergic skin reaction.

### SECTION 12: Ecological information

#### 12.1. Toxicity

Ecology - general : Very toxic to aquatic life with long lasting effects.

Allyl isothiocyanate (57-06-7)	
LC50 fish 1	0.0856 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
LC50 fish 2	0.054 - 0.109 mg/l (Exposure time: 96 h - Species: Oryzias latipes [flow-through])

#### 12.2. Persistence and degradability

No additional information available

#### 12.3. Bioaccumulative potential

No additional information available

#### 12.4. Mobility in soil

No additional information available

#### 12.5. Other adverse effects

No additional information available

### SECTION 13: Disposal considerations

#### 13.1. Disposal methods

Waste treatment methods : Dispose of contents/container in accordance with licensed collector's sorting instructions.

Additional information : Flammable vapors may accumulate in the container.

### SECTION 14: Transport information

#### Department of Transportation (DOT)

In accordance with DOT

Transport document description : UN1545 Allyl isothiocyanate, stabilized, 6.1, II  
UN-No.(DOT) : UN1545  
Proper Shipping Name (DOT) : Allyl isothiocyanate, stabilized  
Class (DOT) : 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132  
Packing group (DOT) : II - Medium Danger  
Hazard labels (DOT) : 6.1 - Poison  
3 - Flammable liquid




Dangerous for the environment : Yes

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Marine pollutant	: Yes
	
DOT Packaging Non Bulk (49 CFR 173.xxx)	: 202
DOT Packaging Bulk (49 CFR 173.xxx)	: 243
DOT Special Provisions (49 CFR 172.102)	: A3 - For combination packaging, if glass inner packaging (including ampoules) are used, they must be packed with absorbent material in tightly closed metal receptacles before packing in outer packaging. A7 - Steel packaging must be corrosion-resistant or have protection against corrosion. IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized. T7 - 4 178.274(d)(2) Normal..... 178.275(d)(3) TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: $t_r$ is the maximum mean bulk temperature during transport, $t_f$ is the temperature in degrees celsius of the liquid during filling, and $a$ is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling ( $t_f$ ) and the maximum mean bulk temperature during transportation ( $t_r$ ) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: $d_{15}$ and $d_{50}$ are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.
DOT Packaging Exceptions (49 CFR 173.xxx)	: None
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: Forbidden
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 60 L
DOT Vessel Stowage Location	: D - The material must be stowed "on deck only" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers or one passenger per each 3 m of overall vessel length, but the material is prohibited on passenger vessels in which the limiting number of passengers is exceeded.
DOT Vessel Stowage Other	: 40 - Stow "clear of living quarters"
Emergency Response Guide (ERG) Number	: 155
Other information	: No supplementary information available.

### Transportation of Dangerous Goods

#### Transport by sea

Transport document description (IMDG)	: UN 1545 ALLYL ISOTHIOCYANATE, STABILIZED, 6.1 (3), II (46°C c.c.)
UN-No. (IMDG)	: 1545
Proper Shipping Name (IMDG)	: ALLYL ISOTHIOCYANATE, STABILIZED
Class (IMDG)	: 6.1 - Toxic substances
Packing group (IMDG)	: II - substances presenting medium danger
Subsidiary risks (IMDG)	: 3 - Flammable liquids
Limited quantities (IMDG)	: 100 ml
Marine pollutant	: Yes



#### Air transport

Transport document description (IATA)	: UN 1545 Allyl isothiocyanate, stabilized, 6.1, II
UN-No. (IATA)	: 1545
Proper Shipping Name (IATA)	: Allyl isothiocyanate, stabilized

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Class (IATA)	: 6.1 - Toxic Substances
Packing group (IATA)	: II - Medium Danger
Subsidiary risks (IATA)	: 3 - Flammable liquids

### SECTION 15: Regulatory information

#### 15.1. US Federal regulations

##### Allyl isothiocyanate (57-06-7)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

#### 15.2. International regulations

##### CANADA

##### Allyl isothiocyanate (57-06-7)

Listed on the Canadian DSL (Domestic Substances List)

##### EU-Regulations

##### Allyl isothiocyanate (57-06-7)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

##### National regulations

##### Allyl isothiocyanate (57-06-7)

Listed on the AICS (Australian Inventory of Chemical Substances)  
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)  
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory  
Listed on the Japanese ISHL (Industrial Safety and Health Law)  
Listed on NZIoC (New Zealand Inventory of Chemicals)  
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)  
Listed on INSQ (Mexican National Inventory of Chemical Substances)  
Listed on the TCSI (Taiwan Chemical Substance Inventory)

#### 15.3. US State regulations

##### Allyl isothiocyanate (57-06-7)

State or local regulations	U.S. - Massachusetts - Right To Know List U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List
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### SECTION 16: Other information

Full text of H-phrases:

H226	Flammable liquid and vapour
H301	Toxic if swallowed
H310	Fatal in contact with skin
H315	Causes skin irritation
H317	May cause an allergic skin reaction
H319	Causes serious eye irritation
H331	Toxic if inhaled
H334	May cause an allergy or asthma symptoms or breathing difficulties if inhaled
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

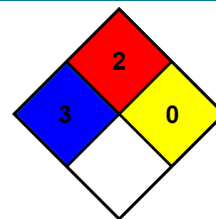


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- NFPA health hazard : 3 - Materials that, under emergency conditions, can cause serious or permanent injury.
- NFPA fire hazard : 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur.
- NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



### Hazard Rating

Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given  
\* - Chronic (long-term) health effects may result from repeated overexposure

Flammability : 2 Moderate Hazard - Materials which must be moderately heated or exposed to high ambient temperatures before ignition will occur. Includes liquids having a flash point at or above 100 F but below 200 F. (Classes II & IIIA)

Physical : 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Personal protection : C  
C - Safety glasses, Gloves, Synthetic apron

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*This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product*