SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: Allyl isothiocyanate

Product Number: W203408
Brand: Aldrich
CAS-No.: 57-06-7

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

- Flammable liquids (Category 3), H226
- Acute toxicity, Oral (Category 4), H302
- Acute toxicity, Inhalation (Category 2), H330
- Acute toxicity, Dermal (Category 2), H310
- Skin corrosion (Category 1B), H314
- Serious eye damage (Category 1), H318
- Skin sensitization (Category 1), H317
- Short-term (acute) aquatic hazard (Category 1), H400
- Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.
2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word

Danger

Hazard statement(s)

H226 Flammable liquid and vapor.
H302 Harmful if swallowed.
H310 + H330 Fatal in contact with skin or if inhaled.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
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.
P260 Do not breathe mist or vapors.
P262 Do not get in eyes, on skin, or on clothing.
P264 Wash skin 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 protective gloves/ protective clothing/ eye protection/ face protection.
P284 Wear respiratory protection.
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302 + P350 + P310 IF ON SKIN: Gently wash with plenty of soap and water. Immediately call a POISON CENTER or doctor/ physician.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam 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.
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS
Vesicant., Lachrymator.

SECTION 3: Composition/information on ingredients

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>Oil of mustard AITC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C₄H₅NS</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>99.15 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>57-06-7</td>
</tr>
<tr>
<td>EC-No.</td>
<td>200-309-2</td>
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</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-isothiocyanato-1-propene</td>
<td>Flam. Liq. 3; Acute Tox. 4; Acute Tox. 2; Skin Corr. 1B; Eye Dam. 1; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H226, H302, H330, H310, H314, H318, H317, H400, H410 M-Factor - Aquatic Acute: 10 - Aquatic Chronic: 10</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.
In case of eye contact
After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed
After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed
The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed
No data available

SECTION 5: Firefighting measures
5.1 Extinguishing media
Suitable extinguishing media
Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Nitrogen oxides (NOx)
Sulfur oxides
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information
Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures
6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions
Do not let product enter drains. Risk of explosion.
6.3 Methods and materials for containment and cleaning up
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Advice on safe handling
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Storage conditions
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage stability
Recommended storage temperature
2 - 8 °C
Handle and open container with care. Store under inert gas.

Storage class
Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-isothiocyanato-1-propene</td>
<td>57-06-7</td>
<td>STEL</td>
<td>1 ppm</td>
<td>USA. Workplace Environmental Exposure Levels (WEEL)</td>
</tr>
</tbody>
</table>

Remarks Skin
8.2 Exposure controls

**Appropriate engineering controls**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

**Skin protection**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

- **Full contact**
  - Material: Viton®
  - Minimum layer thickness: 0.7 mm
  - Break through time: 480 min
  - Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

- **Splash contact**
  - Material: butyl-rubber
  - Minimum layer thickness: 0.7 mm
  - Break through time: 120 min
  - Material tested: Butoject® (KCL 898)

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
Recommended Filter type: Filter A-(P3)
The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains. Risk of explosion.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: clear, liquid
   Color: light orange

b) Odor
   Mustard-like

c) Odor Threshold
   No data available

d) pH
   No data available

e) Melting point/freezing point
   Melting point/range: -80 °C (-112 °F) - lit.

f) Initial boiling point and boiling range
   150 °C 302 °F - lit.

g) Flash point

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   No data available

k) Vapor pressure
   4.5 hPa at 23 °C (73 °F)
   4.930 hPa at 20 °C (68 °F)
   4.9 hPa at 30 °C (86 °F)

l) Vapor density
   No data available

m) Density
   1.013 g/cm³ at 25 °C (77 °F) - lit.
   Relative density
   No data available

n) Water solubility
   2 g/l at 20 °C (68 °F)

o) Partition coefficient: n-octanol/water
   log Pow: 1.83 at 20 °C (68 °F) - (ECHA), Bioaccumulation is not expected.

p) Autoignition temperature
   No data available

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   None

9.2 Other safety information

Surface tension
   53.4 mN/m at 20 °C (68 °F) - OECD Test Guideline 115
SECTION 10: Stability and reactivity

10.1 Reactivity
Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
A risk of explosion and/or of toxic gas formation exists with the following substances:
Strong oxidizing agents
Acids

10.4 Conditions to avoid
Heat.
Heating.

10.5 Incompatible materials
Copper, Copper alloys

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - female - 425.4 mg/kg
(OPPTS 870.1100)
LC50 Inhalation - Rat - male and female - 4 h - 0.206 - 0.508 mg/l - aerosol
(OPPTS 870.1300)
Inhalation: Irritating to respiratory system.
Acute toxicity estimate Inhalation - 4 h - 0.51 mg/l - vapor
(Expert judgment)
LD50 Dermal - Rat - male and female - 200 - 2,000 mg/kg
(OPPTS 870.1200)
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Corrosive
Remarks: (ECHA)

Serious eye damage/eye irritation
Remarks: No data available

Respiratory or skin sensitization
Local lymph node assay (LLNA) - Mouse
Result: Causes sensitization. (OPPTS 870.2600)

**Germ cell mutagenicity**
Test Type: reverse mutation assay
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Result: negative
Remarks: (ECHA)

Test Type: reverse mutation assay
Species: Mouse
Method: OECD Test Guideline 474
Result: negative

**Carcinogenicity**
IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP: No ingredient 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 on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
No data available

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

---

**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish
LC50 - Oryzias latipes (Orange-red killifish) - 0.07 mg/l - 96 h
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates
Remarks: (ECHA)
(3-isothiocyanato-1-propene)
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

12.2 Persistence and degradability
Biodegradability
aerobic - Exposure time 29 d
Result: 0 % - Not readily biodegradable.

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties
No data available

12.7 Other adverse effects
Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

13.1 Waste treatment methods
Product
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)
UN number: 1545  Class: 6.1 (3)  Packing group: II
Proper shipping name: Allyl isothiocyanate, stabilized
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 1545  Class: 6.1 (3)  Packing group: II
Proper shipping name: ALLYL ISOTHIOCYANATE, STABILIZED
Marine pollutant: yes
EMS-No: F-E, S-D

IATA
Aldrich - W203408
SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components
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

<table>
<thead>
<tr>
<th>Component</th>
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<th>Revision Date</th>
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<tr>
<td>3-isothiocyanato-1-propene</td>
<td>57-06-7</td>
<td>2007-03-01</td>
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Pennsylvania Right To Know Components

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<td>2007-03-01</td>
</tr>
</tbody>
</table>

SECTION 16: Other information

Further information
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 Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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