

Revision Date 10-Nov-2010

Revision Number 1

## 1. PRODUCT AND COMPANY IDENTIFICATION

**Product Identifier**

**Product Description:** Allyl isothiocyanate, stabilized  
**Cat No.** 102950000; 102950050; 102951000  
**Synonyms** Allyl isorhodanide; Allyl isosulfocyanate; Isothiocyanic acid, allyl ester

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

**Recommended Use** Laboratory chemicals  
**Uses advised against** No Information available

**Details of the supplier of the safety data sheet**

**Company**

Acros Organics BVBA  
 Janssen Pharmaceuticaaan 3a  
 2440 Geel, Belgium

**E-mail address** begel.sdsdesk@thermofisher.com

**Emergency Telephone Number**

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

## 2. HAZARDS IDENTIFICATION

**Classification of the substance or mixture**

**REGULATION (EC) No 1272/2008**

Acute oral toxicity	Category 3
Acute dermal toxicity	Category 3
Acute Inhalation Toxicity - Dusts and Mists	Category 3
Skin Corrosion / irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2A
Skin Sensitization	Category 1
Specific target organ systemic toxicity (single exposure)	Category 3
Acute aquatic toxicity	Category 1
Chronic aquatic toxicity	Category 1
Flammable liquids.	Category 3

**Classification according to EU Directives 67/548/EEC or 1999/45/EC**

For the full text of the R phrases mentioned in this Section, see Section 16

**Symbol(s)** T - Toxic  
 N - Dangerous for the environment  
**R -phrase(s)** R10 - Flammable  
 R43 - May cause sensitization by skin contact

## 2. HAZARDS IDENTIFICATION

### Risk Combination Phrases

R23/24/25 - Toxic by inhalation, in contact with skin and if swallowed  
 R36/37/38 - Irritating to eyes, respiratory system and skin  
 R50/53 - Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment

### Label Elements



### Signal Word

**Danger**

### Hazard Statements

H315 - Causes skin irritation  
 H317 - May cause an allergic skin reaction  
 H319 - Causes serious eye irritation  
 H410 - Very toxic to aquatic life with long lasting effects  
 H311 - Toxic in contact with skin  
 H335 - May cause respiratory irritation  
 H301 - Toxic if swallowed  
 H331 - Toxic if inhaled  
 H226 - Flammable liquid and vapor

### Precautionary Statements - EU (§28, 1272/2008)

P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
 P280 - Wear protective gloves/protective clothing/eye protection/face protection  
 P312 - Call a POISON CENTER or doctor/physician if you feel unwell  
 P302 + P350 - IF ON SKIN: Gently wash with plenty of soap and water  
 P280 - Wear eye protection/face protection  
 P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing  
 P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
 P273 - Avoid release to the environment  
 P302+ P352 - IF ON SKIN: Wash with plenty of soap and water  
 P280 - Wear protective gloves/protective clothing/eye protection/face protection  
 P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
 P210 - Keep away from heat/sparks/open flames/hot surfaces. - No smoking

### Other Hazards

Lachrymator (substance which increases the flow of tears).

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	EC No.	Weight %	CAS-No	Classification	GHSCLAS	REACH Reg. No.
Allyl isothiocyanate	EEC No. 200-309-2	94	57-06-7	R10 T; R23/24/25 Xi; R36/37/38 R43 N; R50/53;	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Skin Sens. 1 (H317) Acute Tox. 3 (H301) Acute Tox. 3 (H311) Acute Tox. 3 (H331) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)	

**For the full text of the R phrases mentioned in this Section, see Section 16**

### 4. FIRST AID MEASURES

#### Description of first aid measures

##### **Eye Contact**

Immediate medical attention is required Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes

##### **Skin Contact**

Wash off immediately with soap and plenty of water removing all contaminated clothes and shoes Immediate medical attention is required

##### **Ingestion**

Never give anything by mouth to an unconscious person Drink plenty of water Induce vomiting, but only if victim is fully conscious Call a physician immediately Clean mouth with water

##### **Inhalation**

Remove from exposure, lie down Move to fresh air If breathing is difficult, give oxygen If not breathing, give artificial respiration Immediate medical attention is required

##### **Notes to Physician**

Treat symptomatically

### 5. FIRE-FIGHTING MEASURES

#### Extinguishing media

##### **Suitable Extinguishing Media**

Water spray Carbon dioxide (CO<sub>2</sub>) Dry chemical

##### **Extinguishing media which must not be used for safety reasons**

No information available.

#### Special hazards arising from the substance or mixture

Flammable Vapors may travel to source of ignition and flash back

#### Advice for fire-fighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear

## 6. ACCIDENTAL RELEASE MEASURES

### Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation

### Environmental precautions

Prevent further leakage or spillage if safe to do so

### Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust) Prevent product from entering drains  
Keep in suitable and closed containers for disposal Do not flush into surface water or sanitary sewer system

## 7. HANDLING AND STORAGE

### Precautions for Safe Handling

Do not breathe dust Do not breathe vapors or spray mist Do not get in eyes, on skin, or on clothing Take precautionary measures against static discharges Use only in area provided with appropriate exhaust ventilation Use explosion-proof equipment Use only non-sparking tools

### Conditions for safe storage, including any incompatibilities

Keep in a dry place Keep container tightly closed Keep away from heat and sources of ignition Refrigerator/flammables

### Specific End Uses

## 8. EXPOSURE CONTROLS / PERSONAL PROTECTION

### Control parameters

#### Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

#### Derived No Effect Level (DNEL)

No information available.

#### Predicted No Effect Concentration (PNEC)

No information available.

### Exposure controls

#### Engineering Measures

Ensure adequate ventilation, especially in confined areas Ensure that eyewash stations and safety showers are close to the workstation location

### Personal protective equipment

#### Eye Protection

Goggles

#### Hand Protection

Protective gloves

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure

#### Respiratory Protection

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

### Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice

### Environmental exposure controls

No information available.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### Physical State

Liquid

## 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance</b>	Light yellow
<b>odor</b>	pungent
<b>pH</b>	No information available.
<b>Vapor Pressure</b>	5.3 mbar @ 20 °C
<b>Vapor Density</b>	3.41
<b>Boiling Point/Range</b>	151 - 153°C / 303.8 - 307.4°F @ 760 mmHg
<b>Melting Point/Range</b>	-80°C / -112°F
<b>Flash Point</b>	46°C / 114.8°F
<b>Water Solubility</b>	2 g/l water (20°C)
<b>Specific Gravity</b>	1.018
<b>Molecular Formula</b>	C4 H5 N S
<b>Molecular Weight</b>	99.15

## 10. STABILITY AND REACTIVITY

### Reactivity

#### Chemical Stability

Stable under normal conditions.

#### Possibility of Hazardous Reactions

**Hazardous Polymerization** No information available.

**Hazardous Reactions .** No information available.

#### Conditions to Avoid

Keep away from open flames, hot surfaces and sources of ignition, Exposure to air, Exposure to light, Incompatible products, Exposure to moist air or water.

#### Incompatible Materials

Acids, Water, Strong oxidizing agents, Strong bases, Alcohols, Amines.

#### Hazardous Decomposition Products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Sulfur oxides. Hydrogen cyanide (hydrocyanic acid).

## 11. TOXICOLOGICAL INFORMATION

### Information on Toxicological Effects

#### Acute Toxicity

**Product Information** No acute toxicity information is available for this product

#### Component Information

##### Component

Allyl isothiocyanate

LD50 Oral	LD50 Dermal	LC50 Inhalation
112 mg/kg ( Rat )	88 mg/kg ( Rabbit )	

#### Chronic Toxicity

##### Carcinogenicity

There are no known carcinogenic chemicals in this product

##### Sensitization

May cause sensitization by skin contact

##### Mutagenic Effects

No information available

##### Reproductive Effects

No information available.

##### Developmental Effects

No information available.

<b>Target Organs</b>	No information available.
<b>Other Adverse Effects</b>	The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information
<b>Endocrine Disruptor Information</b>	None known

## 12. ECOLOGICAL INFORMATION

### Toxicity

#### **Ecotoxicity effects**

Do not flush into surface water or sanitary sewer system Do not allow material to contaminate ground water system

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Allyl isothiocyanate		0.054-0.109 mg/L LC50 96 h 0.0856 mg/L LC50 96 h	EC50 = 0.099 mg/L 15 min EC50 = 0.106 mg/L 30 min EC50 = 0.11 mg/L 5 min	

### Persistence and degradability

No information available

### Bioaccumulative potential

No information available.

### Mobility in soil

No information available.

### Results of PBT and vPvB assessment

### Other adverse effects

No information available

## 13. DISPOSAL CONSIDERATIONS

### Waste treatment methods

#### **Waste from Residues / Unused Products**

Dispose of in accordance with local regulations

#### **Contaminated Packaging**

Empty containers should be taken for local recycling, recovery or waste disposal

## 14. TRANSPORT INFORMATION

### IMDG/IMO

<b>UN-No</b>	1545
<b>Hazard Class</b>	6.1
<b>Subsidiary Hazard Class</b>	3
<b>Packing Group</b>	II
<b>Proper Shipping Name</b>	ALLYL ISOTHIOCYANATE, STABILIZED

### ADR

<b>UN-No</b>	1545
<b>Hazard Class</b>	6.1
<b>Subsidiary Class</b>	3
<b>Packing Group</b>	II

**14. TRANSPORT INFORMATION**

Proper Shipping Name ALLYL ISOTHIOCYANATE, STABILIZED

**IATA**

UN-No 1545  
 Hazard Class 6.1  
 Subsidiary Hazard Class 3  
 Packing Group II  
 Proper Shipping Name ALLYL ISOTHIOCYANATE, STABILIZED

**15. REGULATORY INFORMATION****Safety, health and environmental regulations/legislation specific for the substance or mixture****International Inventories**

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	CHINA	AICS	KECL
Allyl isothiocyanate	200-309-2	-		X	X	-	X	X	X	X	-

**Legend**

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**EINECS/ELINCS** - European Inventory Lists

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**ENCS** - Japan Existing and New Chemical Substances

**CHINA** - China Inventory of Existing Chemical Substances

**AICS** - Inventory of Chemical Substances

**KECL** - Existing and Evaluated Chemical Substances

**Chemical Safety Assessment****16. OTHER INFORMATION****Text of R phrases mentioned in Section 2-3**

R10 - Flammable

R43 - May cause sensitization by skin contact

R23/24/25 - Toxic by inhalation, in contact with skin and if swallowed

R36/37/38 - Irritating to eyes, respiratory system and skin

R50/53 - Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment

Revision Date 10-Nov-2010

Revision Summary Not applicable

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006

**Disclaimer**

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End of Safety Data Sheet