



SAFETY DATA SHEET

Creation Date 23-Mar-2012

Revision Date 21-Nov-2016

Revision Number 3

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identification

Product Description: Allyl isothiocyanate, stabilized
Cat No. : 102950000; 102950050; 102951000; 102955000
Synonyms Allyl isorhodanide; Allyl isosulfocyanate; Isothiocyanic acid, allyl ester
CAS-No 57-06-7
EC-No. 200-309-2
Molecular Formula C₄ H₅ N S

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

Recommended Use Laboratory chemicals.
Uses advised against No Information available

1.3. 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

1.4. Emergency telephone number

For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - Regulation (EC) No 1272/2008

Physical hazards

Flammable liquids Category 3 (H226)

Health hazards

Acute oral toxicity Category 3 (H301)
Acute dermal toxicity Category 2 (H310)
Acute Inhalation Toxicity - Vapors Category 2 (H330)
Skin Corrosion/irritation Category 2 (H315)
Serious Eye Damage/Eye Irritation Category 2 (H319)
Specific target organ toxicity - (single exposure) Category 3 (H335)

Environmental hazards

Acute aquatic toxicity Category 1 (H400)
Chronic aquatic toxicity Category 1 (H410)

2.2. Label elements

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016



Signal Word

Danger

Hazard Statements

H226 - Flammable liquid and vapor
H301 - Toxic if swallowed
H310 - Fatal in contact with skin
H330 - Fatal if inhaled
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
H410 - Very toxic to aquatic life with long lasting effects

Precautionary Statements

P210 - Keep away from heat/sparks/open flames/hot surfaces. - No smoking
P310 - Immediately call a POISON CENTER or doctor/ physician
P304 + P340 - IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing
P332 + P313 - If skin irritation occurs: Get medical advice/ attention
P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection
P337 + P313 - If eye irritation persists: Get medical advice/ attention

2.3. Other hazards

Lachrymator (substance which increases the flow of tears)

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS-No	EC-No.	Weight %	CLP Classification - Regulation (EC) No 1272/2008
Allyl isothiocyanate	57-06-7	EEC No. 200-309-2	>92	Flam. Liq. 3 (H226) STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 3 (H301) Acute Tox. 2 (H310) Acute Tox. 2 (H330) Aquatic Acute 1 (H400) Aquatic Chronic 1 (H410)

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Ingestion	Do not induce vomiting. Call a physician or Poison Control Center immediately.
Inhalation	Move to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
Protection of First-aiders	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

4.2. Most important symptoms and effects, both acute and delayed

None reasonably foreseeable. .

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

Flammable. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air. Do not allow run-off from fire fighting to enter drains or water courses.

Hazardous Combustion Products

Nitrogen oxides (NO_x), Carbon monoxide (CO), Carbon dioxide (CO₂), Sulfur oxides, Hydrogen cyanide (hydrocyanic acid).

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

6.3. Methods and material for containment and cleaning up

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment. Use only under a chemical fume hood. Do not breathe vapors or spray mist. Do not ingest. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing before re-use. Wash hands before breaks and at the end of workday.

7.2. Conditions for safe storage, including any incompatibilities

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

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s):

Component	Russia	Slovak Republic	Slovenia	Sweden	Turkey
Allyl isothiocyanate	Skin notation MAC: 0.1 mg/m ³				

Biological limit values

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

Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 88 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography

MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

Derived No Effect Level (DNEL)	No information available			
Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral Dermal Inhalation				

Predicted No Effect Concentration (PNEC) No information available.

8.2. Exposure controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting/equipment.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)
Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

Skin and body protection Long sleeved clothing

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls

Prevent product from entering drains. Do not allow material to contaminate ground water system. Local authorities should be advised if significant spillages cannot be contained.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Appearance Light yellow
Physical State Liquid
Odor pungent

ACR10295

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	-80 °C / -112 °F	
Softening Point	No data available	
Boiling Point/Range	151 - 153 °C / 303.8 - 307.4 °F	@ 760 mmHg
Flash Point	46 °C / 114.8 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Vapor Pressure	5.3 mbar @ 20 °C	
Vapor Density	3.41	(Air = 1.0)
Specific Gravity / Density	1.0175	
Bulk Density	Not applicable	Liquid
Water Solubility	2 g/l	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties	No information available	explosive air/vapour mixtures possible
Oxidizing Properties	No information available	

9.2. Other information

Molecular Formula	C4 H5 N S
Molecular Weight	99.15

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Moisture sensitive.

10.3. Possibility of hazardous reactions

Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

10.4. 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.

10.5. Incompatible materials

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

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Sulfur oxides. Hydrogen cyanide (hydrocyanic acid).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on toxicological effects

Product Information

(a) acute toxicity;	
Oral	Category 3
Dermal	Category 2
Inhalation	Category 2

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Allyl isothiocyanate	LD50 = 112 mg/kg (Rat)	LD50 = 88 mg/kg (Rabbit)	

(b) skin corrosion/irritation;	Category 2
(c) serious eye damage/irritation;	Category 2
(d) respiratory or skin sensitization;	
Respiratory	No data available
Skin	No data available
(e) germ cell mutagenicity;	No information available No data available
(f) carcinogenicity;	No data available There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	Category 3
Results / Target organs	Respiratory system.
(i) STOT-repeated exposure;	No data available
Target Organs	None known.
(j) aspiration hazard;	No data available
Other Adverse Effects	The toxicological properties have not been fully investigated.
Symptoms / effects, both acute and delayed	No information available

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects

The product contains following substances which are hazardous for the environment. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
Allyl isothiocyanate	LC50: 0.054 - 0.109 mg/L, 96h flow-through (Oryzias latipes) LC50: = 0.0856 mg/L, 96h flow-through (Pimephales promelas)			EC50 = 0.099 mg/L 15 min EC50 = 0.106 mg/L 30 min EC50 = 0.11 mg/L 5 min

12.2. Persistence and degradability

Persistence

Degradation in sewage treatment plant

Soluble in water, Persistence is unlikely, based on information available.
Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

12.4. Mobility in soil

The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility. Highly mobile in soils

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Other adverse effects

Endocrine Disruptor Information
Persistent Organic Pollutant
Ozone Depletion Potential

This product does not contain any known or suspected endocrine disruptors
This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues / Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

European Waste Catalogue (EWC)

According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.

Other Information

Do not dispose of waste into sewer. Waste codes should be assigned by the user based on the application for which the product was used. Can be incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number

UN1545

14.2. UN proper shipping name

ALLYL ISOTHIOCYANATE, STABILIZED

14.3. Transport hazard class(es)

6.1

Subsidiary Hazard Class

3

14.4. Packing group

II

ADR

14.1. UN number

UN1545

14.2. UN proper shipping name

ALLYL ISOTHIOCYANATE, STABILIZED

14.3. Transport hazard class(es)

6.1

Subsidiary Hazard Class

6.1 3

14.4. Packing group

II

IATA

14.1. UN number

UN1545

14.2. UN proper shipping name

ALLYL ISOTHIOCYANATE, STABILIZED

14.3. Transport hazard class(es)

6.1

Subsidiary Hazard Class

3

14.4. Packing group

II

14.5. Environmental hazards

Dangerous for the environment
Product is a marine pollutant according to the criteria set by IMDG/IMO

14.6. Special precautions for user

No special precautions required

14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

Not applicable, packaged goods

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

SECTION 15: REGULATORY INFORMATION

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

International Inventories

X = listed

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

National Regulations

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment.

Take note of Dir 94/33/EC on the protection of young people at work

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H301 - Toxic if swallowed

H310 - Fatal in contact with skin

H330 - Fatal if inhaled

H315 - Causes skin irritation

H319 - Causes serious eye irritation

H335 - May cause respiratory irritation

H400 - Very toxic to aquatic life

H410 - Very toxic to aquatic life with long lasting effects

H226 - Flammable liquid and vapor

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

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

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

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - Volatile Organic Compounds

Key literature references and sources for data

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and

SAFETY DATA SHEET

Allyl isothiocyanate, stabilized

Revision Date 21-Nov-2016

hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Chemical incident response training.

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Revision Date 21-Nov-2016

Revision Summary SDS sections updated, 2, 3, 11, 16.

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

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet