

Classified as hazardous in accordance with the criteria of EPA New Zealand

Section 1 - Identification

Product Identifier

Product Name	<u>Allyl isothiocyanate</u>
CAS No	57-06-7
Synonyms	Allyl isorhodanide; Allyl isosulfocyanate; Isothiocyanic acid, allyl ester
Molecular Formula	C4 H5 N S
Molecular Weight	99.15
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

Product Code	L02901
Address	Thermo Fisher Scientific New Zealand Ltd 244 Bush Road, Albany, Auckland, New Zealand
Emergency Tel.	CHEMTREC® 09 980 6780 or +64 9 980 6780
Telephone / Fax Numbers	Tel: 09 980 6700 Fax: 09 980 6788
E-mail address	ANZinfo@thermofisher.com

Section 2 - Hazard(s) Identification

Classification under Work Safe New Zealand

Classified as hazardous in accordance with the criteria of EPA New Zealand

HSNO Approval Number **HSR002500**

GHS Classification

Physical hazards

Flammable liquids

Category 3

Health hazards

Acute Oral Toxicity
 Acute Dermal Toxicity
 Acute Inhalation Toxicity - Vapors
 Skin Corrosion/Irritation
 Serious Eye Damage/Eye Irritation
 Specific target organ toxicity - (single exposure)

Category 2
 Category 2
 Category 2
 Category 2
 Category 2
 Category 3

Environmental hazards

Acute aquatic toxicity

Category 1

Chronic aquatic toxicity

Category 1

Label Elements



Signal Word

Danger

Hazard Statements

H226 - Flammable liquid and vapor
 H315 - Causes skin irritation
 H319 - Causes serious eye irritation
 H335 - May cause respiratory irritation
 H410 - Very toxic to aquatic life with long lasting effects
 H300 + H310 + H330 - Fatal if swallowed, in contact with skin or if inhaled

Precautionary Statements

Prevention

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
 P233 - Keep container tightly closed
 P240 - Ground and bond container and receiving equipment
 P241 - Use explosion-proof electrical/ ventilating/ lighting equipment
 P242 - Use non-sparking tools
 P243 - Take action to prevent static discharges
 P262 - Do not get in eyes, on skin, or on clothing
 P264 - Wash face, hands and any exposed 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
 P280 - Wear protective gloves/protective clothing/eye protection/face protection
 P284 - Wear respiratory protection
 P273 - Avoid release to the environment

Response

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or 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 POISON CENTER or doctor
 P330 - Rinse mouth
 P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish
 P362 + P364 - Take off contaminated clothing and wash it before reuse
 P391 - Collect spillage

Storage

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed
 P405 - Store locked up

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Other hazards which do not result in classification

Lachrymator (substance which increases the flow of tears) Toxic to terrestrial vertebrates

Section 3 - Composition and Information on Ingredients

Component	CAS No	Weight %
Allyl isothiocyanate	57-06-7	<100

Section 4 - First Aid Measures

Description of first aid measures

General Advice	Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.
New Zealand Emergency Tel.	CHEMTREC® 09 980 6780 or +64 9 980 6780
Inhalation	Remove 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.
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.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.
First Aid Facilities	Eyewash, safety shower and washroom.
Most important symptoms and effects	None reasonably foreseeable. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting
Notes to Physician	Treat symptomatically.

Section 5 - Fire Fighting Measures

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

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).

Special protective equipment and precautions for fire fighters

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

Personal Precautions, Protective Equipment and Emergency Procedures

Emergency procedures

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

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.

Methods for Containment and Clean Up

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.

Precautions to prevent secondary hazards

Clean contaminated objects and areas thoroughly observing environmental regulations

Reference to Other Sections

Refer to protective measures listed in Sections 8 and 13.

Section 7 - Handling and Storage

Precautions for Safe Handling**Advice on safe handling**

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

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 and gloves, including the inside, before re-use. Wash hands before breaks and after work.

Conditions for Safe Storage, Including any Incompatibilities**Storage Conditions**

Keep away from heat, sparks and flame. Keep container tightly closed in a dry and well-ventilated place. To maintain product quality: Keep refrigerated.

Incompatible Materials

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

AS/NZS 2243.10:2004, Safety in laboratories - Storage of chemicals

AS 1940-2004 - The storage and handling of flammable and combustible liquids

Section 8 - Exposure Controls and Personal Protection

Control parameters**Exposure limits**

The product does not contain any hazardous materials with occupational exposure limits established.

Biological limit values

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

Appropriate engineering 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

Individual protection measures, such as personal protective equipment

Eye Protection Goggles (Australian/New Zealand Standard AS/NZS 1337 - Eye protectors for Industrial applications)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	AUS/NZ Standard	Glove comments
Nitrile rubber, Neoprene, Natural rubber, PVC.	See manufacturers recommendations	-	AS/NZS 2161	(minimum requirement)

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 compatability, 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.

Skin and body protection Long sleeved clothing

Respiratory Protection Use an AS/NZS 1716 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained in line with AS/NZS 1715 on the use and maintenance of respiratory protective devices

Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387 (or AUS/NZ equivalent)

Recommended half mask:- Valve filtering: EN405 or Half mask: EN140 plus filter, EN 141 (or AUS/NZ equivalent) When RPE is used a face piece Fit Test should be conducted

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

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

Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Light yellow	
Odor	pungent	
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
Flammability (liquid)	Flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	46 °C / 114.8 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Water Solubility	2 g/l @20°C	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		

Vapor Pressure	5.3 mbar @ 20 °C	
Density / Specific Gravity	1.0175	
Bulk Density	Not applicable	Liquid
Vapor Density	3.41	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

Other information

Molecular Formula	C4 H5 N S
Molecular Weight	99.15
Explosive Properties	explosive air/vapour mixtures possible
Self-accelerating polymerisation temperature (SAPT)	>50°C (packages up to 50kg)

Section 10 - Stability and Reactivity

Reactivity	None known, based on information available
Stability	Moisture sensitive.
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.
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 ₂). Sulfur oxides. Hydrogen cyanide (hydrocyanic acid).

Section 11 - Toxicological Information

Acute Effects**Information on likely routes of exposure****Product Information**

Inhalation	Not an expected route of exposure.
Eyes	Avoid contact with eyes. Irritating to eyes. Lachrymator (substance which increases the flow of tears).
Skin	Avoid contact with skin. May cause irritation. Harmful in contact with skin.
Ingestion	May be harmful if swallowed.

Numerical measures of toxicity**(a) acute toxicity;**

Oral	Category 3
Dermal	Category 2
Inhalation	Category 2

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Allyl isothiocyanate	LD50 = 112 mg/kg (Rat)	LD50 = 88 mg/kg (Rabbit)	LC50 0.206 - 0.508 mg/L (Rat) 4 h

(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
Sensitization	No information available
(e) germ cell mutagenicity;	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	No information available.
(j) aspiration hazard;	No data available
Other Adverse Effects	The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

Section 12 - Ecological Information

Ecotoxicity

Aquatic ecotoxicity 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

Terrestrial ecotoxicity There is no data for this product

Persistence and Degradability

Persistence	Soluble in water, Persistence is unlikely, based on information available.
Degradation in sewage treatment plant	Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.
Bioaccumulative Potential	Bioaccumulation is unlikely
Mobility	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
<u>Other adverse effects</u>	
Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

Section 13 - Disposal Considerations

Waste treatment methods

Waste from Residues/Unused Products	Do not allow into drains or watercourses or dispose of where ground or surface waters may be affected. Wastes, including emptied containers, are controlled wastes and should be disposed of in accordance with all federal, E.P.A., state and local regulations. Assure conformity with all applicable 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.
Other Information	Disposal agencies or waste contractors must comply with the New Zealand Hazardous Substances (Disposal) Regulations. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations. Do not let this chemical enter the environment. Do not empty into drains. Waste codes should be assigned by the user based on the application for which the product was used.

Section 14 - Transport Information

Component	Hazchem Code
Allyl isothiocyanate 57-06-7 (<100)	3WE

NZS 5433:2020

UN-No	UN1545
Proper Shipping Name	ALLYL ISOTHIOCYANATE, STABILIZED
Hazard Class	6.1
Subsidiary Hazard Class	3
Packing Group	II

IATA

UN-No	UN1545
Proper Shipping Name	ALLYL ISOTHIOCYANATE, STABILIZED
Hazard Class	6.1
Subsidiary Hazard Class	3
Packing Group	II

IMDG/IMO

UN-No	UN1545
Proper Shipping Name	ALLYL ISOTHIOCYANATE, STABILIZED
Hazard Class	6.1
Subsidiary Hazard Class	3
Packing Group	II
Environmental hazards	Dangerous for the environment Product is a marine pollutant according to the criteria set by IMDG/IMO
Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code	Not applicable, packaged goods
Special Precautions	Inhibitors have been added to stabilize this product. Inhibitor levels should be maintained. Hazardous polymerization may occur upon depletion of inhibitor.
Additional information	None known

Section 15 - Regulatory Information

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

HSNO Approval Number	HSR002500
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National Regulations

There are no applicable tolerable exposure limits or environmental exposure limits according to the EPA Controls for Hazardous Substances

Certified handlers, tracking and controlled substance license requirements

Certified handlers are required for some substances. This includes substances requiring a controlled substance license, and most explosives, vertebrates toxic agents, and certain fumigants. Acutely toxic substances which are a Category 1 or 2, such as pesticides also require Certified handlers. Please check the Health and Safety at Work Act 2015 for further information. Tracking is required for some highly hazardous substances. These substances need to be under the control of an appropriately trained person or appropriately secured. Please check the Health and Safety at Work Act 2015 for further information.

Prohibition or notification/licensing requirements

Shown below are details of specific prohibition/notifications or licensing requirements when they apply.

International Regulations

Ozone Depletion Potential	This product does not contain any known or suspected substance
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Rotterdam Convention (PIC)	Not applicable

Authorisation/Restrictions according to EU REACH

Component	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Allyl isothiocyanate	-	Use restricted. See item 75. (see link for restriction details)	-

<https://echa.europa.eu/substances-restricted-under-reach>

International Inventories

New Zealand (NZIoC), Australia (AICS), Europe (EINECS/ELINCS/NLP), Korea (KECL), China (IECSC), Taiwan (TCSI), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	NZIoC	AICS	EINECS	ELINCS	NLP	KECL	IECSC	TCSI
Allyl isothiocyanate	57-06-7	X	X	-	-	-	-	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	PICCS	ISHL	ENCS
Allyl isothiocyanate	57-06-7	X	ACTIVE	X	-	X	X	X

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Section 16 - Other Information

This safety data sheet complies with the requirements of the EPA Hazardous Substances (Hazard Classification) Notice 2020 and WorkSafe New Zealand Regulations

Legend

NZIoC - New Zealand Inventory of Chemicals

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

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

IECSC - Chinese Inventory of Existing Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

NZS 5433:2020 - Transport of Dangerous Goods on Land

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

MARPOL - International Convention for the Prevention of Pollution from Ships

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

WEL - Workplace Exposure Limit

DNEL - Derived No Effect Level

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

VOC - (Volatile Organic Compound)

AICS - Australian Inventory of Chemical Substances

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

ENCS - Japanese Existing and New Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

CAS - Chemical Abstracts Service

ACGIH - American Conference of Governmental Industrial Hygienists

PNEC - Predicted No Effect Concentration

OECD - Organisation for Economic Co-operation and Development

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

ADG - Australian Code for the Transport of Dangerous Goods by Road and Rail

LC50 - Lethal Concentration 50%

ATE - Acute Toxicity Estimate

RPE - Respiratory Protective Equipment

NOEC - No Observed Effect Concentration

BCF - Bioconcentration factor

PBT - Persistent, Bioaccumulative, Toxic

Key literature references and sources for data

HSNO classifications provided in the New Zealand Chemical Classification Information Database (CCID).

<https://echa.europa.eu/information-on-chemicals>

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

EPA Guide to classifying hazardous substances in New Zealand

EPA - Assigning a product to an existing HSNO approval guide

Training Advice

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

Revision Date

16-Mar-2023

Revision Summary

Not applicable

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