

ALFAAL02901

Allyl isothiocyanate

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

产品说明: Product Description:	异硫代氰酸烯丙酯 Allyl isothiocyanate
Cat No. :	L02901
Synonyms	Allyl isorhodanide; Allyl isosulfocyanate; Isothiocyanic acid, allyl ester
CAS No	57-06-7
Molecular Formula	C4 H5 N S
Supplier	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
Emergency Telephone Number	For information US call: 001-800-227-6701 / 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
E-mail address	begel.sdsdesk@thermofisher.com
Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State Liquid	Appearance Light yellow	Odor pungent
Emergency Overview Causes serious eye irritation. Fatal if inhaled. May cause respiratory irritation. Moisture sensitive. Lachrymator (substance which increases the flow of tears). Flammable liquid and vapor. Toxic if swallowed. Causes skin irritation. May cause an allergic skin reaction. Suspected of damaging fertility or the unborn child. May cause damage to organs. Harmful to aquatic life. Very toxic to aquatic life with long lasting effects. Fatal in contact with skin.		

Classification of the substance or mixture

Flammable liquids.	Category 3
Acute Oral Toxicity	Category 3
Acute Dermal Toxicity	Category 2
Acute Inhalation Toxicity - Vapors	Category 2
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Skin Sensitization	Category 1
Reproductive Toxicity	Category 2
Specific target organ toxicity - (single exposure)	Category 3 Category 2
Acute aquatic toxicity	Category 1 Category 3
Chronic aquatic toxicity	Category 1

Label Elements**Signal Word****Danger****Hazard Statements**

H226 - Flammable liquid and vapor
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
H301 - Toxic if swallowed
H315 - Causes skin irritation
H317 - May cause an allergic skin reaction
H361 - Suspected of damaging fertility or the unborn child
H371 - May cause damage to organs
H410 - Very toxic to aquatic life with long lasting effects
H310 + H330 - Fatal 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
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

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

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

Physical and Chemical Hazards

Vapors may cause flash fire or explosion. Flammable liquid.

Health Hazards

Causes serious eye irritation. Fatal if inhaled. May cause respiratory irritation. Toxic if swallowed. Causes skin irritation. May cause an allergic skin reaction. Suspected of damaging fertility or the unborn child. May cause damage to organs. Fatal in contact with skin.

Environmental hazards

Harmful to aquatic life. Very toxic to aquatic life with long lasting effects. Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

Allyl isothiocyanate

Other Hazards

Lachrymator (substance which increases the flow of tears)

Toxic to terrestrial vertebrates. This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

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

SECTION 4. FIRST AID MEASURES**General Advice**

Show this safety data sheet to the doctor in attendance. 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.

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.

Ingestion

Do NOT induce vomiting. Call a physician or poison control center immediately.

Most important symptoms and effects

None reasonably foreseeable. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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.

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.

Protective Equipment and Precautions 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

Personal Precautions

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.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**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.

Storage

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

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters****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

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	See manufacturers recommendations		EN 374	(minimum requirement)

Allyl isothiocyanate

Natural rubber
PVC

-

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

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

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**Appearance**

Light yellow

Physical State

Liquid

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

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 @20°C

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

explosive air/vapour mixtures possible

Oxidizing Properties

No information available

Allyl isothiocyanate

Molecular Formula C4 H5 N S
Molecular Weight 99.15

SECTION 10. STABILITY AND REACTIVITY

Stability Moisture sensitive.

Hazardous Reactions None under normal processing.
Hazardous Polymerization 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.

Materials to avoid Acids. Water. Strong oxidizing agents. Strong bases. Alcohols. Amines.

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

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;

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
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.

Allyl isothiocyanate

(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 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

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.

Bioaccumulative Potential

Bioaccumulation is unlikely

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

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**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.

Other Information

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**Road and Rail Transport****UN-No**

UN1545

Proper Shipping Name

ALLYL ISOTHIOCYANATE, STABILIZED

Hazard Class

6.1

SAFETY DATA SHEET**Allyl isothiocyanate**

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

IATA

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

Special Precautions for User Inhibitors have been added to stabilize this product Inhibitor levels should be maintained
Hazardous polymerization may occur upon depletion of inhibitor

SECTION 15. REGULATORY INFORMATION**International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Allyl isothiocyanate	X	X	X	X	200-309-2	X	X	X	X	X	X	-

National Regulations**SECTION 16. OTHER INFORMATION**

Prepared By Health, Safety and Environmental Department
Creation Date 23-Mar-2012
Revision Date 06-Mar-2024
Revision Summary New emergency telephone response service provider.

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.

Legend

Allyl isothiocyanate

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**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road**OECD** - Organisation for Economic Co-operation and Development**BCF** - Bioconcentration factor**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code**MARPOL** - International Convention for the Prevention of Pollution from Ships**ATE** - Acute Toxicity Estimate**VOC** - (Volatile Organic Compound)**Key literature references and sources for data**<https://echa.europa.eu/information-on-chemicals>

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

Disclaimer

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End of Safety Data Sheet