

SAFETY DATA SHEET

Creation Date 23-Mar-2012

Revision Date 18-Dec-2025

Revision Number 7

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

Product Name Allyl isothiocyanate, stabilized

Cat No. : AC102950000; AC102950050; AC102951000; AC102955000

CAS No 57-06-7

Synonyms Allyl isorhodanide; Allyl isosulfocyanate; Isothiocyanic acid, allyl ester

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

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

2. Hazard(s) identification

Classification

This chemical is considered hazardous according to [US] OSHA (29 CFR 1910.1200, 2024)

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
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Respiratory system.	

Label Elements

Signal Word

Danger

Hazard Statements

Flammable liquid and vapor
Toxic if swallowed
Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation
Fatal in contact with skin or if inhaled

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product
Do not get in eyes, on skin, or on clothing
Wear protective gloves/protective clothing/eye protection/face protection
Do not breathe dust/fume/gas/mist/vapors/spray
Use only outdoors or in a well-ventilated area
Wear respiratory protection
Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
Keep container tightly closed
Ground and bond container and receiving equipment
Use explosion-proof electrical/ventilating/lighting equipment
Keep cool
Take action to prevent static discharges
Use non-sparking tools

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing
Immediately call a POISON CENTER or doctor
Call a POISON CENTER or doctor if you feel unwell

Skin

Immediately call a POISON CENTER or doctor
Take off contaminated clothing and wash before reuse
If skin irritation occurs: Get medical advice/attention
IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Immediately call a POISON CENTER or doctor
Rinse mouth

Fire

In case of fire: Use CO₂, dry chemical, or foam to extinguish

Storage

Store locked up
Store in a well-ventilated place. Keep container tightly closed

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Very toxic to aquatic life with long lasting effects

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

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

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
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO ₂), dry chemical, alcohol-resistant foam. Water mist may be used to cool closed containers.
Unsuitable Extinguishing Media	No information available
Flash Point	46 °C / 114.8 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available
Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	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).

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.

NFPA
Health
3

Flammability
2

Instability
1

Physical hazards
N/A

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.

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

8. Exposure controls / personal protection

Exposure Guidelines

This product does not contain any hazardous materials with occupational exposure limit established by the region specific regulatory bodies.

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.

Personal Protective Equipment
Eyeface Protection

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

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.

Recommended Filter type:

Organic gases and vapours filter. Type A. Brown. conforming to EN14387.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State	Liquid		
Color	Light yellow		
Odor	pungent		
Odor Threshold	No information available		
Property	Values	Remarks	• Method
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	
Flammability (liquid)	Flammable	On basis of test data	
Flammability (solid,gas)	Not applicable	Liquid	
Explosion Limits	No data available		
Autoignition Temperature	No data available		
Decomposition Temperature	No data available		
pH	No information 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)		

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Moisture sensitive.
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)
Hazardous Polymerization	No information available.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Information on expected route of exposure

Inhalation	Not an expected route of exposure.
Ingestion	May be harmful if swallowed.
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.

Toxicology data for the components

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

Toxicologically Synergistic Products No information available

(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;

The table below indicates whether each agency has listed any ingredient as a carcinogen

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Allyl isothiocyanate	57-06-7	Not listed	Not listed	Not listed	Not listed	Not listed

(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.

Other Adverse Effects The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

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 Algae	Freshwater Fish	Microtox	Water Flea
Allyl isothiocyanate	Not listed	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	Not listed

Persistence and Degradability Soluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility Will likely be mobile in the environment due to its water solubility.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

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

TDG

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

15. Regulatory Information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Allyl isothiocyanate	57-06-7	X	ACTIVE	-

Legend:

TSCA - US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Not applicable

Substances & Mixtures, Under TSCA Section 6(h) (PBT)

TSCA 12(b) - Notices of Export

Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Allyl isothiocyanate	57-06-7	X	-	200-309-2	X	X	X	X	X	-

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

U.S. Federal Regulations**SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Allyl isothiocyanate	X	X	X	-	-

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security

This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH

Component	CAS No	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	57-06-7	-	Use restricted. See entry 75. (see link for restriction details)	-

REACH links

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

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Allyl isothiocyanate	57-06-7	Not applicable	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Allyl isothiocyanate	57-06-7	Not applicable	Not applicable	Not applicable	Not applicable

16. Other Information

Prepared By

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Revision Summary

Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

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 SDS