ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

Allyl isothiocyanate

Revision Date:2026-05-31 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name	: Allyl isothiocyanate
CBnumber	: CB8853857
CAS	: 57-06-7
EINECS Number	: 200-309-2
Synonyms	: allyl isothiocyanate,3-isothiocyanato-1-propene

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word Danger

Precautionary statements

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P273 Avoid release to the environment.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H226 Flammable liquid and vapour

H302 Harmful if swallowed

H314 Causes severe skin burns and eye damage

H317 May cause an allergic skin reaction

H410 Very toxic to aquatic life with long lasting effects

SECTION 3: Composition/information on ingredients

Substance

Product name	: Allyl isothiocyanate
Synonyms	: allyl isothiocyanate,3-isothiocyanato-1-propene
CAS	: 57-06-7
EC number	: 200-309-2
MF	: C4H5NS
MW	: 99.16

SECTION 4: First aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Water Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting

Combustible. Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air at elevated temperatures. Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products

Carbon oxides Nitrogen oxides (NOx) Sulfur oxides

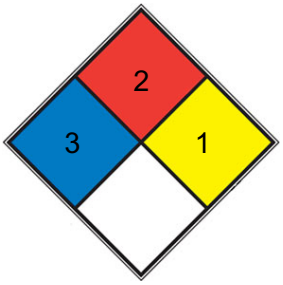
Specific extinguishing methods

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

NFPA 704



■	HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen, sulfuric acid, calcium hypochlorite, hexafluorosilicic acid)
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
■	REACT	1	Normally stable, but can become unstable at elevated temperatures and pressures (e.g. propene)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency

responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material . Dispose of properly. Clean up affected area.

SECTION 7: Handling and storage

Handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Avoidance of contact

Copper Copper alloys

Storage

Further information on storage conditions

Keep container tightly closed in a dry and wellventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Storage class

3, Flammable liquids

Recommended storage temperature

Recommended storage temperature see product label.

Further information on storage stability

Handle and open container with care.

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

No data available

Personal protective equipment

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other

accompanying standards relating to the used respiratory protection system.

Recommended Filter type

Filter A-(P3)

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Tightly fitting safety goggles

Skin and body protection

Flame retardant antistatic protective clothing.

Hand protection

Material

Viton®

Break through time

480 min

Glove thickness

0.7 mm

Protective index

Full contact

Manufacturer

Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Material

butyl-rubber

Break through time

120 min

Glove thickness

0.7 mm

Protective index

Splash contact

Manufacturer

Butoject® (KCL 898)

Remarks

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D- 36124 Eichenzell, Internet: www.kcl.de).

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

clear, liquid

Color

light orange

Odor

mustard-like

Odor Threshold

No data available

pH

No data available

pH

7

pH

7 (ECHA) Bioaccumulation is not expected.

Melting point/ range

-80 °C

Method: lit.

Boiling point/boiling range

150 °C

Method: lit.

Flash point

45 °C (1,013 hPa)

Method: Regulation (EC) No. 440/2008, Annex, A.9, closed cup

GLP: yes

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

No data available

Lower explosion limit / Lower flammability limit

No data available

Vapor pressure

4.5 hPa (23 °C) 0.493 kPa (20 °C) 4.9 hPa (30 °C)

Relative vapor density

No data available

Relative density

1.013 g/mL at 25 °C(lit.)

Density

1.013 g/cm3 (25 °C)

Method: lit.

Water solubility

2 g/l (20 °C)

Partition coefficient: n-octanol/water

log Pow: 1.83 (20 °C)

Autoignition temperature

404 °C (101 kPa)

Method: Regulation (EC) No. 440/2008, Annex, A.15

GLP: yes

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

Not classified as explosive.

Oxidizing properties : Method: Regulation (EC) No. 440/2008, Annex, A.21

GLP: yes none

Surface tension

53.4 mN/m, 20 °C, OECD Test Guideline 115, GLP: yes

Molecular weight

99.15 g/mol

Particle characteristics Particle size

No data available

Solubility

Chloroform (Sparingly), Methanol (Slightly)

Physical state

Fine Crystalline Powder

Dielectric constant

17.199999999999999

SECTION 10: Stability and reactivity

Reactivity

Vapor/air-mixtures are explosive at intense warming.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

A risk of explosion and/or of toxic gas formation exists with the following substances: Strong oxidizing agents acids

Conditions to avoid

Heat. Heating.

Incompatible materials

Copper Copper alloys

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - female - 425.4 mg/kg (OPPTS 870.1100)

LC50 Inhalation - Rat - male and female - 4 h - 0.206 - 0.508 mg/l - aerosol (OPPTS 870.1300)

Inhalation: Irritating to respiratory system.

Acute toxicity estimate Inhalation - 4 h - 0.51 mg/l - vapor (Expert judgment)

LD50 Dermal - Rat - male and female - 200 - 2,000 mg/kg (OPPTS 870.1200)

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive

Remarks: (ECHA)

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: Causes sensitization.

(OPPTS 870.2600)

Germ cell mutagenicity

Test Type: reverse mutation assay

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Test Type: reverse mutation assay

Species: Mouse

Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

SECTION 12: Ecological information

Ecotoxicity

Toxicity to fish

Remarks: No data available

Components:

3-isothiocyanato-1-propene:

Toxicity to fish

LC50 (Oryzias latipes (Orange-red killifish)): 0.07 mg/l Exposure time: 96 h Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates

EC50: 0.73 mg/l Exposure time: 48 h Remarks: (ECHA)

M-Factor (Acute aquatic toxicity)

10

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

NOEC (Oryzias latipes (Orange-red killifish)): 8.5 µg/l Exposure time: 28 d Test Type: mortality

M-Factor (Chronic aquatic toxicity)

10

Persistence and degradability

Biodegradability

Remarks: No data available

Components:

3-isothiocyanato-1-propene:

Biodegradability

aerobic Result: Not readily biodegradable. Biodegradation: 0 % Exposure time: 29 d

Bioaccumulative potential

Bioaccumulation

Remarks: No data available

Components:

3-isothiocyanato-1-propene:

Partition coefficient: noctanol/water

log Pow: 1.83 (20 °C) pH: 7 Remarks: (ECHA) Bioaccumulation is not expected.

Mobility in soil

Stability in soil

Remarks: No data available

Other adverse effects

Components:

3-isothiocyanato-1-propene:

Additional ecological information

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : UN 1545

Proper shipping name : Allyl isothiocyanate, stabilized

Class : 6.1

Subsidiary risk : 3

Packing group : II

Labels : Division 6.1 - Toxic substances, Class 3 - Flammable liquids

Packing instruction (cargo aircraft) : 661

Packing instruction (passenger aircraft) : Not permitted for transport

IMDG-Code

UN number : UN 1545

Proper shipping name : ALLYL ISOTHIOCYANATE, STABILIZED

Class : 6.1

Subsidiary risk : 3

Packing group : II

Labels : 6.1 (3)

EmS Code : F-E, S-D

Marine pollutant : yes

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National regulation GB 6944/12268

UN number : UN 1545

Proper shipping name : ALLYL ISOTHIOCYANATE, STABILIZED

Class : 6.1

Subsidiary risk : 3

Packing group : II

Labels : 6.1 (3)

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15: Regulatory information

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

Listed

No. / Code Chemical name / Category Threshold quantity

J5 Acute toxic 500 t

Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

No. / Code Chemical name / Category Threshold quantity

W5.4 Flammable liquids 5,000 t

Hazardous Chemicals for Priority Management

Listed under SAWS

Regulations on Occupational Labor Protection in the at workplaces where

Toxic Substances Are Used

Catalogue of Highly Toxic Chemicals

Not listed

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not listed

Regulation on the Administration of Precursor Chemicals

Catalogue and Classification of Precursor Chemicals

Not listed

SECTION 16: Other information

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency forTransport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN -Standard of the German Institute for Standardisation

DSL - Domestic SubstancesList (Canada)

ECx - Concentration associated with x% response

ELx - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and NewChemical Substances (Japan)

ErCx - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonized System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Can- cer

IATA - International Air Transport Association

IBC - International Code for theConstruction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC50 -Half maximal inhibitory concentration

ICAO - International Civil Aviation Organiza- tion

IECSC - Inventory of Existing Chemical Substances in China

IMDG - Interna- tional Maritime Dangerous Goods

IMO - International Maritime Organization

ISHL -Industrial Safety and Health Law (Japan)

ISO - International Organisation forStandardization

KECI - Korea Existing Chemicals Inventory

LC50 - Lethal Concen- tration to 50 % of a test population

LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)

MARPOL - International Convention for the Prevention of Pol- lution from Ships

n.o.s. - Not Otherwise Specified

Nch - Chilean Norm

NO(A)EC -No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Ef- fect Level

NOELR - No Observable Effect Loading Rate

NOM - Official MexicanNorm

NTP - National Toxicology Program

NZIoC - New Zealand Inventory of Chem- icals

OECD - Organization for Economic Co-operation and Development

OPPTS - Of- fice of Chemical Safety and Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic substance

PICCS - Philippines Inventory of Chemicals and Chemical Sub- stances

(Q)SAR - (Quantitative) Structure Activity Relationship

REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning theRegistration, Evaluation, Authorisation and Restriction of Chemicals

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - TaiwanChemical Substance Inventory

TDG - Transportation of Dangerous Goods

TECI -Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (UnitedStates)

UN - United Nations

UNRTDG - United Nations Recommendations on theTransport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

WHMIS - Workplace Hazardous Materials Information System