

SAFETY DATA SHEETS

According to the UN GHS revision 10

Version: 1.1
Creation Date: July 15, 2024
Revision Date: January 08, 2025

SECTION 1: Identification

1.1 GHS Product identifier

Product name Allyl Isothiocyanate

1.2 Other means of identification

Product number CCHM702478
Other names FEMA 2034; Redskin; AITK

1.3 Recommended use of the chemical and restrictions on use

Identified uses For laboratory and Industrial use only.
Uses advised against no data available

1.4 Supplier's details

Company CATO Research Chemicals Inc.
Address 3/F,Building B,No.179 BASIGO, Guangpu Rd East,Huangpu Dist,Guangzhou
Telephone +86-20-81960175

1.5 Emergency phone number

Emergency phone number +86-20-81960175
Service hours 'Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

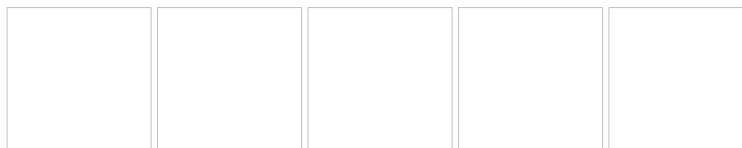
SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Flammable liquids, Category 3
Acute toxicity - Category 4, Oral
Acute toxicity - Category 3, Dermal
Skin corrosion, Sub-category 1C
Skin sensitization, Category 1
Serious eye damage, Category 1
Acute toxicity - Category 2, Inhalation
Respiratory sensitization, Category 1
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H226 Flammable liquid and vapour
H302 Harmful if swallowed
H311 Toxic in contact with skin
H314 Causes severe skin burns and eye damage
H317 May cause an allergic skin reaction
H330 Fatal if inhaled
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

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.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] 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 affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P363 Wash contaminated clothing before reuse.
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.
P333+P317 If skin irritation or rash occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P320 Specific treatment is urgent (see ... on this label).
P342+P316 If experiencing respiratory symptoms: Get emergency medical help immediately.
P391 Collect spillage.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.
P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Allyl Isothiocyanate	Allyl isothiocyanate	57-06-7	200-309-2	≈ 99%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention.

4.2 Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: TOXIC; inhalation, ingestion or contact (skin, eyes) with vapors, dusts or substance may cause severe injury, burns or death. Bromoacetates and chloroacetates are extremely irritating/lachrymators. Reaction with water or moist air will release toxic, corrosive or flammable gases. Reaction with water may generate much heat that will increase the concentration of fumes in the air. Fire will produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Isocyanates, aliphatic thiocyanates, and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use foam, dry chemical, or carbon dioxide. Keep run-off water out of sewers and water sources.

5.2 Specific hazards arising from the chemical

Excerpt from ERG Guide 155 [Substances - Toxic and/or Corrosive (Flammable / Water-Sensitive)]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapors may travel to source of ignition and flash back. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Substance will react with water (some violently) releasing flammable, toxic or corrosive gases and runoff. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated or if contaminated with water. (ERG, 2016)

5.3 Special protective actions for fire-fighters

Use powder, AFFF, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Personal protection: complete protective clothing including self-contained breathing apparatus. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

6.2 Environmental precautions

Evacuate danger area! Personal protection: complete protective clothing including self-contained breathing apparatus. Ventilation. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

6.3 Methods and materials for containment and cleaning up

Environmental considerations: Land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames, NO sparks and NO smoking. Above 46°C use a closed system, ventilation and explosion-proof electrical equipment. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong oxidants, acids and food and feedstuffs. Well closed. Store only if stabilized. Safe Storage: Fireproof. Separated from strong oxidants, acids and food and feedstuffs. Well closed. Store only if stabilized.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-

elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Allyl isothiocyanate, stabilized is a colorless to pale-yellow oily liquid with an irritating odor. Flash point 135°F. Boiling point 300°F. Poisonous by ingestion and skin absorption. Emits toxic fumes when heated to high temperature. Insoluble in water and slightly denser than water. Hence sinks in water. Used to make other chemicals and as a fumigant.
Colour	Colorless to pale yellow, oily liquid
Odour	Very pungent
Melting point/freezing point	-80°C
Boiling point or initial boiling point and boiling range	150°C(lit.)
Flammability	Flammable. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	46°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	less than 0.1 mg/mL at 66° F (NTP, 1992)
Partition coefficient n-octanol/water	log Kow = 2.15 (est)
Vapour pressure	5 mm Hg at 77.5° F ; 10 mm Hg at 100.9° F (NTP, 1992)
Density and/or relative density	1.013g/mL at 25°C(lit.)
Relative vapour density	3.41 (NTP, 1992) (Relative to Air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Decomposes on heating and on burning. Decomposes on contact with acids. This produces highly toxic fumes including nitrogen oxides and sulfur oxides. Reacts with strong oxidants.

10.2 Chemical stability

Tends to darken on aging.

10.3 Possibility of hazardous reactions

Fire risk; combustible. A routine preparation by interaction of allyl chloride and sodium thiocyanate in an autoclave at 5.5 bar exploded violently at the end of the reaction. Peroxides were not present or involved and no other cause could be found, but extensive decomposition occurred when allyl isothiocyanate was heated to 250°C. in glass ampoules [Ind. Eng. Chem. 1941:19 1408].

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Dangerous...on contact with acid or acid fumes, it emits highly toxic fumes of /cyanides, oxides of sulfur, and oxides of nitrogen/.

10.6 Hazardous decomposition products

When heated to decomposition or on contact with acid or acid fumes it emits highly toxic fumes of /cyanides, oxides of sulfur, and oxides of nitrogen/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 339 mg/kg (10% solution in corn oil)
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Evaluation: There is inadequate evidence in humans for the carcinogenicity of allyl isothiocyanate. There is limited evidence in experimental animals for the carcinogenicity of allyl isothiocyanate. Overall evaluation: Allyl isothiocyanate is not classifiable as to its carcinogenicity to humans (Group 3).

Reproductive toxicity

no data available

STOT-single exposure

Lachrymation. The substance is irritating to the eyes, skin and respiratory tract.

STOT-repeated exposure

Repeated or prolonged contact with skin may cause dermatitis. Repeated or prolonged contact may cause skin sensitization. The substance may have effects on the liver, kidneys, stomach, thyroid and bladder.

Aspiration hazard

No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20°C.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50; Species: *Pimephales promelas* (fathead minnow); Conditions: flow-through bioassay with measured concentrations, 25.1 deg C, dissolved oxygen 6.9 mg/L, and pH 7.8; Concentration: 85.6 ug/L for 96 hr
- Toxicity to daphnia and other aquatic invertebrates: no data available
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC: A mean half-life of 2 days in 6 different soils maintained at 75% moisture capacity and 20 deg C was reported for allyl isothiocyanate, present at 500 ug/g wet soil. When maintained under aerobic conditions, transformation rates were not affected(1), suggesting that biodegradation is not an important environmental fate process(SRC).

12.3 Bioaccumulative potential

An estimated BCF of 12 was calculated in fish for allyl isothiocyanate(SRC), using an estimated log Kow of 2.15(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4 Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of allyl isothiocyanate can be estimated to be 260(SRC). According to a classification scheme(2), this estimated Koc value suggests that allyl isothiocyanate is expected to have moderate mobility in soil.

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN1545 (For reference only, please check.) IMDG: UN1545 (For reference only, please check.) IATA: UN1545 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: ALLYL ISOTHIOCYANATE, STABILIZED (For reference only, please check.) IMDG: ALLYL ISOTHIOCYANATE, STABILIZED (For reference only, please check.) IATA: ALLYL ISOTHIOCYANATE, STABILIZED (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.) IMDG: 6.1 (For reference only, please check.) IATA: 6.1 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: II (For reference only, please check.) IMDG: II (For reference only, please check.) IATA: II (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: Yes IMDG: Yes IATA: Yes

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Allyl isothiocyanate	Allyl isothiocyanate	57-06-7	200-309-2
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Not Listed.

SECTION 16: Other information

Information on revision

Creation Date July 15, 2024
Revision Date January 08, 2025

Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:



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- http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
 - ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
 - ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
 - Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
 - ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Other Information

An added stabilizer or inhibitor can influence the toxicological properties of this substance, consult an expert.

Any questions regarding this SDS, Please send your inquiry to info@cato-chem.com

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