

Safety data sheet
according to Regulation (EC) No 1907/2006, Article 31

Printing date 25.01.2025

Version number 1

Revision: 04.09.2020

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

- **1.1 Product identifier**
- **Trade name: Allyl Isothiocyanate (Mustard Oil) synthetic**
- **Product number: 4083**
- **CAS Number:**
57-06-7
- **EC number:**
200-309-2
- **1.2 Relevant identified uses of the substance or mixture and uses advised against**
No further relevant information available.
- **Application of the substance / the mixture** Flavoring Ingredients
- **1.3 Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Advanced Biotech
10 Taft Road
Totowa, NJ 07512 USA
- **Further information obtainable from:**
Product Safety Department
productsafety@adv-bio.com
- **1.4 Emergency telephone number:**
Infotrac: 1-800-535-5053 (Domestic) & 1-352-323-3500 (International)
Email: responders@infotrac.net & During normal business hours: 1-973-339-6242

SECTION 2: Hazards identification

- **2.1 Classification of the substance or mixture**
- **Classification according to Regulation (EC) No 1272/2008**



GHS02 flame

Flam. Liq. 3 H226 Flammable liquid and vapour.



GHS06 skull and crossbones

Acute Tox. 3 H311 Toxic in contact with skin.
Acute Tox. 2 H330 Fatal if inhaled.



GHS08 health hazard

Resp. Sens. 1 H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.



GHS05 corrosion

Skin Corr. 1C H314 Causes severe skin burns and eye damage.
Eye Dam. 1 H318 Causes serious eye damage.

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GHS09 environment

Aquatic Acute 1 H400 Very toxic to aquatic life.
 Aquatic Chronic 1 H410 Very toxic to aquatic life with long lasting effects.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.
 Skin Sens. 1B H317 May cause an allergic skin reaction.

- **Labelling according to Regulation (EC) No 1272/2008**
 The substance is classified and labelled according to the CLP regulation.
- **Hazard pictograms**



GHS02 GHS05 GHS06 GHS08 GHS09

- **Signal word** Danger
- **Hazard-determining components of labelling:**
 Allyl isothiocyanate
- **Hazard statements**
 H226 Flammable liquid and vapour.
 H302 Harmful if swallowed.
 H311 Toxic in contact with skin.
 H330 Fatal if inhaled.
 H314 Causes severe skin burns and eye damage.
 H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
 H317 May cause an allergic skin reaction.
 H410 Very toxic to aquatic life with long lasting effects.

- **Precautionary statements**
 P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
 P260 Do not breathe dusts or mists.
 P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].
 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/doctor.
 P320 Specific treatment is urgent (see on this label).
 P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
 P405 Store locked up.
 P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **2.3 Other hazards**
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.

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· **vPvB:** Not applicable.

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SECTION 3: Composition/information on ingredients

- **3.1 Substances**
- **CAS No. Description**
CAS: 57-06-7 Allyl isothiocyanate
- **Identification number(s)**
- **EC number:** 200-309-2
- **Acute toxicity estimate (ATE) values**
LD50 oral: 425 mg/kg
LD50 dermal: 300 mg/kg
LC50/4 h inhalative: 0.05 mg/l

SECTION 4: First aid measures

- **4.1 Description of first aid measures**
- **General information:**
Immediately remove any clothing soiled by the product.
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
Remove breathing equipment only after contaminated clothing have been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.
- **After inhalation:**
Supply fresh air or oxygen; call for doctor.
In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
- **After swallowing:** Call for a doctor immediately.
- **4.2 Most important symptoms and effects, both acute and delayed**
No further relevant information available.
- **4.3 Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

SECTION 5: Firefighting measures

- **5.1 Extinguishing media**
- **Suitable extinguishing agents:**
CO₂, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **For safety reasons unsuitable extinguishing agents:** Water with full jet
- **5.2 Special hazards arising from the substance or mixture**
During heating or in case of fire poisonous gases are produced.
- **5.3 Advice for firefighters**
- **Protective equipment:** Mouth respiratory protective device.
- **Additional information**
Cool endangered receptacles with water spray.
Collect contaminated fire fighting water separately. It must not enter the sewage system.

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SECTION 6: Accidental release measures

- **6.1 Personal precautions, protective equipment and emergency procedures**
Mount respiratory protective device.
Wear protective equipment. Keep unprotected persons away.
- **6.2 Environmental precautions:**
Do not allow product to reach sewage system or any water course.
Inform respective authorities in case of seepage into water course or sewage system.
Do not allow to enter sewers/ surface or ground water.
- **6.3 Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Use neutralising agent.
Dispose contaminated material as waste according to section 13.
Ensure adequate ventilation.
- **6.4 Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

SECTION 7: Handling and storage

- **7.1 Precautions for safe handling**
Ensure good ventilation/exhaustion at the workplace.
Open and handle receptacle with care.
Prevent formation of aerosols.
- **Information about fire - and explosion protection:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
Keep respiratory protective device available.
- **7.2 Conditions for safe storage, including any incompatibilities**
- **Storage:**
- **Requirements to be met by storerooms and receptacles:**
Please refer to the product specification and/or Certificate of Analysis for product storage requirements.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:** Keep container tightly sealed.
- **7.3 Specific end use(s)** No further relevant information available.

SECTION 8: Exposure controls/personal protection

- **8.1 Control parameters**
- **Ingredients with limit values that require monitoring at the workplace:** Not required.
- **Additional information:** The lists valid during the making were used as a basis.
- **8.2 Exposure controls**
- **Appropriate engineering controls** No further data; see section 7.
- **Individual protection measures, such as personal protective equipment**
- **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing
Wash hands before breaks and at the end of work.
Store protective clothing separately.

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Avoid contact with the skin.
Avoid contact with the eyes and skin.

· **Respiratory protection:**

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use self-contained respiratory protective device.

· **Hand protection**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material should be based on consideration of the penetration times, rates of diffusion and the degradation

· **Material of gloves**

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

· **Penetration time of glove material**

The exact break through time has to be determined by the manufacturer of the protective gloves and has to be observed.

· **Eye/face protection**



Tightly sealed goggles

SECTION 9: Physical and chemical properties

· **9.1 Information on basic physical and chemical properties**

· General Information	Molecular Weight: 99.16 g/mol
· Physical state	Liquid
· Colour:	According to product specification
· Odour:	According to product specification
· Odour threshold:	Not determined.
· Melting point/freezing point:	-100 °C
· Boiling point or initial boiling point and boiling range	148-154 °C
· Flammability	Flammable.
· Lower and upper explosion limit	
· Lower:	Not determined.
· Upper:	Not determined.
· Flash point:	45 °C
· Decomposition temperature:	Not determined.
· pH	Not determined.
· Viscosity:	
· Kinematic viscosity	Not determined.
· Dynamic:	Not determined.
· Solubility	
· water at 20 °C:	2 g/l

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- **Partition coefficient n-octanol/water (log value)** Not determined.
- **Vapour pressure at 38 °C:** 13 hPa
- **Density and/or relative density**
- **Density at 20 °C:** 1.005-1.035 g/cm³
- **Relative density** Not determined.
- **Specific Gravity** 1.005-1.035 @ 20 °C
- **Refractive Index**
- **Vapour density** Not determined.

- **9.2 Other information**
- **Appearance:**
- **Form:** Liquid
- **Important information on protection of health and environment, and on safety.**
- **Ignition temperature:** Not determined.
- **Explosive properties:** Product is not explosive. However, formation of explosive air/vapour mixtures are possible.
- **Solvent content:**
- **VOC (EC)** 0.00 %
- **Change in condition**
- **Evaporation rate** Not determined.

- **Information with regard to physical hazard classes**
- **Explosives** Void
- **Flammable gases** Void
- **Aerosols** Void
- **Oxidising gases** Void
- **Gases under pressure** Void
- **Flammable liquids** Flammable liquid and vapour.
- **Flammable solids** Void
- **Self-reactive substances and mixtures** Void
- **Pyrophoric liquids** Void
- **Pyrophoric solids** Void
- **Self-heating substances and mixtures** Void
- **Substances and mixtures, which emit flammable gases in contact with water** Void
- **Oxidising liquids** Void
- **Oxidising solids** Void
- **Organic peroxides** Void
- **Corrosive to metals** Void
- **Desensitised explosives** Void

SECTION 10: Stability and reactivity

- **10.1 Reactivity** No further relevant information available.
- **10.2 Chemical stability**
- **Thermal decomposition / conditions to be avoided:**
 No decomposition if used according to specifications.
- **10.3 Possibility of hazardous reactions** No dangerous reactions known.
- **10.4 Conditions to avoid** No further relevant information available.

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- **10.5 Incompatible materials:** No further relevant information available.
- **10.6 Hazardous decomposition products:** No dangerous decomposition products known.

SECTION 11: Toxicological information

- **11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008**

- **Acute toxicity**

Toxic if swallowed.
 Fatal in contact with skin.

- **LD/LC50 values relevant for classification:**

ATE (Acute Toxicity Estimates)

Oral	LD50	112 mg/kg (rat)
Dermal	LD50	88 mg/kg (rabbit)
Inhalative	LC50/4 h	0.5 mg/l

CAS: 57-06-7 Allyl isothiocyanate

Oral	LD50	425 mg/kg (ATE) 112 mg/kg (rat)
Dermal	LD50	300 mg/kg (ATE) 88 mg/kg (rabbit)

- **Primary irritant effect:**
- **Skin corrosion/irritation** Causes severe skin burns and eye damage.
- **Serious eye damage/irritation** Causes serious eye damage.
- **Respiratory or skin sensitisation**
 May cause allergy or asthma symptoms or breathing difficulties if inhaled.
 May cause an allergic skin reaction.
- **Germ cell mutagenicity** Based on available data, the classification criteria are not met.
- **Carcinogenicity** Based on available data, the classification criteria are not met.
- **Reproductive toxicity** Based on available data, the classification criteria are not met.
- **STOT-single exposure** Based on available data, the classification criteria are not met.
- **STOT-repeated exposure** Based on available data, the classification criteria are not met.
- **Aspiration hazard** Based on available data, the classification criteria are not met.
- **11.2 Information on other hazards**

- **Endocrine disrupting properties**

Substance is not listed.

SECTION 12: Ecological information

- **12.1 Toxicity**
- **Aquatic toxicity:** No further relevant information available.
- **12.2 Persistence and degradability** No further relevant information available.
- **12.3 Bioaccumulative potential** No further relevant information available.
- **12.4 Mobility in soil** No further relevant information available.
- **12.5 Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **12.6 Endocrine disrupting properties**
 The product does not contain substances with endocrine disrupting properties.

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· **12.7 Other adverse effects**

· **Remark:** Very toxic for fish

· **Additional ecological information:**

· **General notes:**

Water hazard class 2 (German Regulation) (Self-assessment): hazardous for water

Do not allow product to reach ground water, water course or sewage system.

Must not reach sewage water or drainage ditch undiluted or unneutralised.

Danger to drinking water if even small quantities leak into the ground.

Also poisonous for fish and plankton in water bodies.

Very toxic for aquatic organisms

SECTION 13: Disposal considerations

· **13.1 Waste treatment methods**

· **Recommendation**

Must not be disposed together with household garbage. Do not allow product to reach sewage system.

· **Uncleaned packaging:**

· **Recommendation:** Disposal must be made according to official regulations.

SECTION 14: Transport information

· **14.1 UN number or ID number**

· **ADR, IMDG, IATA**

UN1545

· **14.2 UN proper shipping name**

· **ADR**

1545 ALLYL ISOTHIOCYANATE, STABILIZED,
ENVIRONMENTALLY HAZARDOUS

· **IMDG, IATA**

ALLYL ISOTHIOCYANATE, STABILIZED

· **14.3 Transport hazard class(es)**

· **ADR**



· **Class**

6.1 (TF1) Toxic substances.

· **Label**

6.1+3

· **IMDG**



· **Class**

6.1 Toxic substances.

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· Label	6.1/3
· IATA	
	
· Class	6.1 Toxic substances.
· Label	6.1 (3)
· 14.4 Packing group · ADR, IMDG, IATA	II
· 14.5 Environmental hazards: · Marine pollutant:	No Symbol (fish and tree)
· Special marking (ADR):	Symbol (fish and tree)
· 14.6 Special precautions for user · Hazard identification number (Kemler code): · EMS Number: · Stowage Category · Stowage Code	Warning: Toxic substances. 639 F-E,S-D D SW1 Protected from sources of heat. SW2 Clear of living quarters.
· 14.7 Maritime transport in bulk according to IMO instruments	Not applicable.
· Transport/Additional information:	
· ADR · Limited quantities (LQ) · Excepted quantities (EQ)	100 ml Code: E0 Not permitted as Excepted Quantity
· Transport category · Tunnel restriction code	2 D/E
· IMDG · Limited quantities (LQ) · Excepted quantities (EQ)	100 ml Code: E4 Maximum net quantity per inner packaging: 1 ml Maximum net quantity per outer packaging: 500 ml
· UN "Model Regulation":	UN 1545 ALLYL ISOTHIOCYANATE, STABILIZED, 6.1 (3), II, ENVIRONMENTALLY HAZARDOUS

SECTION 15: Regulatory information

- 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture
- Labelling according to Regulation (EC) No 1272/2008
The substance is classified and labelled according to the CLP regulation.

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· **Hazard pictograms**



GHS02 GHS05 GHS06 GHS08 GHS09

· **Signal word** Danger

· **Hazard-determining components of labelling:**

Allyl isothiocyanate

· **Hazard statements**

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

· **Precautionary statements**

- P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
- P260 Do not breathe dusts or mists.
- P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower].
- 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/doctor.
- P320 Specific treatment is urgent (see on this label).
- P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
- P405 Store locked up.
- P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

· **Directive 2012/18/EU**

· **Named dangerous substances - ANNEX I** Substance is not listed.

· **Seveso category**

H2 ACUTE TOXIC
 E1 Hazardous to the Aquatic Environment
 P5c FLAMMABLE LIQUIDS

· **Qualifying quantity (tonnes) for the application of lower-tier requirements** 50 t

· **Qualifying quantity (tonnes) for the application of upper-tier requirements** 200 t

· **REGULATION (EC) No 1907/2006 ANNEX XVII** Conditions of restriction: 3

· **DIRECTIVE 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment – Annex II**

Substance is not listed.

· **REGULATION (EU) 2019/1148**

· **Annex I - RESTRICTED EXPLOSIVES PRECURSORS (Upper limit value for the purpose of licensing under Article 5(3))**

Substance is not listed.

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· **Annex II - REPORTABLE EXPLOSIVES PRECURSORS**

Substance is not listed.

· **Regulation (EC) No 273/2004 on drug precursors**

Substance is not listed.

· **Regulation (EC) No 111/2005 laying down rules for the monitoring of trade between the Community and third countries in drug precursors**

Substance is not listed.

· **15.2 Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

· **Department issuing SDS:** Product safety department

· **Contact:**

Product Safety Department
productsafety@adv-bio.com

· **Abbreviations and acronyms:**

ADR: Accord relatif au transport international des marchandises dangereuses par route (European Agreement Concerning the International Carriage of Dangerous Goods by Road)
 IMDG: International Maritime Code for Dangerous Goods
 IATA: International Air Transport Association
 GHS: Globally Harmonised System of Classification and Labelling of Chemicals
 EINECS: European Inventory of Existing Commercial Chemical Substances
 CAS: Chemical Abstracts Service (division of the American Chemical Society)
 VOC: Volatile Organic Compounds (USA, EU)
 LC50: Lethal concentration, 50 percent
 LD50: Lethal dose, 50 percent
 PBT: Persistent, Bioaccumulative and Toxic
 vPvB: very Persistent and very Bioaccumulative
 ATE: Acute toxicity estimate values
 Flam. Liq. 3: Flammable liquids – Category 3
 Acute Tox. 4: Acute toxicity – Category 4
 Acute Tox. 3: Acute toxicity – Category 3
 Acute Tox. 2: Acute toxicity – Category 2
 Skin Corr. 1C: Skin corrosion/irritation – Category 1C
 Eye Dam. 1: Serious eye damage/eye irritation – Category 1
 Resp. Sens. 1: Respiratory sensitisation – Category 1
 Skin Sens. 1B: Skin sensitisation – Category 1B
 Aquatic Acute 1: Hazardous to the aquatic environment - acute aquatic hazard – Category 1
 Aquatic Chronic 1: Hazardous to the aquatic environment - long-term aquatic hazard – Category 1