

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

Printing date 25.01.2025



Version number 1

Revision: 25.01.2025

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

- **1.1 Product identifier**
- **Trade name:** 3-(methylthio) Propyl Isothiocyanate synthetic
- **Product number:** 4087
- **CAS Number:**
505-79-3
- **EC number:**
208-020-3
- **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**
-  GHS07
- Acute Tox. 4 H302 Harmful if swallowed.
- Skin Sens. 1 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**
-  GHS07
- **Signal word** Warning
- **Hazard-determining components of labelling:**
3-(methylthio) Propyl Isothiocyanate
- **Hazard statements**
H302 Harmful if swallowed.
H317 May cause an allergic skin reaction.
- **Precautionary statements**
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves.

(Contd. on page 2)

Safety data sheet

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 1)

P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.

P330 Rinse mouth.

P333+P313 If skin irritation or rash occurs: Get medical advice/attention.

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.
- **vPvB:** Not applicable.

SECTION 3: Composition/information on ingredients

- **3.1 Substances**
- **CAS No. Description**
CAS: 505-79-3 3-(methylthio) Propyl Isothiocyanate
- **Identification number(s)**
- **EC number:** 208-020-3
- **Acute toxicity estimate (ATE) values** LD50 oral: 540 mg/kg

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.
- **After inhalation:**
Supply fresh air and be sure to call for a 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.
- **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.
- **5.2 Special hazards arising from the substance or mixture** No further relevant information available.
- **5.3 Advice for firefighters**
- **Protective equipment:** No special measures required.
- **Additional information**
Cool endangered receptacles with water spray.
Collect contaminated fire fighting water separately. It must not enter the sewage system.

(Contd. on page 3)

Safety data sheet

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 2)

SECTION 6: Accidental release measures

- **6.1 Personal precautions, protective equipment and emergency procedures** Not required.
- **6.2 Environmental precautions:** No special measures required.
- **6.3 Methods and material for containment and cleaning up:**
 Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
 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.
 Prevent formation of aerosols.
- **Information about fire - and explosion protection:** No special measures required.
- **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:** None.
- **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.
- **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.

(Contd. on page 4)

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 3)

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** Goggles recommended during refilling

SECTION 9: Physical and chemical properties

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

· **General Information**

· **Physical state**

Liquid

· **Colour:**

According to product specification

· **Odour:**

According to product specification

· **Odour threshold:**

Not determined.

· **Melting point/freezing point:**

Undetermined.

· **Boiling point or initial boiling point and boiling range**

Undetermined.

· **Flammability**

Not applicable.

· **Lower and upper explosion limit**

· **Lower:**

Not determined.

· **Upper:**

Not determined.

· **Flash point:**

86.6 °C

· **Decomposition temperature:**

Not determined.

· **pH**

Not determined.

· **Viscosity:**

· **Kinematic viscosity**

Not determined.

· **Dynamic:**

Not determined.

· **Solubility**

· **water:**

Not miscible or difficult to mix.

· **Partition coefficient n-octanol/water (log value)**

Not determined.

· **Vapour pressure:**

Not determined.

· **Density and/or relative density**

· **Density at 20 °C:**

1.111 g/cm³

· **Relative density**

Not determined.

· **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 does not present an explosion hazard.

(Contd. on page 5)

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 4)

- **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** Void
- **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.
- **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** Harmful if swallowed.

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

ATE (Acute Toxicity Estimates)

Oral	LD50	540 mg/kg (ATE)
------	------	-----------------

CAS: 505-79-3 3-(methylthio) Propyl Isothiocyanate

Oral	LD50	540 mg/kg (ATE)
------	------	-----------------

- **Primary irritant effect:**
- **Skin corrosion/irritation** Based on available data, the classification criteria are not met.

(Contd. on page 6)

Safety data sheet

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 5)

- **Serious eye damage/irritation** Based on available data, the classification criteria are not met.
- **Respiratory or skin sensitisation** 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.
- **12.7 Other adverse effects**
- **Additional ecological information:**
- **General notes:** Not hazardous for water.

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

- | | |
|--|---|
| <ul style="list-style-type: none"> · 14.1 UN number or ID number · ADR, IMDG, IATA | <p>UN2206</p> |
| <ul style="list-style-type: none"> · 14.2 UN proper shipping name · ADR | <p>2206 ISOCYANATES, TOXIC, N.O.S. (3-(methylthio) Propyl Isothiocyanate)</p> |
| <ul style="list-style-type: none"> · IMDG, IATA | <p>ISOCYANATES, TOXIC, N.O.S. (3-(methylthio) Propyl Isothiocyanate)</p> |

(Contd. on page 7)

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 6)

· **14.3 Transport hazard class(es)**

· **ADR, IMDG, IATA**



· **Class** 6.1 Toxic substances.
· **Label** 6.1

· **14.4 Packing group**

· **ADR, IMDG, IATA** II

· **14.5 Environmental hazards:**

· **Marine pollutant:** No

· **14.6 Special precautions for user**

· **Stowage Category** E
· **Stowage Code** 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)** 100 ml
· **Excepted quantities (EQ)** Code: E4
Maximum net quantity per inner packaging: 1 ml
Maximum net quantity per outer packaging: 500 ml

· **IMDG**

· **Limited quantities (LQ)** 100 ml
· **Excepted quantities (EQ)** Code: E4
Maximum net quantity per inner packaging: 1 ml
Maximum net quantity per outer packaging: 500 ml

· **UN "Model Regulation":**

UN 2206 ISOCYANATES, TOXIC, N.O.S. (3-(METHYLTHIO) PROPYL ISOTHIOCYANATE), 6.1, II

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.

· **Hazard pictograms**



GHS07

(Contd. on page 8)

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 7)

- **Signal word** Warning
- **Hazard-determining components of labelling:**
3-(methylthio) Propyl Isothiocyanate
- **Hazard statements**
H302 Harmful if swallowed.
H317 May cause an allergic skin reaction.
- **Precautionary statements**
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves.
P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P330 Rinse mouth.
P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
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.
- **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.

· **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)

(Contd. on page 9)

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

Printing date 25.01.2025

Version number 1

Revision: 25.01.2025

Trade name: 3-(methylthio) Propyl Isothiocyanate synthetic

(Contd. of page 8)

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
Acute Tox. 4: Acute toxicity – Category 4
Skin Sens. 1: Skin sensitisation – Category 1

IE

Advanced Biotech