

According to Regulation (EC) No 1907/2006

# Ethyl isothiocyanate

Version number: 1  
Issued: 2023-11-15



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

### 1.1. Product identifier

**Trade name**

Ethyl isothiocyanate

**CAS number**

542-85-8

**EC number**

208-831-2

**Synonyms**

1-Isothiocyanatoethane

### 1.2. Relevant identified uses of the substance or mixture and uses advised against

**Relevant identified uses**

Research and development.

**Not suitable for use in**

Not suitable for human consumption or veterinary purposes.

### 1.3. Details of the supplier of the safety data sheet

**Supplier**

Molekula Group

Address

Molekula Ltd, Lingfield Way, Darlington,  
DL1 4XX Darlington  
United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

**Contact person**

Kevin Banks

**Email**

+44 (0) 7769276927

### 1.4. Emergency telephone number

**Poison center/Additional emergency number**

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

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## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

#### Classification

Serious eye damage, hazard category 1  
Hazardous to the aquatic environment — Acute hazard category 1  
Respiratory sensitisation, hazard category 1  
Acute toxicity, oral, hazard category 3  
Acute toxicity, dermal, hazard category 3  
Acute toxicity, inhalation, hazard category 2  
Skin corrosion, hazard category 1  
Flammable liquids, hazard category 3

#### Hazard statements

H226, H301 + H311 + H331, H314, H334, H400

### 2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

#### Hazard pictograms



#### Signal word

Danger

#### Hazard statements

H226 Flammable liquid and vapour.  
H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled  
H314 Causes severe skin burns and eye damage.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
H400 Very toxic to aquatic life.

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## Precautionary statements

P202 Do not handle until all safety precautions have been read and understood.  
P260 Do not breathe dust/fumes/gas/mist/vapours/spray.  
P262 Do not get in eyes, on skin, or on clothing.  
P264 Wash skin thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P271 Use only outdoors or in a well-ventilated area.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P284 wear respiratory protection.  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.  
P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.  
P302 + P352 IF ON SKIN: Wash with plenty of water/.  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.  
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.  
P314 Get medical advice/attention if you feel unwell.  
P320 Specific treatment is urgent (see on this label).  
P342 + P311 If experiencing respiratory symptoms: Call a POISON CENTER/doctor.  
P361 + P364 Take off immediately all contaminated clothing and wash it before reuse.  
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P405 Store locked up.  
P501 Dispose of contents/container to local regulations.

## 2.3. Other hazards

No data available

## SECTION 3: Composition/information on ingredients

### 3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrases M factor acute M factor chronic	Note
Ethyl isothiocyanate	542-85-8 208-831-2 - -	100%	Flam. Liq. 3, Acute Tox. 3 - oral, Acute Tox. 3 - dermal, Acute Tox. 3 - inhala- tion, Skin Corr. 1, Resp. Sens. 1, Aquatic Acute 1	H226, H301 + H311 + H331, H314, H334, H400 - -	-

## Molecular weight

87.14

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## **Substance additional information**

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

## **SECTION 4: First aid measures**

### **4.1. Description of first aid measures**

IF exposed or concerned: Get medical advice/attention. First aiders/ medical personnel need to protect themselves. Show this Safety Data Sheet (SDS) to medical personnel.

#### **Inhalation**

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/doctor. If breathing stops, provide artificial respiration. For breathing difficulties oxygen may be necessary.

#### **Skin contact**

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water [or shower]. Immediately call a POISON CENTER/doctor.

#### **Eye contact**

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

#### **Ingestion**

IF SWALLOWED: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only if the persons are fully conscious and awake). Administer activated charcoal (20 - 40g in a 10% slurry) and consult a doctor as quickly as possible. Do not attempt to neutralise.

#### **Information for doctors**

No data available.

### **4.2. Most important symptoms and effects, both acute and delayed**

The severity of the symptoms described will vary dependant of the concentration and the length of exposure. Causes burns by all exposure routes.

See section 11 for more detailed information on health effects and symptoms.

#### **Inhalation**

Single exposure may cause the following adverse effects: Causes severe burns. Difficulty in breathing. Unconsciousness, possibly death.

#### **Skin contact**

Single exposure may cause the following adverse effects: Causes severe burns. Blistering may occur. May be absorbed in the body and cause dizziness, nausea and vomiting. Unconsciousness, death.

#### **Eye contact**

Single exposure may cause the following adverse effects: Causes serious eye damage. Unconsciousness, possibly death.

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## Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. May cause severe internal injury. Unconsciousness, possibly death.

## 4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically. Immediately call a POISON CENTER/doctor.

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

#### Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

#### Unsuitable extinguishing media

No specific fire fighting procedure given.

### 5.2. Special hazards arising from the substance or mixture

Specific hazards: FLAMMABLE. Corrosive. Toxic. Combustible.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

Nitrous gases (NO<sub>x</sub>).

Sulphur oxides

Vapours are heavier than air and may travel along the floor and in the bottom of containers.

Explosive mixtures may be formed at elevated temperatures

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3. Advice for firefighters

#### Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Prevent skin contact by maintaining a safe distance and by wearing suitable protective equipment/ clothing. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

Do not breathe vapour/spray. Avoid contact with skin and eyes. For personal protection, see section 8.

In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

### 6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground. Risk of explosion.

### 6.3. Methods and material for containment and cleaning up

Collect with absorbent, non-combustible material into suitable containers. Use spark-proof tools and explosion-proof equipment.

### 6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

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## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Preventive handling precautions

For precautions see section 2.2. Work under hood. Keep away from open flames and hot surfaces. No smoking. Take action to prevent static discharges. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

#### General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Wash contaminated skin thoroughly after handling. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use.

### 7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container.  
Store at ambient temperature.  
Keep away from heat and sources of ignition.  
Toxic storage. Flammable liquid storage. Corrosive storage.

Moisture Sensitive.

### 7.3. Specific end use(s)

No specific usage precautions noted.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No data available

### 8.2. Exposure controls

#### Personal Protective Equipment Symbols



#### Eye / face protection

Wear eye protection.

#### Hand protection

Wear protective gloves. Recommended gloves: Viton rubber (fluor rubber).  
Glove Thickness: 0.7mm  
Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

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## Other skin protection

Wash skin thoroughly after handling.

## Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

## Environmental exposure controls

Avoid discharge into drains.

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

#### Physical state

Liquid

#### Colour

Light yellow

#### Odour

Rotten eggs.

#### Melting point / freezing point

-6 °C

#### Boiling point or initial boiling point and boiling range

130 - 132 °C

#### Flammability

No data available

#### Lower and upper explosion limit

No data available

#### Flash point

31 °C

#### **Method**

CC (Closed cup).

#### Auto-ignition temperature

No data available

#### Decomposition temperature

No data available

#### pH

6.3

#### Kinematic viscosity

No data available

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## Solubility

Insoluble.

## Partition coefficient n-octanol/water

No data available

## Vapour pressure

No data available

## Density and/or relative density

0.995 g/cm<sup>3</sup>

## Relative vapour density

3

## Particle characteristics

No data available

## 9.2. Other information

No data available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

Vapor/air-mixtures are explosive at intense warming.

### 10.2. Chemical stability

Stable under the prescribed storage conditions. Moisture Sensitive.

### 10.3. Possibility of hazardous reactions

Violent reactions possible with:

Alcohols

Amines.

oxidising agents

Hot concentrated sulphuric acid.

### 10.4. Conditions to avoid

Heating.

### 10.5. Incompatible materials

Strong oxidising agents. Acids. Water Strong bases Alcohols Amines.

### 10.6. Hazardous decomposition products

See section 5.

## SECTION 11: Toxicological information

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

#### Acute toxicity



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Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Duration of exposure
Ethyl isothiocyanate 542-85-8 / 208-831-2	LD50	100 mg/kg	Oral	-
Ethyl isothiocyanate 542-85-8 / 208-831-2	LC50	3.1 mg/l	Inhalation.	4 hours
Ethyl isothiocyanate 542-85-8 / 208-831-2	LD50	300 mg/kg	Dermal	-

## Aspiration hazard

Based on available data, the classification criteria are not met.

## 11.2. Information on other hazards

No data available

## SECTION 12: Ecological information

### 12.1. Toxicity

#### Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
Ethyl isothiocyanate 542-85-8 / 208-831-2	EC50	0.4 mg/l	48 hours	Daphnia magna
Ethyl isothiocyanate 542-85-8 / 208-831-2	LC50	0.43 mg/l	48 hours	Daphnia magna

### 12.2. Persistence and degradability

No data available

### 12.3. Bioaccumulative potential

No data available

### 12.4. Mobility in soil

No data available

### 12.5. Results of PBT and vPvB assessment

No data available

### 12.6. Endocrine disrupting properties

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

### 12.7. Other adverse effects

No data available

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## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

#### Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

## SECTION 14: Transport information

### 14.1. UN number

3286

### 14.2. UN proper shipping name

#### ADR / RID / ADN proper shipping name

FLAMMABLE LIQUID, TOXIC, CORROSIVE, N.O.S. (Ethyl isothiocyanate)

#### IMDG proper shipping name

FLAMMABLE LIQUID, TOXIC, CORROSIVE, N.O.S. (Ethyl isothiocyanate)

#### IATA proper shipping name

Flammable liquid, toxic, corrosive, n.o.s. (Ethyl isothiocyanate)

### 14.3. Transport hazard class(es)

#### Label

ADR/RID/ADN



3

6.1

8

IMDG



3

6.1

8

IATA



3

6.1

8

#### ADR / RID Class

3

#### ADR / RID Classification code

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## ADR / RID hazard identification number

368

## IMDG Class

3 (6.1/8)

## IATA Class

3 (6.1, 8)

## ADN Class

3

## ADN Class Code

FTC

### 14.4. Packing group

ADR / RID / ADN: II

IMDG: II

IATA: II

### 14.5. Environmental hazards

#### IMDG EmS

F-E, S-C

### 14.6. Special precautions for user

Tunnel restriction code: D/E

Transport category: 2

### 14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC99

## SECTION 15: Regulatory information

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

#### EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### National regulations

Directive: 2012/18/EU

H2 ACUTE TOXIC

E1 ENVIRONMENTAL HAZARDS

P5c FLAMMABLE LIQUIDS

### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

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## SECTION 16: Other information

### Phrase meaning

Eye Dam. 1 - Serious eye damage, hazard category 1  
Aquatic Acute 1 - Hazardous to the aquatic environment — Acute hazard category 1  
Resp. Sens. 1 - Respiratory sensitisation, hazard category 1  
Acute Tox. 3 - oral - Acute toxicity, oral, hazard category 3  
Acute Tox. 3 - dermal - Acute toxicity, dermal, hazard category 3  
Acute Tox. 2 - inhalation - Acute toxicity, inhalation, hazard category 2  
Skin Corr. 1 - Skin corrosion, hazard category 1  
Flam. Liq. 3 - Flammable liquids, hazard category 3  
Acute Tox. 3 - inhalation - Acute toxicity, inhalation, hazard category 3  
H226 Flammable liquid and vapour.  
H301 + H311 + H331 Toxic if swallowed, in contact with skin or if inhaled  
H314 Causes severe skin burns and eye damage.  
H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled.  
H400 Very toxic to aquatic life.