

# Safety Data Sheet

#50147670 · Full 16-section SDS

According to Regulation (EC) No 1907/2006  
According to Regulation (EC) No 2020/878

| PRODUCT                                    | CAS NUMBER     | FORMULA                                                                 | VERSION   | REVISION DATE      |
|--------------------------------------------|----------------|-------------------------------------------------------------------------|-----------|--------------------|
| <b>Ethyl (ethoxymethylene)cyanoacetate</b> | <b>94-05-3</b> | <b>C<sub>2</sub>H<sub>5</sub>OCH=C(CN)COOC<sub>2</sub>H<sub>5</sub></b> | <b>10</b> | <b>05 Oct 2026</b> |

## SECTION 1

### Identification

#### 1.1 Product identifier

|                           |                                                                         |
|---------------------------|-------------------------------------------------------------------------|
| <b>Product name</b>       | Ethyl (ethoxymethylene)cyanoacetate                                     |
| <b>CAS number</b>         | 94-05-3                                                                 |
| <b>EC / EINECS number</b> | 202-299-5                                                               |
| <b>Chemical formula</b>   | C <sub>2</sub> H <sub>5</sub> OCH=C(CN)COOC <sub>2</sub> H <sub>5</sub> |
| <b>Molecular weight</b>   | 169.18                                                                  |
| <b>SMILES</b>             | CCO\C=C(\C#N)C(=O)OCC                                                   |

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

Research and development. Laboratory Chemicals. Manufacture of substances.  
Not suitable for human consumption or veterinary purposes.

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

Molekula Limited  
1 Millennium Way, Newton Aycliffe  
Durham, DL5 6JW, United Kingdom  
info@molekula.com · +44 (0) 3302 000333

#### 1.4 Emergency telephone number

**0344 892 0111** — National Poisons Information Service (NPIS) (United Kingdom — for healthcare professionals (via TOXBASE))

## SECTION 2

### Hazard identification

#### 2.1 Classification of the substance or mixture

Acute Tox. 4 (oral), H302  
Skin Irrit. 2, H315  
Eye Irrit. 2, H319  
STOT SE 3 (respiratory tract irritation), H335

## 2.2 Label elements



### WARNING

| CODE         | HAZARD STATEMENT                                                                                                    |
|--------------|---------------------------------------------------------------------------------------------------------------------|
| H302         | Harmful if swallowed                                                                                                |
| H315         | Causes skin irritation                                                                                              |
| H317         | May cause an allergic skin reaction                                                                                 |
| H318         | Causes serious eye damage                                                                                           |
| H334         | May cause allergy or asthma symptoms or breathing difficulties if inhaled                                           |
| H335         | May cause respiratory irritation                                                                                    |
| CODE         | PRECAUTIONARY STATEMENT                                                                                             |
| P261         | Avoid breathing dust/fume/gas/mist/vapours/spray                                                                    |
| P280         | Wear protective gloves/protective clothing/eye protection/face protection                                           |
| P301+312     | IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell                                           |
| P304+340     | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing                     |
| P305+351+338 | IF IN EYES: Rinse with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing |
| P310         | Immediately call a POISON CENTER or doctor/physician                                                                |
| P342+311     | Call a POISON CENTER or doctor                                                                                      |

## 2.3 Other hazards

Does not meet the PBT or vPvB criteria of REACH Annex XIII.  
This product does not contain any known or suspected Endocrine disruptors.

## SECTION 3

### Composition / information on ingredients

#### 3.1 Substances

|                                                          |                                                                                                                          |
|----------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| Name                                                     | Ethyl (ethoxymethylene)cynoacetate                                                                                       |
| CAS number                                               | 94-05-3                                                                                                                  |
| EC number                                                | 202-299-5                                                                                                                |
| Concentration / purity                                   | ~100.0%                                                                                                                  |
| Classification according to Regulation (EC) No 1272/2008 | Acute Tox. 4 (oral), H302<br>Skin Irrit. 2, H315<br>Eye Irrit. 2, H319<br>STOT SE 3 (respiratory tract irritation), H335 |
| Hazard statements                                        | H302, H315, H317, H318, H334, H335                                                                                       |
| Acute toxicity estimate (ATE)                            | Not reported                                                                                                             |
| Impurities / stabilising additives                       | Not applicable                                                                                                           |

## SECTION 4

### First-aid measures

#### 4.1 Description of first aid measures

|                     |                                                                                                                                                                                                                                                                                                       |
|---------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Inhalation</b>   | If breathing is difficult, remove to fresh air and keep at rest; give oxygen or artificial respiration if necessary; get medical advice if breathing difficulties persist. Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention. |
| <b>Skin contact</b> | Remove contaminated clothing immediately and wash with plenty of water; do not remove clothing stuck to skin; consult a doctor if irritation persists. Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.                   |
| <b>Eye contact</b>  | Rinse immediately with plenty of water, remove contact lenses if easy, continue rinsing; get medical attention if irritation persists.                                                                                                                                                                |
| <b>Ingestion</b>    | Rinse mouth with water; do not induce vomiting; get medical advice/attention.                                                                                                                                                                                                                         |

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel. First aiders/ medical personnel need to protect themselves.

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

Causes eye burns. May cause allergy or asthma symptoms or breathing difficulties if inhaled. May cause allergic skin reaction. Causes severe eye damage. Symptoms of allergic reaction may include rash, itching, swelling, trouble breathing, tingling of the hands and feet, dizziness, lightheadedness, chest pain, muscle pain or flushing

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

Get immediate medical advice/attention. Treat symptomatically.

## SECTION 5

### Fire-fighting measures

#### 5.1 Extinguishing media

|                                       |                                                      |
|---------------------------------------|------------------------------------------------------|
| <b>Suitable extinguishing media</b>   | Foam, dry powder, carbon dioxide, water spray, sand. |
| <b>Unsuitable extinguishing media</b> | Do not use a heavy water stream.                     |

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

Corrosive  
Combustible  
Carbon monoxide (CO)  
Carbon dioxide (CO<sub>2</sub>)  
Nitrogen oxides (NO<sub>x</sub>)  
Vapours are heavier than air and may spread along floors or in the bottom of containers.  
Forms explosive mixtures with air on intense heating.  
Development of hazardous combustion gases or vapours possible in the event of fire.

#### 5.3 Advice for firefighters

Use water spray to cool exposed containers; do not enter fire area without proper protective equipment including respiratory protection; prevent firefighting water from entering the environment.

## SECTION 6

### Accidental release measures

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

Evacuate unnecessary personnel, eliminate ignition sources, avoid dust formation and contact with skin/eyes; responders use self-contained breathing apparatus and chemically protective clothing.

#### 6.2 Environmental precautions

Prevent entry to sewers and public waters; notify authorities if product enters them.

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

Sweep or shovel up into suitable closed containers for disposal.

#### 6.4 Reference to other sections

For specific precautions, see Section 8 and Section 13.

## SECTION 7

### Handling & storage

#### 7.1 Precautions for safe handling

Avoid creating or spreading dust; provide local exhaust or general ventilation; do not eat, drink or smoke when using; wash hands after handling.

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

**Storage temperature** Ambient

**Conditions for safe storage (incompatibilities)** Store below 20 °C in original closed container in a cool, dry, well-ventilated place away from heat, sunlight and ignition sources; incompatible with strong oxidizing agents, strong acids, strong bases and strong reducing agents.

#### 7.3 Specific end use(s)

See Section 1.2.

## SECTION 8

### Exposure controls / personal protection

#### 8.1 Control parameters

**Occupational exposure limits (OEL / WEL)** No additional information available

**DNEC/PNEC data** Handle in accordance with good industrial hygiene and safety procedures.

## 8.2 Exposure controls

|                                        |                                                                                                                                                                                                                                                                                                                              |
|----------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Eye / face protection</b>           | Chemical splash goggles<br>Wear eye/face protection as recommended. All eye/face protection should comply with EN ISO 16321-1:2022.                                                                                                                                                                                          |
| <b>Skin / hand protection</b>          | Disposable nitrile rubber (NBR) gloves, 0.11 mm, breakthrough >480 min (EN 374); protective clothing with elasticated cuffs and closed neck (EN ISO 13982).                                                                                                                                                                  |
| <b>Respiratory protection</b>          | Dust mask (FFP2/FFP3)<br>Keep self-contained breathing apparatus readily available for emergency use. Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided. Respiratory equipment: Reusable Air-Purifying Respirator (APR). Filter type: ABEK. Standard: EN 14387. |
| <b>Other protection</b>                | Do not eat, drink or smoke during use; emergency safety showers should be available.                                                                                                                                                                                                                                         |
| <b>Environmental exposure controls</b> | Avoid release to the environment.                                                                                                                                                                                                                                                                                            |

## SECTION 9

### Physical & chemical properties

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

|                                                          |                                                                     |
|----------------------------------------------------------|---------------------------------------------------------------------|
| <b>Appearance / physical state</b>                       | Solid<br><b>DERIVED FROM: LITERATURE</b>                            |
| <b>Colour</b>                                            | White to off-white, light yellow<br><b>DERIVED FROM: LITERATURE</b> |
| <b>Odour</b>                                             | Not known<br><b>DERIVED FROM: LITERATURE</b>                        |
| <b>Melting / freezing point</b>                          | 48 - 52 °C (lit.)<br><b>DERIVED FROM: LITERATURE</b>                |
| <b>Boiling point</b>                                     | 190 - 191 (lit.)<br><b>DERIVED FROM: LITERATURE</b>                 |
| <b>Flammability</b>                                      | Non flammable<br><b>DERIVED FROM: LITERATURE</b>                    |
| <b>Lower and upper explosion limit</b>                   | <i>No data available</i>                                            |
| <b>Flash point</b>                                       | 130 °C<br><b>DERIVED FROM: LITERATURE</b>                           |
| <b>Auto-ignition temperature</b>                         | <i>No data available</i>                                            |
| <b>Decomposition temperature</b>                         | <i>No data available</i>                                            |
| <b>pH</b>                                                | <i>No data available</i>                                            |
| <b>Acidity</b>                                           | Neutral<br><b>DERIVED FROM: LITERATURE</b>                          |
| <b>Kinematic viscosity</b>                               | <i>No data available</i>                                            |
| <b>Solubility</b>                                        | Water: <0.01 g/L (20°C)<br><b>DERIVED FROM: LITERATURE</b>          |
| <b>Partition coefficient n-octanol/water (log value)</b> | <i>No data available</i>                                            |

|                 |                   |
|-----------------|-------------------|
| Vapour pressure | No data available |
|-----------------|-------------------|

|                |                                        |
|----------------|----------------------------------------|
| Density (g/mL) | 1.076 g/mL<br>DERIVED FROM: LITERATURE |
|----------------|----------------------------------------|

|                         |                   |
|-------------------------|-------------------|
| Relative vapour density | No data available |
|-------------------------|-------------------|

|                          |                   |
|--------------------------|-------------------|
| Particle characteristics | No data available |
|--------------------------|-------------------|

## 9.2 Other information

No data available

## SECTION 10

### Stability & reactivity

#### 10.1 Reactivity

The product is non-reactive under normal conditions of use, storage and transport.  
Forms explosive mixtures with air on intense heating.  
A range from ~15 Kelvin below the flash point is rated as critical.

#### 10.2 Chemical stability

Stable under the prescribed storage conditions

#### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Strong oxidising agents  
Strong acids  
Strong bases  
Strong reducing agents

#### 10.4 Conditions to avoid

Protect from sunlight; keep away from heat, hot surfaces, sparks, open flames and other ignition sources; no smoking.

#### 10.5 Incompatible materials

Strong oxidizers, strong acids, strong bases, strong reducing agents.

#### 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 (LD50 / LC50) | LD50 (Oral): <2000 mg/kg (Rat) |
|------------------------------|--------------------------------|

|                             |                         |
|-----------------------------|-------------------------|
| Skin corrosion / irritation | Causes skin irritation. |
|-----------------------------|-------------------------|

|                            |                           |
|----------------------------|---------------------------|
| Eye corrosion / irritation | Causes serious eye damage |
|----------------------------|---------------------------|

|                                  |                                                                                       |
|----------------------------------|---------------------------------------------------------------------------------------|
| Respiratory / skin sensitisation | Respiratory: Category 1<br>Skin: Category 1- may cause sensitisation by skin contact. |
|----------------------------------|---------------------------------------------------------------------------------------|

|                 |                |
|-----------------|----------------|
| Carcinogenicity | Not classified |
|-----------------|----------------|

|              |                |
|--------------|----------------|
| Mutagenicity | Not classified |
|--------------|----------------|

**Reproductive toxicity**

Not classified

**STOT (single / repeated exposure)**Single exposure: may cause respiratory irritation  
Repeated exposure: not classified.**Aspiration hazard**

Solid.

**11.2 Information on other hazards**

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

## SECTION 12

**Ecological information****12.1 Toxicity**

Fish:

LC50: 135 mg/L/96h (Brachydanio rerio)

Crustacea:

EC50: 211.4 mg/L/48h

Algae:

EC50: 104 mg/L/72h (Scenedesmus subspicatus)

**12.2 Persistence and degradability***No data available***12.3 Bioaccumulative potential***No data available***12.4 Mobility in soil**

No additional information available

**12.5 Results of PBT and vPvB assessment**

Does not meet the PBT or vPvB criteria of REACH Annex XIII.

**12.6 Endocrine disrupting properties***See Section 11.2.***12.7 Other adverse effects***No data available*

## SECTION 13

**Disposal considerations****13.1 Waste treatment methods**

Dispose of in accordance with local/national regulations

## SECTION 14

**Transport information****14.1 UN number or ID number***Not applicable*

#### 14.2 UN proper shipping name

Not applicable

#### 14.3 Transport hazard class(es)

Not applicable

#### 14.4 Packing group

Not applicable

#### 14.5 Environmental hazards

Not applicable

#### 14.6 Special precautions for user

Special precautions for user Not applicable

Transport category Not applicable

Tunnel code Not applicable

Packing instruction (ADR) Not applicable

Packing instruction (IMDG) Not applicable

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

No data available

### SECTION 15

#### Regulatory information

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

Substance-specific regulations (e.g. licences) No REACH Annex XVII restrictions; not on the REACH Candidate List.

REACH code Y110

ECHA notification Not applicable

##### 15.2 Chemical safety assessment

No

### SECTION 16

#### Other information

Revision notes / other information This version (v10) was created on 05.10.2026 and replaces version 1 (26.11.2019).

This Safety Data Sheet was generated automatically from the data Molekula holds against this product, in the 16-section GHS/CLP format. Fields shown as "No data available" carry no recorded value; fields shown as "Not applicable" were assessed as not relevant to this substance. For queries, contact Molekula at [info@molekula.com](mailto:info@molekula.com).