

Safety Data Sheet

#90028383 · 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
Allyl mercaptan	870-23-5	C3H6S	10	03 Sep 2026

SECTION 1

Identification

1.1 Product identifier

Product name Allyl mercaptan

CAS number 870-23-5

EC / EINECS number 212-792-7

Chemical formula C3H6S

Molecular weight 74.14

SMILES C=CCS

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

For research and development. Laboratory chemicals. Manufacture of substances. Not suitable for human 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

Flam. Liq. 2; H225
Acute Tox. 4; H302
Acute Tox. 4; H312
Acute Tox. 4; H332

2.2 Label elements



DANGER

CODE	HAZARD STATEMENT
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H225	Highly flammable liquid and vapour
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H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled
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CODE	PRECAUTIONARY STATEMENT
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P210	Keep away from heat/sparks/open flames/hot surfaces - No smoking
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P261	Avoid breathing dust/fume/gas/mist/vapours/spray
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P280	Wear protective gloves/protective clothing/eye protection/face protection
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P301+P312	IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
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P302+P350	IF ON SKIN: Gently wash with soap and water
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P304+P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
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P307+P311	IF exposed: Call a POISON CENTER or doctor/physician
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2.3 Other hazards

Not applicable

SECTION 3

Composition / information on ingredients

3.1 Substances

Name	Allyl mercaptan
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CAS number	870-23-5
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EC number	212-792-7
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Concentration / purity	~100%
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Classification according to Regulation (EC) No 1272/2008	Flam. Liq. 2; H225 Acute Tox. 4; H302 Acute Tox. 4; H312 Acute Tox. 4; H332
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Hazard statements	H225, H302 + H312 + H332
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Acute toxicity estimate (ATE)	<i>No data available</i>
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Impurities / stabilising additives	<i>Not applicable</i>
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SECTION 4

First-aid measures

4.1 Description of first aid measures

Inhalation	Remove victim to fresh air; give oxygen/artificial respiration if needed; seek medical attention if breathing difficulties persist
Skin contact	Remove contaminated clothing (unless stuck to skin); wash immediately with plenty of water; consult doctor if irritation persists
Eye contact	Rinse immediately with water for at least 15 minutes; remove contact lenses if safe; seek medical attention if irritation persists
Ingestion	Rinse mouth with water; do not induce vomiting; seek immediate medical 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

Treat symptomatically.

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5

Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media Dry powder, sand, water spray, carbon dioxide, foam.

Unsuitable extinguishing media Heavy water stream.

5.2 Special hazards arising from the substance or mixture

Carbon oxides, Sulphur oxides

Combustible.

Pay attention to flashback.

Vapours are heavier than air and may spread along floors.

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

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Use water spray to cool exposed containers. Prevent fire-fighting water from entering the environment. Wear self-contained breathing apparatus and protective clothing.

SECTION 6

Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Ventilate area thoroughly, especially low-lying areas. Wear protective equipment. Evacuate unnecessary personnel.

6.2 Environmental precautions

Prevent entry into sewers or public waters. Notify authorities if contamination occurs.

6.3 Methods and material for containment and cleaning up

Contain spills with bunding. Soak up with inert solids (e.g., clay, diatomaceous earth). Stop release if safe.

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 vapor formation. Ensure proper ventilation. Do not handle in confined spaces. Handle empty containers with care due to residual flammable vapors.

7.2 Conditions for safe storage, including any incompatibilities

Storage temperature	Ambient
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Conditions for safe storage (incompatibilities)	Keep tightly closed, away from heat/sparks/flames. Store in a well-ventilated area. Avoid incompatible materials (not specified).
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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)	<i>Not applicable</i>
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DNEC/PNEC data	<i>Not applicable</i>
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8.2 Exposure controls

Eye / face protection	Safety glasses Wear eye/face protection as recommended. All eye/face protection should comply with EN ISO 16321-1:2022.
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Skin / hand protection	Recommended gloves: Viton rubber (fluor rubber), 0.7mm (480mins).
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Respiratory protection	Full-face respirator 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.
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Other protection	<i>No data available</i>
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Environmental exposure controls	<i>No data available</i>
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SECTION 9

Physical & chemical properties**9.1 Information on basic physical and chemical properties**

Appearance / physical state	Liquid DERIVED FROM: LITERATURE
Colour	Colourless to pale yellow DERIVED FROM: LITERATURE
Odour	Pungent DERIVED FROM: LITERATURE
Melting / freezing point	<i>Not applicable</i>
Boiling point	66 - 68 °C at 1,013 hPa DERIVED FROM: LITERATURE
Flammability	<i>No data available</i>
Lower and upper explosion limit	<i>No data available</i>
Flash point	18 °C DERIVED FROM: LITERATURE
Auto-ignition temperature	<i>Not applicable</i>
Decomposition temperature	<i>No data available</i>
pH	<i>Not applicable</i>
Acidity	<i>Not applicable</i>
Kinematic viscosity	<i>No data available</i>
Solubility	Insoluble in water DERIVED FROM: LITERATURE
Partition coefficient n-octanol/water (log value)	<i>Not applicable</i>
Vapour pressure	<i>Not applicable</i>
Density (g/mL)	0.93 g/mL DERIVED FROM: LITERATURE
Relative vapour density	<i>No data available</i>
Particle characteristics	<i>No data available</i>

9.2 Other information*No data available*

SECTION 10

Stability & reactivity**10.1 Reactivity***No data available***10.2 Chemical stability***Not applicable*

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, sparks, open flames, and confined spaces.

10.5 Incompatible materials

Oxidising agents

10.6 Hazardous decomposition products

Carbon oxides (CO, CO₂) and sulfur oxides.

SECTION 11

Toxicological information

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

Acute toxicity (LD50 / LC50)	Oral LD50: Harmful (Category 4): 500.1 mg/kg Dermal/Inhalation LC50: Harmful (Category 4): 11.1 mg/l (4 h) Vapour.
Skin corrosion / irritation	May cause moderate skin irritation
Eye corrosion / irritation	May cause eye irritation
Respiratory / skin sensitisation	Not applicable
Carcinogenicity	Not applicable
Mutagenicity	Not applicable
Reproductive toxicity	Not applicable
STOT (single / repeated exposure)	Not applicable
Aspiration hazard	Not applicable

11.2 Information on other hazards

Not applicable

SECTION 12

Ecological information

12.1 Toxicity

Not applicable

12.2 Persistence and degradability

Not applicable

12.3 Bioaccumulative potential

Not applicable

12.4 Mobility in soil

Not applicable

12.5 Results of PBT and vPvB assessment

Not applicable

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

UN3336

14.2 UN proper shipping name

MERCAPTANS, LIQUID, FLAMMABLE, N.O.S.

14.3 Transport hazard class(es)

3



14.4 Packing group

II

14.5 Environmental hazards

Not applicable

14.6 Special precautions for user

Special precautions for user *Not applicable*

Transport category 2

Tunnel code (D/E)

Packing instruction (ADR) P001

Packing instruction (IMDG) P001

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 data available*

REACH code Y110

ECHA notification *Not applicable*

15.2 Chemical safety assessment

Not applicable

SECTION 16

Other information

Revision notes / other information This SDS replaces version 1.0, issued 13/09/2019

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.