

According to Regulation (EC) No 1907/2006

4-Octyne

Version number: 1
Issued: 2023-10-09



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

1.1. Product identifier

Trade name

4-Octyne

CAS number

1942-45-6

EC number

217-730-2

Synonyms

Oct-4-yne

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

Street 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 address

+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

Skin irritation, hazard category 2

Eye irritation, hazard category 2

Specific Target Organ Toxicity — Single exposure, hazard category 3

Flammable liquids, hazard category 3

Aspiration hazard, hazard category 1

Hazard statements

H226, H304, H315, H319, H335

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Danger

Hazard statements

H226 Flammable liquid and vapour.

H304 May be fatal if swallowed and enters airways.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

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Precautionary statements

P202 Do not handle until all safety precautions have been read and understood.
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
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.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P302 + P352 IF ON SKIN: Wash with plenty of water/.
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.
P312 Call a POISON CENTER/doctor if you feel unwell.
P332 + P313 If skin irritation occurs: Get medical advice/attention.
P337 + P313 If eye irritation persists: Get medical advice/attention.
P362 + P364 Take off contaminated clothing and wash it before reuse.
P403 Store in a well-ventilated place.
P405 Store locked up.
P501 Dispose of contents/container to .

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.1. Substances

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-pharse M factor acute M factor chronic	Note
4-Octyne	1942-45-6 217-730-2 - -	100%	Flam. Liq. 3, Asp. Tox. 1, Skin Irrit. 2, Eye Irrit. 2, STOT SE 3	H226, H304, H315, H319, H335 - -	-

Molecular weight

110.20

Substance additional information

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

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SECTION 4: First aid measures

4.1. Description of first aid measures

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel.

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. In case of persistent throat irritation or coughing: Seek medical attention and bring these instructions.

Skin contact

IF ON SKIN: Wash with plenty of soap and water. Continue to rinse for at least 15 minutes. Get medical advice/attention if you feel unwell.

Eye contact

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

Ingestion

Rinse mouth. Do NOT induce vomiting. Get medical advice/attention if you feel unwell. Risk of aspiration upon vomiting

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.

Inhalation

Single exposure may cause the following adverse effects: Upper respiratory irritation. Difficulty in breathing.

Skin contact

Single exposure may cause the following adverse effects: Severe skin irritation.

Eye contact

May cause temporary eye irritation.

Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. Nausea, vomiting.

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

Treat symptomatically. No special treatment requirement.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Use alcohol resistant foam, carbon dioxide or dry powder to extinguish.

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Unsuitable extinguishing media

No specific fire fighting procedure given.

5.2. Special hazards arising from the substance or mixture

Specific hazards: FLAMMABLE.

Containers can burst violently when heated, due to excess pressure build-up.

Vapours may form explosive mixture with air at room temperature.

Carbon monoxide (CO). Carbon dioxide (CO₂).

Combustible.

Combustible liquid.

Vapours are heavier than air and may travel along the floor and 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

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

Avoid inhalation of vapours and spray mist and contact with skin and eyes. For personal protection, see section 8. Provide adequate ventilation. Remove sources of ignition. Beware of the explosion danger. Take action to prevent static discharges.

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. Remove sources of ignition. Beware of the explosion danger. 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.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take action to prevent static discharges. Use spark-proof tools and explosion-proof equipment. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Avoid ingestion and inhalation.

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General hygiene

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

7.2. Conditions for safe storage, including any incompatibilities

Store at room temperature. Store in a dry place. Store in a closed container. Handle and store contents under inert gas. Moisture Sensitive.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Exposure limits

No occupational exposure limit assigned.

8.2. Exposure controls

Personal Protective Equipment Symbols



Eye / face protection

Wear eye protection.

Hand protection

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

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. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Liquid

Colour

Colourless.

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Odour

Characteristic.

Melting point / freezing point

-103 °C

Boiling point or initial boiling point and boiling range

131 - 132 °C

Flammability

No data available

Lower and upper explosion limit

0.8 - 37 %

Flash point

29 °C

Auto-ignition temperature

No data available

Decomposition temperature

No data available

pH

No data available

Kinematic viscosity

No data available

Solubility

Insoluble.

Partition coefficient n-octanol/water

3.55

Vapour pressure

12.9 hPa

Density and/or relative density

0.751 g/cm³

Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

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SECTION 10: Stability and reactivity

10.1. Reactivity

There are no known reactivity hazards associated with this product.

10.2. Chemical stability

Stable under normal temperature conditions. Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

There are no known conditions that are likely to result in a hazardous situation.

10.4. Conditions to avoid

Heat, sparks, flames.

10.5. Incompatible materials

oxidising 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

Product / Substance name CAS / EC no.	Exposure route	Remarks
4-Octyne 1942-45-6 / 217-730-2	Inhalation.	May cause irritation to the respiratory system.

STOT-single exposure

Product / Substance name CAS / EC no.	Exposure route	Result
4-Octyne 1942-45-6 / 217-730-2	Inhalation.	May cause respiratory irritation.

Aspiration hazard

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

11.2. Information on other hazards

Endocrine disrupting properties

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

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SECTION 12: Ecological information

12.1. Toxicity

No data available

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

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

3295

14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

HYDROCARBONS, LIQUID, N.O.S. (4-Octyne)

IMDG proper shipping name

HYDROCARBONS, LIQUID, N.O.S. (4-Octyne)

IATA proper shipping name

Hydrocarbons, liquid, n.o.s. (4-Octyne)

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14.3. Transport hazard class(es)

Label

ADR/RID/ADN



3

IMDG



3

IATA



3

ADR / RID Class

3

ADR / RID Classification code

F1

ADR / RID hazard identification number

30

IMDG Class

3

IATA Class

3

ADN Class

3

ADN Class Code

F1

14.4. Packing group

ADR / RID / ADN: III

IMDG: III

IATA: III

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14.5. Environmental hazards

IMDG EmS

F-E, S-D

14.6. Special precautions for user

Tunnel restriction code: D/E

Transport category: 3

14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC03

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: FLAMMABLE LIQUIDS

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

Phrase meaning

Skin Irrit. 2 - Skin irritation, hazard category 2

Eye Irrit. 2 - Eye irritation, hazard category 2

STOT SE 3 - Specific Target Organ Toxicity — Single exposure, hazard category 3

Flam. Liq. 3 - Flammable liquids, hazard category 3

Asp. Tox. 1 - Aspiration hazard, hazard category 1

H226 Flammable liquid and vapour.

H304 May be fatal if swallowed and enters airways.

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