

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

| | |
|---------------------------|-------------------|
| Product Description: | 4-Octyne |
| Cat No. : | 43157 |
| Synonyms | Dipropylacetylene |
| CAS No | 1942-45-6 |
| Molecular Formula | C8 H14 |
| REACH registration number | - |

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

| | |
|----------------------|--------------------------|
| Recommended Use | Laboratory chemicals. |
| Uses advised against | No Information available |

1.3. Details of the supplier of the safety data sheet

| | |
|---------|--|
| Company | Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608 |
|---------|--|

| | |
|----------------|--------------------------------|
| E-mail address | begel.sdsdesk@thermofisher.com |
|----------------|--------------------------------|

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Flammable liquids

Category 3 (H226)

Health hazards

Based on available data, the classification criteria are not met

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H226 - Flammable liquid and vapor

Precautionary Statements

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

| Component | CAS No | EC No | Weight % | CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567 |
|-----------|-----------|-------------------|----------|---|
| Oct-4-yne | 1942-45-6 | EEC No. 217-730-2 | >95 | Flam. Liq. 3 (H226) |

REACH registration number

-

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

Eye Contact

Immediate medical attention is required. Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention. Take off contaminated clothing and shoes immediately.

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

| | |
|---|--|
| Ingestion | Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. Call a physician immediately. If possible drink milk afterwards. |
| Inhalation | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required. |
| Self-Protection of the First Aider | Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination. |

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

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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

Notes to Physician Treat symptomatically. Symptoms may be delayed.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

Do not use a solid water stream as it may scatter and spread fire.

5.2. Special hazards arising from the substance or mixture

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Thermal decomposition can lead to release of irritating gases and vapors, Carbon monoxide (CO), Carbon dioxide (CO₂).

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Sweep up and shovel into suitable containers for disposal. Remove all sources of ignition. Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Refrigerator/flammables. Keep away from heat/sparks/open flames/hot surfaces. - No smoking. Keep away from heat, sparks and flame. Flammables area. Keep container tightly closed in a dry and well-ventilated place.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s):

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ventilation systems. Use explosion-proof electrical/ventilating/lighting equipment.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

control hazardous materials at source

Personal protective equipment

Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand Protection

Protective gloves

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments |
|----------------|-----------------------------------|-----------------|-------------|-----------------------|
| Nitrile rubber | See manufacturers recommendations | - | EN 374 | (minimum requirement) |
| Viton (R) | | | | |

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection

No protective equipment is needed under normal use conditions.

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Small scale/Laboratory use

Maintain adequate ventilation

Environmental exposure controls

No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

| | | |
|---|---------------------------------|-----------------------------------|
| Physical State | Liquid | |
| Appearance | Clear | |
| Odor | Odorless | |
| Odor Threshold | No data available | |
| Melting Point/Range | -103 °C / -153.4 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | 131 - 132 °C / 267.8 - 269.6 °F | @ 760 mmHg |
| Flammability (liquid) | Flammable | On basis of test data |
| Flammability (solid,gas) | Not applicable | Liquid |
| Explosion Limits | No data available | |
| Flash Point | 29 °C / 84 °F | Method - No information available |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | No data available | |
| pH | No information available | |
| Viscosity | No data available | |
| Water Solubility | No information available | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Vapor Pressure | 35 mmHg @ 37.7 °C | |
| Density / Specific Gravity | 0.750 | |
| Bulk Density | Not applicable | Liquid |
| Vapor Density | 3.8 | (Air = 1.0) |
| Particle characteristics | Not applicable (liquid) | |

9.2. Other information

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

| | |
|-----------------------------|--|
| Molecular Formula | C8 H14 |
| Molecular Weight | 110.2 |
| Explosive Properties | explosive air/vapour mixtures possible |

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity None known, based on information available

10.2. Chemical stability Stable under normal conditions.

10.3. Possibility of hazardous reactions

| | |
|---------------------------------|---------------------------|
| Hazardous Polymerization | No information available. |
| Hazardous Reactions | No information available. |

10.4. Conditions to avoid Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.

10.5. Incompatible materials Oxidizing agent.

10.6. Hazardous decomposition products Thermal decomposition can lead to release of irritating gases and vapors. Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information No acute toxicity information is available for this product

(a) acute toxicity;

| | |
|-------------------|-------------------|
| Oral | No data available |
| Dermal | No data available |
| Inhalation | No data available |

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

| | |
|--------------------|-------------------|
| Respiratory | No data available |
| Skin | No data available |

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available
There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

12.4. Mobility in soil No information available

12.5. Results of PBT and vPvB assessment No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

**Persistent Organic Pollutant
Ozone Depletion Potential**

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

European Waste Catalogue (EWC) According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN1993
14.2. UN proper shipping name Flammable liquid, n.o.s.
Technical Shipping Name 4-Octyne
14.3. Transport hazard class(es) 3
14.4. Packing group III

ADR

14.1. UN number UN1993
14.2. UN proper shipping name Flammable liquid, n.o.s.
Technical Shipping Name 4-Octyne
14.3. Transport hazard class(es) 3
14.4. Packing group III

IATA

14.1. UN number UN1993
14.2. UN proper shipping name Flammable liquid, n.o.s.
Technical Shipping Name 4-Octyne
14.3. Transport hazard class(es) 3
14.4. Packing group III

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

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

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

| Component | CAS No | EINECS | ELINCS | NLP | IECSC | TCSI | KECL | ENCS | ISHL |
|-----------|-----------|-----------|--------|-----|-------|------|----------|------|------|
| Oct-4-yne | 1942-45-6 | 217-730-2 | - | - | - | X | KE-26783 | - | - |

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | DSL | NDSL | AICS | NZIoC | PICCS |
|-----------|-----------|------|---|-----|------|------|-------|-------|
| Oct-4-yne | 1942-45-6 | X | ACTIVE | - | X | - | X | X |

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

Authorisation/Restrictions according to EU REACH Not applicable

| Component | CAS No | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|-----------|-----------|---|---|---|
| Oct-4-yne | 1942-45-6 | - | - | - |

Seveso III Directive (2012/18/EC)

| Component | CAS No | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements |
|-----------|-----------|---|--|
| Oct-4-yne | 1942-45-6 | Not applicable | Not applicable |

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification Water endangering class = 3 (self classification)

| Component | Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81) | Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC) | Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure |
|------------------------------|--|---|---|
| Oct-4-yne 1942-45-6 (>95) | Prohibited and Restricted Substances | | |

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H226 - Flammable liquid and vapor

Legend

SAFETY DATA SHEET

4-Octyne

Revision Date 10-Feb-2024

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.

Chemical incident response training.

Prepared By

Health, Safety and Environmental Department

Creation Date

23-Feb-2012

Revision Date

10-Feb-2024

Revision Summary

New emergency telephone response service provider.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet