ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

4-Octyne

Revision Date:2026-05-31 Revision Number:1

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

Product identifier

Product name	: 4-Octyne
CBnumber	: CB3853276
CAS	: 1942-45-6
EINECS Number	: 217-730-2
Synonyms	: 4-Octyne,oct-4-yne

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

Relevant identified uses	: For R&D use only. Not for medicinal, household or other use.
Uses advised against	: none

Company Identification

Company	: Chemicalbook
Address	: Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone	: 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)

Signal word Danger

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P233 Keep container tightly closed.

P240 Ground/bond container and receiving equipment.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P331 Do NOT induce vomiting.

Hazard statements

H226 Flammable liquid and vapour

H304 May be fatal if swallowed and enters airways

H319 Causes serious eye irritation

H335 May cause respiratory irritation

SECTION 3: Composition/information on ingredients

Substance

Product name	: 4-Octyne
Synonyms	: 4-Octyne,oct-4-yne
CAS	: 1942-45-6
EC number	: 217-730-2
MF	: C8H14
MW	: 110.2

SECTION 4: First aid measures

General advice

Show this safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

Protection of first-aiders

For personal protection see section 8.

Notes to physician

No data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Foam Carbon dioxide (CO2) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extin- guishing agents are given.

Specific hazards during fire fighting

Combustible liquid. Combustible. Vapours are heavier than air and may spread along floors. Forms explosive mixtures with air at elevated temperatures. Development of hazardous combustion gases or vapours possible in the event of fire.

Hazardous combustion products

Carbon oxides

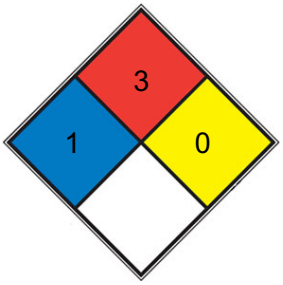
Specific extinguishing methods

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters

In the event of fire, wear self-contained breathing apparatus.

NFPA 704



■	HEALTH	1	Exposure would cause irritation with only minor residual injury (e.g. acetone, sodium bromate, potassium chloride)
■	FIRE	3	Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions . Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, acetone)
■	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium,N2)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains. Risk of explosion.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material . Dispose of properly. Clean up affected area.

SECTION 7: Handling and storage

Handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Avoidance of contact

Oxidizing agents

Storage

Further information on storage conditions

Keep container tightly closed in a dry and wellventilated place. Keep away from heat and sources of ignition.

Storage class

3, Flammable liquids

Recommended storage temperature

Recommended storage temperature see product label.

Packaging material

Suitable material: Mild Steel Drum

SECTION 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures

No data available

Personal protective equipment

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type

Filter type ABEK

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Safety glasses

Skin and body protection

Flame retardant antistatic protective clothing.

Hand protection

Remarks

required

Hygiene measures

Change contaminated clothing. Wash hands after working with substance.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

liquid

Color

colourless

Odor

characteristic

Odor Threshold

No data available

pH

No data available

Melting point/ range

-103 °C

Method: lit.

Boiling point/boiling range

131 - 132 °C

Method: lit.

Flash point

29 °C

Method: closed cup

Evaporation rate

No data available

Flammability (solid, gas)

No data available

Flammability (liquids)

No data available

Burning rate

No data available

Upper explosion limit / Upper flammability limit

37 %(V)

Lower explosion limit / Lower flammability limit

0.8 %(V)

Vapor pressure

12.9 hPa (25 °C)

Relative vapor density

1.4 (25 °C)

Relative density

0.751 g/mL at 25 °C(lit.)

Density

0.751 g/cm3 (25 °C)

Method: lit.

Water solubility

insoluble (20 °C)

Partition coefficient: n-octanol/water

log Pow: 3.55

Method: (calculated) (Lit.) Bioaccumulation is not expected.

Autoignition temperature

No data available

Decomposition temperature

No data available

Viscosity, dynamic

No data available

Viscosity, kinematic

No data available

Flow time

No data available

Explosive properties

No data available

Oxidizing properties

none

Molecular weight

110.20 g/mol

Particle characteristics Particle size

No data available

Refractive index

1.425 (20 °C) 589 nm

Physical state

Liquid

SECTION 10: Stability and reactivity

Reactivity

Vapour/air-mixtures are explosive at intense warming.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

No data available

Conditions to avoid

Heating.

Incompatible materials

Oxidizing agents

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Oral: No data available

Inhalation: Irritating to respiratory system.

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

Remarks: No data available

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

The substance or mixture is known to cause human aspiration toxicity hazards or has to be regarded as if it causes a human aspiration toxicity hazard.

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

Ecotoxicity

No data available

Persistence and degradability

No data available

Bioaccumulative potential

Components:

4-Octyne:

Partition coefficient: noctanol/water

log Pow: 3.55 Method: (calculated) Remarks: (Lit.) Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Components:

4-Octyne:

Additional ecological information

We have no quantitative data concerning the ecological effects of this product. Further information on ecology Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

International Regulations

IATA-DGR

UN/ID No. : UN 3295

Proper shipping name : Hydrocarbons, liquid, n.o.s.

Class : 3

Packing group : III

Labels : Class 3 - Flammable liquids

Packing instruction (cargo aircraft) : 366

Packing instruction (passenger aircraft) : 355

IMDG-Code

UN number : UN 3295

Proper shipping name : HYDROCARBONS, LIQUID, N.O.S.

Class : 3

Packing group : III

Labels : 3

EmS Code : F-E, S-D

Marine pollutant : no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National Regulations

JT/T 617

UN number : UN 3295

Proper shipping name : HYDROCARBONS, LIQUID, N.O.S.

Class : 3

Packing group : III

Labels : 3

Environmentally hazardous : no

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15: Regulatory information

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals

Identification of Major Hazard Installations for Hazardous Chemicals (GB 18218)

No. / Code Chemical name / Category Threshold quantity

W5.3 Flammable liquids 1,000 t

Hazardous Chemicals for Priority Management

Not applicable under SAWS

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

Not applicable

SECTION 16: Other information

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals

ANTT - National Agency forTransport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN -Standard of the German Institute for Standardisation

DSL - Domestic SubstancesList (Canada)

ECx - Concentration associated with x% response

ELx - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and NewChemical Substances (Japan)

ErCx - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonised System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Can- cer

IATA - International Air Transport Association

IBC - International Code for theConstruction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC50 -Half maximal inhibitory concentration

ICAO - International Civil Aviation Organiza- tion

IECSC - Inventory of Existing Chemical Substances in China

IMDG - Interna- tional Maritime Dangerous Goods

IMO - International Maritime Organisation

ISHL -Industrial Safety and Health Law (Japan)

ISO - International Organisation forStandardisation

KECI - Korea Existing Chemicals Inventory

LC50 - Lethal Concen- tration to 50 % of a test population

LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)

MARPOL - International Convention for the Prevention of Pol- lution from Ships

MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods

n.o.s. - Not Otherwise Specified

Nch - Chilean Norm

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Ef- fect Level

NOELR - No Observable Effect Loading Rate

NOM - Official MexicanNorm

NTP - National Toxicology Program

NZIoC - New Zealand Inventory of Chem- icals

OECD - Organisation for Economic Co-operation and Development

OPPTS - Of- fice of Chemical Safety and Pollution Prevention

PBT - Persistent, Bioaccumulative and Toxic substance

PICCS - Philippines Inventory of Chemicals and Chemical Sub- stances

(Q)SAR - (Quantitative) Structure Activity Relationship

REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning theRegistration, Evaluation, Authorisation and Restriction of Chemicals

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - TaiwanChemical Substance Inventory

TDG - Transportation of Dangerous Goods

TECI -Thailand Existing Chemicals Inventory

TSCA - Toxic Substances Control Act (UnitedStates)

UN - United Nations

UNRTDG - United Nations Recommendations on theTransport of Dangerous Goods

vPvB - Very Persistent and Very Bioaccumulative

WHMIS - Workplace Hazardous Materials Information System