

Chemical Safety Data Sheet MSDS / SDS

1-BUTEN-3-YNE

Revision Date:2024-12-21 Revision Number:1

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

Product identifier

Product name : 1-BUTEN-3-YNE
CBnumber : CB2454902
CAS : 689-97-4
EINECS Number : 211-713-3
Synonyms : but-1-en-3-yne, 1-Buten-3-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 : 400-158-6606

SECTION 2: Hazards identification

Classification of the substance or mixture

Flammable gases, Category 1A, Flammable gas

Label elements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H220 Extremely flammable gas

H280 Contains gas under pressure; may explode if heated

Precautionary statement(s)

Prevention

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

Response

P377 Leaking gas fire: Do not extinguish, unless leak can be stopped safely.

P381 In case of leakage, eliminate all ignition sources.

Storage

P403 Store in a well-ventilated place.

Disposal

none

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1-BUTEN-3-YNE
Synonyms	: but-1-en-3-yne, 1-Buten-3-yne
CAS	: 689-97-4
EC number	: 211-713-3
MF	: C ₄ H ₄
MW	: 52.07

SECTION 4: First aid measures

Description of first aid measures**If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms and effects, both acute and delayed

Excerpt from ERG Guide 115 [Gases - Flammable (Including Refrigerated Liquids)]: Vapors may cause dizziness or asphyxiation without warning. Some may be irritating if inhaled at high concentrations. Contact with gas or liquefied gas may cause burns, severe injury and/or frostbite. Fire may produce irritating and/or toxic gases. (ERG, 2016)

Indication of any immediate medical attention and special treatment needed

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary. Anticipate seizures and treat if necessary. For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport. Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow,

SECTION 5: Firefighting measures

Extinguishing media

Excerpt from ERG Guide 115 [Gases - Flammable (Including Refrigerated Liquids)]: DO NOT EXTINGUISH A LEAKING GAS FIRE UNLESS LEAK CAN BE STOPPED. CAUTION: Hydrogen (UN1049), Deuterium (UN1957) and Hydrogen, refrigerated liquid (UN1966) burn with an invisible flame. Hydrogen and Methane mixture, compressed (UN2034) may burn with an invisible flame. SMALL FIRE: Dry chemical or CO₂. LARGE FIRE: Water spray or fog. Move containers from fire area if you can do it without risk. FIRE INVOLVING TANKS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Do not direct water at source of leak or safety devices; icing may occur. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

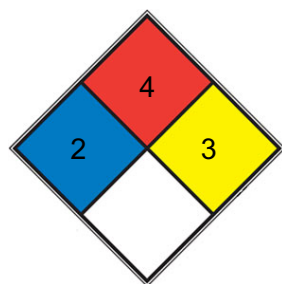
Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 115 [Gases - Flammable (Including Refrigerated Liquids)]: EXTREMELY FLAMMABLE. Will be easily ignited by heat, sparks or flames. Will form explosive mixtures with air. Vapors from liquefied gas are initially heavier than air and spread along ground. CAUTION: Hydrogen (UN1049), Deuterium (UN1957), Hydrogen, refrigerated liquid (UN1966) and Methane (UN1971) are lighter than air and will rise. Hydrogen and Deuterium fires are difficult to detect since they burn with an invisible flame. Use an alternate method of detection (thermal camera, broom handle, etc.) Vapors may travel to source of ignition and flash back. Cylinders exposed to fire may vent and release flammable gas through pressure relief devices. Containers may explode when heated. Ruptured cylinders may rocket. (ERG, 2016)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 4 Will rapidly or completely vaporize at normal atmospheric pressure and temperature, or is readily dispersed in air and will burn readily. Includes pyrophoric substances. Flash point below room temperature at 22.8 °C (73 °F). (e.g. acetylene, propane, [hydrogen gas](#))

REACT 3 Capable of detonation or explosive decomposition but requires a strong initiating source, must be heated under confinement before initiation, reacts explosively with water, or will detonate if severely shocked (e.g. [ammonium nitrate](#), cesium, hydrogen peroxide)

SPEC.
HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	Butenyne			
CAS No.	689-97-4			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m ³	ppm	mg/m ³
Latvia	?	20	?	?
	Remarks			

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-

elimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	1-buten-3-yne is a colorless gas or liquid. Derived by the dimerization of acetylene. Used in the synthesis of neoprene and for other organic syntheses.
Colour	Colorless gas or liquid
Odour	acetylene-like odor
Melting point/freezing point	-118°C
Boiling point or initial boiling point and boiling range	5°C
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	no data available
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Sol in benzene
Partition coefficient n-octanol/water	no data available
Vapour pressure	1,350 mm Hg @ 25 deg C
Density and/or relative density	0.71
Relative vapour density	1.80 (AIR= 1)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Highly flammable. Oxidizes in air to form unstable peroxides that may explode spontaneously.

Chemical stability

no data available

Possibility of hazardous reactions

1-BUTEN-3-YNE may react vigorously with strong oxidizing agents. May react exothermically with reducing agents In the presence of various catalysts (such as acids) or initiators, may undergo exothermic addition polymerization reactions. Forms an explosive salt with silver nitrate.

Thermally unstable, under pressure, in combination with 1,3-butadiene [Loss Prev., 1971, 5, 67].

Conditions to avoid

no data available

Incompatible materials

Forms explosive peroxides with air or oxygen. ... Reacts explosively when heated with 1,3-butadiene or oxygen. Reacts with silver nitrate to form the explosive silver buten-3-ynide.

Hazardous decomposition products

Very exothermic decomposition when heated. ... When heated to decomposition it emits acrid smoke and irritating fumes.

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- Inhalation: LC50 Mouse inhalation 97,200 mg/cu m/2 hr
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

no data available

Bioaccumulative potential

An estimated BCF of 10 was calculated for 1-buten-3-yne(SRC), using an estimated log Kow of 1.4(1) and a regression-derived equation(2).

According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of 1-buten-3-yne is estimated as 70(SRC), using a measured water solubility of 1,790 mg/l(1) and a regression-derived equation(2).

According to a classification scheme(3), this Koc value suggests that 1-buten-3-yne is expected to have high mobility in soil.

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN1954 (For reference only, please check.)

IMDG: UN1954 (For reference only, please check.)

IATA: UN1954 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: COMPRESSED GAS, FLAMMABLE, N.O.S. (For reference only, please check.)

IMDG: COMPRESSED GAS, FLAMMABLE, N.O.S. (For reference only, please check.)

IATA: COMPRESSED GAS, FLAMMABLE, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 2.1 (For reference only, please check.)

IMDG: 2.1 (For reference only, please check.)

IATA: 2.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: (For reference only, please check.)

IMDG: (For reference only, please check.)

IATA: (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Not Listed.

Korea Existing Chemicals List (KECL)

Not Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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