

Chemical Safety Data Sheet MSDS / SDS

But-3-en-3-olide SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: But-3-en-3-olide

CAS: 674-82-8

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.in

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Flammable liquids, Category 3

Acute toxicity - Category 4, Inhalation

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H226 Flammable liquid and vapour

H332 Harmful if inhaled

Precautionary statement(s)

Prevention

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.

P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharges.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].

P370+P378 In case of fire: Use ... to extinguish.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P317 Get medical help.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	But-3-en-3-olide
Common names and synonyms:	But-3-en-3-olide
CAS number:	674-82-8
EC number:	211-617-1
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Half-upright position. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Do NOT induce vomiting. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 131P [Flammable Liquids - Toxic]: TOXIC; may be fatal if inhaled, ingested or absorbed through skin. Inhalation or contact with some of these materials will irritate or burn skin and eyes. Fire will produce irritating, corrosive and/or toxic gases. Vapors may cause dizziness or suffocation. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

Indication of immediate medical attention and special treatment needed, if necessary

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Approach fire from upwind to avoid hazardous vapors and toxic decomposition products. Fight fire from protected location or maximum possible distance. Use water spray to keep fire-exposed containers cool. Use flooding quantities of water as fog or spray. Carbon dioxide may be used. Extinguish fire using agent suitable for surrounding fire.

Specific hazards arising from the chemical

Excerpt from ERG Guide 131P [Flammable Liquids - Toxic]: HIGHLY FLAMMABLE: Will be easily ignited by heat, sparks or flames. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Most vapors are heavier than air. They will spread along ground and collect in low or confined areas (sewers, basements, tanks). Vapor explosion and poison hazard indoors, outdoors or in sewers. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Many liquids are lighter than water. (ERG, 2016)

Special protective actions for fire-fighters

Use carbon dioxide, dry sand. NO hydrous agents. NO water. In case of fire: keep drums, etc., cool by spraying with water. NO direct contact with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations. NEVER direct water jet on liquid.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and

dispose of according to local regulations. NEVER direct water jet on liquid.

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

NO open flames, NO sparks and NO smoking. Above 33°C use a closed system, ventilation and explosion-proof electrical equipment. 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

Fireproof. Separated from acids, bases and food and feedstuffs. Cooled. Dry. Store only if stabilized. Store at 32 deg F (0 deg C) in a standard flammable liquids storage warehouse, room, or cabinet. Special vented containers may be required. Separate from oxidizing materials, acids, and alkalis.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Appropriate engineering 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, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Diketene, stabilized is a colorless liquid with a disagreeable odor. Slightly less dense than water. Irritates skin and eyes. Used to make paints and pharmaceuticals.
Colour:	Light colored liquid
Odour:	PUNGENT ODOR
Melting point/freezing point:	-7.5°C
Boiling point or initial boiling point and boiling range:	127.4°C
Flammability:	Flammable.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	34
Auto-ignition temperature:	275°C

Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	0.88 mPa.s
Solubility:	SOL IN COMMON ORGANIC SOLVENTS; SOL IN WATER
Partition coefficient n-octanol/water:	no data available
Vapour pressure:	7.9 mm Hg (20 °C)
Density and/or relative density:	1.1
Relative vapour density:	2.9 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance slowly polymerizes. The substance violently polymerizes due to warming or under the influence of acids and bases. This generates fire or explosion hazard. Reacts violently with water.

Chemical stability

Readily polymerizes on standing

Possibility of hazardous reactions

MODERATE WHEN EXPOSED TO HEAT OR FLAMEDIKETENE is a very reactive dimer, it may undergo a spontaneous decomposition followed by explosion or ignition [Vervalin, 1973, p.86]. In the presence of bases, amines, mineral acids or Lewis acids a violent polymerization will occur, accompanied by gas evolution [Zdenek, F. et al., Czech Pat. 156 584, 1975].

Conditions to avoid

no data available

Incompatible materials

Reacts with water to form acetone and carbon dioxide.

Hazardous decomposition products

Diketene residues in a tank trailer awaiting incineration decomposed violently on standing, blew off the dome cover and ignited.

SECTION 11: Toxicological information

Acute toxicity

Oral: no data available

Inhalation: no data available

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

The substance is severely irritating to the eyes, skin and respiratory tract. Inhalation of the vapour may cause lung oedema. See Notes.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C.

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

In a 4 week closed bottle biodegradation study, using 100 mg/L acetyl ketene and 30 mg/L sludge, acetyl ketene had a theoretical BOD of 95-102%(1).

Bioaccumulative potential

Based upon an estimated water solubility of 5.30×10^{-5} mg/L(1,SRC), the BCF for acetyl ketene can be estimated to be 0.365(1,SRC). This BCF value suggests that bioconcentration in aquatic organisms of acetyl ketene is not expected to be an important fate process(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indexes(1), the Koc for acetyl ketene can be estimated to be about 6.3(1,SRC). Based on an estimated water solubility of 5.30×10^{-5} (2,SRC) and a regression derived equation(2), the Koc for acetyl ketene can be estimated to be 3.1(2,SRC). According to a suggested classification scheme(3), these estimated Koc values suggest that acetyl ketene has very high soil mobility(SRC).

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: UN2521 (For reference only, please check.)

IMDG: UN2521 (For reference only, please check.)

IATA: UN2521 (For reference only, please check.)

UN Proper Shipping Name

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

IMDG: DIKETENE, STABILIZED (For reference only, please check.)

IATA: DIKETENE, STABILIZED (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)
IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

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

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

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?pageID=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/>

Other Information

Reacts violently with fire extinguishing agents such as water. The symptoms of lung oedema often do not become manifest until a few hours have passed and they are aggravated by physical effort. Rest and medical observation are therefore essential. Immediate administration of an appropriate inhalation therapy by a doctor or a person authorized by him/her, should be considered. An added stabilizer or inhibitor can influence the toxicological properties of this substance, consult an expert. Vinylaceto-beta-lactone is also used as a synonym.

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any