

## Chemical Safety Data Sheet MSDS / SDS

## But-3-en-3-olide SDS

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

|           |            |            |            |            |            |            |            |
|-----------|------------|------------|------------|------------|------------|------------|------------|
| Section 1 | Section 2  | Section 3  | Section 4  | Section 5  | Section 6  | Section 7  | Section 8  |
| Section 9 | Section 10 | Section 11 | Section 12 | Section 13 | Section 14 | Section 15 | Section 16 |

**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  
Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090  
Telephone: +91 9550333722

**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  $5.30 \times 10^{-5}$  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  $5.30 \times 10^{-5}$ (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](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