

## SAFETY DATA SHEET

Version 3.6  
Revision Date 02/02/2015  
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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : Diketene

Product Number : 422363

Brand : Aldrich

Index-No. : 606-017-00-5

CAS-No. : 674-82-8

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

Identified uses : Laboratory chemicals, Manufacture of substances

## 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

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2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

**GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226  
Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 3), H331

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Danger

Hazard statement(s)

H226 Flammable liquid and vapour.  
H302 Harmful if swallowed.  
H331 Toxic if inhaled.

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.  
P233 Keep container tightly closed.  
P240 Ground/bond container and receiving equipment.  
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.  
P242 Use only non-sparking tools.  
P243 Take precautionary measures against static discharge.  
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

|                    |   |
|--------------------|---|
| P264               | Wash skin thoroughly after handling.  |
| P270               | Do not eat, drink or smoke when using this product.   |
| P271               | Use only outdoors or in a well-ventilated area.   |
| P280               | Wear protective gloves/ eye protection/ face protection.  |
| P301 + P312 + P330 | IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell. Rinse mouth.                              |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.                   |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER or doctor/ physician. |
| P370 + P378        | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.                                  |
| P403 + P233        | Store in a well-ventilated place. Keep container tightly closed.  |
| P403 + P235        | Store in a well-ventilated place. Keep cool.  |
| P405               | Store locked up.  |
| P501               | Dispose of contents/ container to an approved waste disposal plant.   |

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |  |
|------------------|--|
| Formula          | : C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> |
| Molecular weight | : 84.07 g/mol                                  |
| CAS-No.          | : 674-82-8                                     |
| EC-No.           | : 211-617-1                                    |
| Index-No.        | : 606-017-00-5                                 |

#### Hazardous components

| Component       | Classification   | Concentration |
|-----------------|--|---------------|
| <b>Diketene</b> |  |               |
|                 | Flam. Liq. 3; Acute Tox. 4; Acute Tox. 3; H226, H302, H331 | <= 100 %      |

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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## 5. FIREFIGHTING MEASURES

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations.

Vapours can accumulate in low areas.

For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### 6.4 Reference to other sections

For disposal see section 13.

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## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature 2 - 8 °C

Handle and open container with care. Reacts violently with water.

Storage class (TRGS 510): Flammable liquids

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

#### **Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### **Appropriate engineering controls**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

## Personal protective equipment

### Eye/face protection

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

### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |   |  |
|---|--|
| a) Appearance                                   | Form: clear, liquid<br>Colour: yellow                                      |
| b) Odour  | No data available  |
| c) Odour Threshold                              | No data available  |
| d) pH   | No data available  |
| e) Melting point/freezing point                 | No data available  |
| f) Initial boiling point and boiling range      | 69 - 70 °C (156 - 158 °F) at 133 hPa (100 mmHg) - lit.                     |
| g) Flash point                                  | 34 °C (93 °F) - closed cup   |
| h) Evaporation rate                             | No data available  |
| i) Flammability (solid, gas)                    | No data available  |
| j) Upper/lower flammability or explosive limits | No data available  |
| k) Vapour pressure                              | 10.5 hPa (7.9 mmHg) at 20 °C (68 °F)<br>68 hPa (51 mmHg) at 55 °C (131 °F) |
| l) Vapour density                               | 2.9 - (Air = 1.0)  |
| m) Relative density                             | 1.09 g/cm <sup>3</sup> at 25 °C (77 °F)                                    |
| n) Water solubility                             | No data available  |
| o) Partition coefficient: n-octanol/water       | No data available  |
| p) Auto-ignition temperature                    | No data available  |
| q) Decomposition temperature                    | No data available  |
| r) Viscosity                                    | No data available  |

- s) Explosive properties      No data available
- t) Oxidizing properties      No data available

## 9.2 Other safety information

Relative vapour density    2.9 - (Air = 1.0)

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Strong oxidizing agents, acids, Bases, Amines, glass, Soda glass, Oxidizing agents

### 10.6 Hazardous decomposition products

Other decomposition products - No data available  
In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 614 mg/kg

LC50 Inhalation - Guinea pig - 2 h - 3,000 mg/m<sup>3</sup>

LD50 Dermal - Rabbit - 3,105 mg/kg

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Skin - Rabbit

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitisation

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

IARC:      No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

ACGIH:      No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP:      No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA:      No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

#### Reproductive toxicity

No data available

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: RQ8225000

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## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

No data available

### 12.2 Persistence and degradability

No data available

### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Other adverse effects

No data available

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

**Product**

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

**DOT (US)**

UN number: 2521      Class: 6.1 (3)      Packing group: I

Proper shipping name: Diketene, stabilized

Reportable Quantity (RQ):

Poison Inhalation Hazard: Hazard zone B

**IMDG**

UN number: 2521      Class: 6.1 (3)      Packing group: I      EMS-No: F-E, S-D

Proper shipping name: DIKETENE, STABILIZED

**IATA**

UN number: 2521      Class: 6.1 (3)

Proper shipping name: Diketene, stabilized

IATA Passenger: Not permitted for transport

IATA Cargo: Not permitted for transport

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## 15. REGULATORY INFORMATION

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

### Massachusetts Right To Know Components

|          | CAS-No.  | Revision Date |
|----------|----------|---------------|
| Diketene | 674-82-8 | 1993-04-24    |

### Pennsylvania Right To Know Components

|          | CAS-No.  | Revision Date |
|----------|----------|---------------|
| Diketene | 674-82-8 | 1993-04-24    |

### New Jersey Right To Know Components

|          | CAS-No.  | Revision Date |
|----------|----------|---------------|
| Diketene | 674-82-8 | 1993-04-24    |

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

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

|            |                              |
|------------|------------------------------|
| Acute Tox. | Acute toxicity               |
| Flam. Liq. | Flammable liquids            |
| H226       | Flammable liquid and vapour. |
| H302       | Harmful if swallowed.        |
| H331       | Toxic if inhaled.            |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 2 |
| Chronic Health Hazard: |   |
| Flammability:          | 3 |
| Physical Hazard        | 0 |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 3 |
| Fire Hazard:       | 3 |
| Reactivity Hazard: | 0 |

### Further information

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### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

