

## SAFETY DATA SHEET

Version 5.2

Revision Date 03/07/2018

Print Date 10/04/2019

---

1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : Cyrene, 99%

Product Number : 807796  
Brand : Sigma-Aldrich

CAS-No. : 53716-82-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

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

Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USATelephone : +1 800-325-5832  
Fax : +1 800-325-5052

## 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

---

2. HAZARDS IDENTIFICATION

## 2.1 Classification of the substance or mixture

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

Eye irritation (Category 2A), H319

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 : Warning

Hazard statement(s)

H319 : Causes serious eye irritation.

Precautionary statement(s)

P264 : Wash skin thoroughly after handling.  
P280 : Wear eye protection/ face protection.  
P305 + P351 + P338 : IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P337 + P313 : If eye irritation persists: Get medical advice/ attention.

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

---

3. COMPOSITION/INFORMATION ON INGREDIENTS

## 3.1 Substances

Synonyms : Dihydrolevoglucosenone

Formula : C<sub>6</sub>H<sub>8</sub>O<sub>3</sub>  
Molecular weight : 128.13 g/mol  
CAS-No. : 53716-82-8

#### Hazardous components

Component	Classification	Concentration
<b>(1S,5R)-6,8-dioxabicyclo[3.2.1]octan-4-one</b>		
	Eye Irrit. 2A; H319	90 - 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

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

#### 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. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

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

---

## 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

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

---

## 6. ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.  
For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

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

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

## 6.4 Reference to other sections

For disposal see section 13.

---

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.  
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.  
Storage class (TRGS 510): 10: Combustible liquids

### 7.3 Specific end use(s)

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

---

## 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

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### Personal protective equipment

##### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with impervious gloves. Wash and dry hands. 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.

##### Body Protection

Impervious 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 by a qualified industrial hygienist 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. For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges.

##### Control of environmental exposure

Do not let product enter drains.

---

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                                 |  |
|---------------------------------|--|
| a) Appearance                   | Form: liquid<br>Colour: colourless, light yellow   |
| b) Odour                        | No data available  |
| c) Odour Threshold              | No data available  |
| d) pH                           | No data available  |
| e) Melting point/freezing point | Melting point/range: < -19.99 °C (< -3.98 °F) at ca.1,013 hPa (760 mmHg) - OECD Test Guideline 102 |
| f) Initial boiling point and    | 227 °C (441 °F) at 1,007.0 hPa (755.3 mmHg) - OECD Test Guideline 103                              |

boiling range

- g) Flash point 108 °C (226 °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 0.28 hPa (0.21 mmHg) at 25 °C (77 °F) - OECD Test Guideline 104
- l) Vapour density No data available
- m) Relative density 1.25 g/cm<sup>3</sup> at 20 °C (68 °F) - OECD Test Guideline 109
- n) Water solubility No data available
- o) Partition coefficient: n-octanol/water log Pow: -1.519 at 22 °C (72 °F) - OECD Test Guideline 107
- p) Auto-ignition temperature 296 °C (565 °F) at 1,003.0 - 1,013.0 hPa (752.3 - 759.8 mmHg)
- 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

Surface tension 72.5 mN/m at 22 °C (72 °F)

---

## 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

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents, Strong reducing agents, Strong acids

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

---

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - female - > 2,000 mg/kg  
(OECD Test Guideline 423)

Inhalation: No data available

Dermal: No data available

No data available

**Skin corrosion/irritation**

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

**Serious eye damage/eye irritation**

No data available

**Respiratory or skin sensitisation**

in vivo assay - Mouse

Result: Did not cause sensitisation on laboratory animals.

(OECD Test Guideline 429)

**Germ cell mutagenicity**

reverse mutation assay

Salmonella typhimurium

Result: negative

**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 on OSHA's list of regulated carcinogens.

**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: Not available

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

---

**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

No data available

Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - 100 mg/l - 48 h (OECD Test Guideline 202)
---	---

Toxicity to algae	Growth inhibition EC50 - Pseudokirchneriella subcapitata - > 100 mg/l - 72 h (OECD Test Guideline 201)
-------------------	---

**12.2 Persistence and degradability**

Biodegradability	aerobic - Exposure time 28 d (OECD Test Guideline 301A)
------------------	--

**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

---

### 13. DISPOSAL CONSIDERATIONS

#### 13.1 Waste treatment methods

##### Product

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.

---

### 14. TRANSPORT INFORMATION

#### DOT (US)

Not dangerous goods

#### IMDG

Not dangerous goods

#### IATA

Not dangerous goods

---

### 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

Acute Health Hazard

#### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

#### Pennsylvania Right To Know Components

(1S,5R)-6,8-dioxabicyclo[3.2.1]octan-4-one

CAS-No.  
53716-82-8

Revision Date

#### New Jersey Right To Know Components

(1S,5R)-6,8-dioxabicyclo[3.2.1]octan-4-one

CAS-No.  
53716-82-8

Revision Date

#### 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.

---

### 16. OTHER INFORMATION

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

Eye Irrit.  
H319

Eye irritation  
Causes serious eye irritation.

**HMIS Rating**

Health hazard:	2
Chronic Health Hazard:	
Flammability:	1
Physical Hazard	0

**NFPA Rating**

Health hazard:	2
Fire Hazard:	1
Reactivity Hazard:	0

**Further information**

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

**Preparation Information**

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

Version: 5.2

Revision Date: 03/07/2018

Print Date: 10/04/2019