

SAFETY DATA SHEET

Version 6.8
Revision Date 04/28/2025
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SECTION 1. 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

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Eye irritation : Category 2A

Other hazards

None known.

GHS label elements

Hazard pictograms

:



Signal Word

: Warning

Hazard Statements

: H319 Causes serious eye irritation.

Precautionary Statements

: **Prevention:**

P264 Wash skin thoroughly after handling.

P280 Wear eye protection/ face protection.

Response:

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.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture

: Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
(1S,5R)-6,8-dioxabicyclo[3.2.1]octan-4-one	53716-82-8*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice

: Show this material safety data sheet to the doctor in attendance.

If inhaled

: After inhalation: fresh air.

In case of skin contact

: In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

: After eye contact: rinse out with plenty of water. Call in ophthalmologist.

	Remove contact lenses.
If swallowed	: After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.
	Vapors are heavier than air and may spread along floors.
	Forms explosive mixtures with air on intense heating.
	Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Nature of decomposition products not known.
Specific extinguishing methods	: No data available
Further information	: Prevent fire extinguishing water from contaminating surface water or the ground water system.

Special protective equipment for fire-fighters : In the event of fire, wear self-contained breathing apparatus.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:
Do not breathe vapors, aerosols.
Avoid substance contact.
Ensure adequate ventilation.
Evacuate the danger area, observe emergency procedures, consult an expert.
Advice for emergency responders:
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.

Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills.
Observe possible material restrictions (see sections 7 and 10).
Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions : Tightly closed.

Storage class : 10, Combustible liquids

Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

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.

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material : butyl-rubber
Break through time : 480 min
Glove thickness : 0.7 mm
Protective index : Full contact
Manufacturer : Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Material : Nitrile rubber
Break through time : 120 min
Glove thickness : 0.4 mm
Protective index : Splash contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Remarks : This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards

such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Change contaminated clothing. Wash hands after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid (68 °F / 20 °C, 1,013 hPa)

Color : transparent

Odor : No data available

Odor Threshold : No data available

pH : No data available

Melting point/ range : < -4 °F / < -20 °C
(ca. 1,013 hPa)
Method: OECD Test Guideline 102
GLP: yes

Boiling point/boiling range : 441 °F / 227 °C (1,007 hPa)
Method: OECD Test Guideline 103
GLP: yes

Flash point : 226 °F / 108 °C
(1019.0 hPa)
Method: Regulation (EC) No. 440/2008, Annex, A.9,
closed cup
GLP: yes

Evaporation rate : No data available

Burning rate : No data available

Self-ignition : 565 °F / 296 °C
ca. 100.3 - 101.3 kPa
GLP: yes

Upper explosion limit /
Upper flammability limit : No data available

Lower explosion limit /
Lower flammability limit : No data available

Vapor pressure : 0.28 hPa (77 °F / 25 °C)

Sigma-Aldrich - 807796

Page 6 of 13

Method: OECD Test Guideline 104
GLP: yes

Relative vapor density	: No data available
Relative density	: No data available
Density	: 1.25 g/cm ³ (68 °F / 20 °C) Method: OECD Test Guideline 109 GLP: yes
Solubility(ies) Water solubility	: ca. 52.6 g/l (68 °F / 20 °C) Method: OECD Test Guideline 105 GLP: yes
Partition coefficient: n-octanol/water	: log Pow: -1.52 (72 °F / 22 °C) Method: OECD Test Guideline 107 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Surface tension	: 72.5 mN/m, 72 °F / 22 °C, OECD Test Guideline 115, GLP: yes
Molecular weight	: 128.13 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity : Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Strong heating.
Incompatible materials	: Strong oxidizing agents Strong reducing agents Strong acids
Hazardous decomposition products	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

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

LC50 Inhalation - Rat - male and female - 4 h - > 5.16 mg/l - dust/mist

(OECD Test Guideline 436)

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - In vitro study

Result: irritating

(OECD Test Guideline 437)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: Did not cause sensitization on laboratory animals.

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Micronucleus test

Test system: Human lymphocytes

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 487

Result: negative

Sigma-Aldrich - 807796

Page 8 of 13

Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative

Carcinogenicity

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

NTP: No ingredient 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

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Repeated dose toxicity - Rat - male and female - Oral - 14 d - NOAEL (No observed adverse effect level) - 1,000 mg/kg

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

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

Toxicity to fish : EC50 (Oncorhynchus mykiss (rainbow trout)): > 100 mg/l
End point: mortality
Exposure time: 96 h
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 203
GLP: yes

Toxicity to daphnia and other aquatic : EC50 (Daphnia magna (Water flea)): > 100 mg/l
End point: Immobilization

invertebrates	Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes
Toxicity to algae/aquatic plants	: ErC50 (<i>Pseudokirchneriella subcapitata</i>): > 100 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes
Toxicity to microorganisms	: EC50 (activated sludge): > 1,000 mg/l Exposure time: 3 h Test Type: static test Method: OECD Test Guideline 209 GLP: yes

Persistence and degradability

Components:

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

Biodegradability	: aerobic Inoculum: activated sludge, non-adapted Result: Readily biodegradable. Biodegradation: 99 % Exposure time: 28 d Method: OECD Test Guideline 301A GLP: yes
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Bioaccumulative potential

Components:

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

Partition coefficient: n-octanol/water	: log Pow: -1.52 (72 °F / 22 °C) pH: 5.18 - 5.24 Method: OECD Test Guideline 107 GLP: yes Remarks: Bioaccumulation is not expected.
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Mobility in soil

No data available

Other adverse effects

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National regulation

49 CFR Road

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard

SARA 313

: 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.

US State Regulations**Massachusetts Right To Know**

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

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION**Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention

Sigma-Aldrich - 807796

Page 12 of 13

of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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