

# • SAFETY DATA SHEET

Version 6.9  
Revision Date 10/15/2025  
Print Date 10/16/2025

## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : (3S)-cis-3,6-Dimethyl-1,4-dioxane-2,5-dione  
Product Number : 367044  
Brand : Aldrich  
CAS-No. : 4511-42-6

### 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 number

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)**


**Hazards for the product as supplied**

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 protective gloves/ 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.

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**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

CAS-No. : 4511-42-6

**Components**

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
(3S-cis)-3,6-Dimethyl-1,4-dioxane-2,5-dione	4511-42-6*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.

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**SECTION 4. FIRST AID MEASURES**

General advice : Show this 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

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## SECTION 5. FIREFIGHTING MEASURES

Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Hazardous combustion products	: Carbon oxides
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.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Avoid inhalation of dusts. 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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Further information on storage conditions : Tightly closed.  
Dry.

Storage class : 13, Non Combustible Solids

Recommended storage temperature : 36 - 46 °F / 2 - 8 °C

Further information on storage stability : Hydrolyses readily.  
Handle and store under inert gas.

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## 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 : required when dusts 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 P2

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

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Material	: Nitrile rubber
Break through time	: 480 min
Glove thickness	: 0.11 mm
Protective index	: Full contact
Manufacturer	: Dermatril® (KCL 740 / Aldrich Z677272, Size M)
Material	: Nitrile rubber
Break through time	: 480 min
Glove thickness	: 0.11 mm
Protective index	: Splash contact
Manufacturer	: Dermatril® (KCL 740 / Aldrich Z677272, Size M)
Manufacturer	: data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
Remarks	: 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. If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.
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.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: solid
Color	: No data available
Odor	: No data available

Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: 198 - 201 °F / 92 - 94 °C Method: lit.
Boiling point/boiling range	: 511 °F / 266 °C (1,019 hPa) Method: OECD Test Guideline 103
Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: The product is not flammable. Method: Flammability (solids)
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.33 g/cm <sup>3</sup> (68 °F / 20 °C) Method: OECD Test Guideline 109
Solubility(ies)	
Water solubility	: 16.7 g/l soluble (68.2 °F / 20.1 °C) Method: OECD Test Guideline 105
Solubility in other solvents	: > 167 mg/l soluble Solvent: Toluene
Partition coefficient: n- octanol/water	: No data available
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 : No data available

Molecular weight : 144.13 g/mol

Particle characteristics  
Particle size : No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity : No data available

Chemical stability : The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions : No data available

Conditions to avoid : Avoid moisture.  
no information available

Incompatible materials : Strong oxidizing agents

Hazardous decomposition products : In the event of fire: see section 5

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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

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

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 402)

#### Skin corrosion/irritation

Remarks: No data available

#### Serious eye damage/eye irritation

Remarks: No data available

#### Respiratory or skin sensitization

in vivo assay - Mouse

Result: Does not cause skin sensitisation.  
(OECD Test Guideline 429)

#### Germ cell mutagenicity

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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 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**

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

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## **SECTION 12. ECOLOGICAL INFORMATION**

### **Ecotoxicity**

#### **Components:**

#### **(3S-cis)-3,6-Dimethyl-1,4-dioxane-2,5-dione:**

Toxicity to fish : Remarks: No data available

### **Persistence and degradability**

#### **Components:**

#### **(3S-cis)-3,6-Dimethyl-1,4-dioxane-2,5-dione:**

Biodegradability : Remarks: No data available

### **Bioaccumulative potential**

#### **Components:**

#### **(3S-cis)-3,6-Dimethyl-1,4-dioxane-2,5-dione:**

Bioaccumulation : Remarks: No data available



## **Mobility in soil**

### **Components:**

#### **(3S-cis)-3,6-Dimethyl-1,4-dioxane-2,5-dione:**

Stability in soil : Remarks: No data available

## **Other adverse effects**

### **Components:**

#### **(3S-cis)-3,6-Dimethyl-1,4-dioxane-2,5-dione:**

Additional ecological information : No data available

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## **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.

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## **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 Regulations**

#### **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.

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## 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

Components	CAS-No.	Component TPQ (lbs)
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**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.

#### Pennsylvania Right To Know

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#### New Jersey Right To Know

(3S-cis)-3,6-Dimethyl-1,4-dioxane-2,5-dione 4511-42-6

#### California Prop. 65

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

### The components of this product are reported in the following inventories:

TSCA : All substances listed as active on the 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.

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## 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 Harmonised 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 Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; 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 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 - Organisation 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](http://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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