

## SAFETY DATA SHEET

Version 5.5  
Revision Date 06/02/2016  
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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Bis(methylcyclopentadienyl)zirconium(IV) dichloride

Product Number : 481238  
Brand : Aldrich

CAS-No. : 12109-71-6

**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  
USA

Telephone : +1 800-325-5832  
Fax : +1 800-325-5052

**1.4 Emergency telephone number**

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

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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)**

Substances and mixtures, which in contact with water, emit flammable gases (Category 2), H261  
Skin corrosion (Category 1B), H314  
Serious eye damage (Category 1), H318

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)

H261

In contact with water releases flammable gases.

H314

Causes severe skin burns and eye damage.

Precautionary statement(s)

P223

Keep away from any possible contact with water, because of violent reaction and possible flash fire.

P231 + P232

Handle under inert gas. Protect from moisture.

P260

Do not breathe dust or mist.

P264

Wash skin thoroughly after handling.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P301 + P330 + P331

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310	Immediately call a POISON CENTER/doctor.
P321	Specific treatment (see supplemental first aid instructions on this label).
P335 + P334	Brush off loose particles from skin. Immerse in cool water/ wrap in wet bandages.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P402 + P404	Store in a dry place. Store in a closed container.
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>12</sub> H <sub>14</sub> Cl <sub>2</sub> Zr
Molecular weight	: 320.37 g/mol
CAS-No.	: 12109-71-6

#### Hazardous components

Component	Classification	Concentration
<b>Bis(methylcyclopentadienyl)zirconium(IV) dichloride</b>		
	Water-react. 2; Skin Corr. 1B; Eye Dam. 1; H261, H314	<= 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

Take off contaminated clothing and shoes immediately. 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. Continue rinsing eyes during transport to hospital.

#### 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

No data available

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

### 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 formation of dust and aerosols.

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

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.

### 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

Component	CAS-No.	Value	Control parameters	Basis
Bis(methylcyclopentadienyl)zirconium(IV) dichloride	12109-71-6	TWA	5.000000 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	5.000000 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		STEL	10.000000 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		

		TWA	5.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	10.000000 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	5 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	5 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		
		STEL	10 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		
		TWA	5 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	10 mg/m3	USA. NIOSH Recommended Exposure Limits
		PEL	5 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	10 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

## 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

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, 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 particle respirator type N100 (US) or type P3 (EN 143) 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

Do not let product enter drains.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |                           |   |
|---------------------------|---|
| a) Appearance             | Form: solid   |
| b) Odour                  | No data available   |
| c) Odour Threshold        | No data available   |
| d) pH                     | No data available   |
| e) Melting point/freezing | Melting point/range: 180.5 - 184 °C (356.9 - 363 °F) - lit. |

point

- |   |                   |
|---|-------------------|
| f) Initial boiling point and boiling range      | No data available |
| g) Flash point                                  | No data available |
| 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                              | No data available |
| l) Vapour density                               | No data available |
| m) Relative density                             | No data available |
| 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

No data available

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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

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents, acids, Bases, Chemically active metals

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas, Zirconium oxides

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

No data available

Inhalation: No data available

Dermal: No data available

No data available

**Skin corrosion/irritation**

No data available

**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.

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: Not available

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea

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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

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 3261      Class: 8      Packing group: III  
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (Bis(methylcyclopentadienyl)zirconium(IV) dichloride)

Poison Inhalation Hazard: No

### IMDG

UN number: 3261      Class: 8      Packing group: III      EMS-No: F-A, S-B  
Proper shipping name: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (Bis(methylcyclopentadienyl)zirconium(IV) dichloride)

### IATA

UN number: 3261      Class: 8      Packing group: III  
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (Bis(methylcyclopentadienyl)zirconium(IV) dichloride)

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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

Acute Health Hazard

### Massachusetts Right To Know Components

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

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Bis(methylcyclopentadienyl)zirconium(IV) dichloride	12109-71-6	1993-02-16

### New Jersey Right To Know Components

	CAS-No.	Revision Date
Bis(methylcyclopentadienyl)zirconium(IV) dichloride	12109-71-6	1993-02-16

### 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.

Eye Dam.	Serious eye damage
H261	In contact with water releases flammable gases.
H314	Causes severe skin burns and eye damage.

H318 Causes serious eye damage.  
Skin Corr. Skin corrosion  
Water-react. Substances and mixtures, which in contact with water, emit flammable gases

**HMIS Rating**

Health hazard: 3  
Chronic Health Hazard:  
Flammability: 0  
Physical Hazard 0

**NFPA Rating**

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

**Further information**

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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

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