



BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE

Safety Data Sheet OMZR016

Date of issue: 19/02/2016 Version: 1.0

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form	: Substance
Physical state	: Solid
Substance name	: BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE
Product code	: OMZR016
Formula	: C ₂₀ H ₃₀ Cl ₂ Zr
Synonyms	: DECAMETHYLZIRCONOCENE DICHLORIDE
Chemical family	: METAL COMPOUND

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

1.2.1. Relevant identified uses

Use of the substance/mixture : Chemical intermediate

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

GELEST, INC.

11 East Steel Road
Morrisville, PA 19067

USA

T 215-547-1015 - F 215-547-2484 - (M-F): 8:00 AM - 5:30 PM EST

info@gelest.com - www.gelest.com

GELEST INC.

Fritz-Klatte-Strasse 8
65933 Frankfurt

Germany

T +49 (0) 69 3535106-500 - F +49 (0) 69 3535106-501 - (M-F): 8:00 AM - 4:00 PM

info@gelestde.com - www.gelestde.com

1.4. Emergency telephone number

Emergency number : CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Skin corrosion/irritation, Category 2	H315
Serious eye damage/eye irritation, Category 2	H319
Full text of H statements : see section 16	

Adverse physicochemical, human health and environmental effects

No additional information available

2.2. Label elements

Labelling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



GHS07

Signal word (CLP) :

Warning

Hazard statements (CLP) :

H315 - Causes skin irritation.
H319 - Causes serious eye irritation.

Precautionary statements (CLP) :

P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P264 - Wash hands thoroughly after handling.

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE

Safety Data Sheet

P302+P352 - IF ON SKIN: Wash with plenty of soap and water.
P332+P313 - If skin irritation occurs: Get medical advice/attention.
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. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type : Mono-constituent
Name : BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE
CAS-No. : 54039-38-3

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
Bis(pentamethylcyclopentadienyl)zirconium dichloride	(CAS-No.) 54039-38-3	95 - 100	Skin Irrit. 2, H315 Eye Irrit. 2, H319

Full text of H-statements: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general : Remove contaminated clothing and shoes. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). If possible show this sheet; if not available show packaging or label.

First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing. If you feel unwell, seek medical advice.

First-aid measures after skin contact : Wash with plenty of water/.... Get medical advice/attention.

First-aid measures after eye contact : Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention.

First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Get medical advice/attention.

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

Symptoms/effects after inhalation : May cause irritation to the respiratory tract.

Symptoms/effects after skin contact : Causes skin irritation.

Symptoms/effects after eye contact : Causes serious eye irritation.

Symptoms/effects after ingestion : May be harmful if swallowed.

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

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : Water spray. Water fog. Foam. Carbon dioxide. Dry chemical.

Unsuitable extinguishing media : None known.

5.2. Special hazards arising from the substance or mixture

Fire hazard : Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.

5.3. Advice for firefighters

Firefighting instructions : Exercise caution when fighting any chemical fire. Use water spray or fog for cooling exposed containers.

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection. Avoid contact with skin and eyes. Do not breathe dust.

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE

Safety Data Sheet

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Protective equipment : Wear protective equipment as described in Section 8.
Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment : Do not attempt to take action without suitable protective equipment. Equip cleanup crew with proper protection. For further information refer to section 8: "Exposure controls/personal protection".

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

6.3. Methods and material for containment and cleaning up

For containment : Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams.
Methods for cleaning up : Sweep or shovel spills into appropriate container for disposal.

6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Avoid contact with skin and eyes. Do not breathe dust. Avoid dust formation. Provide local exhaust or general room ventilation to minimize exposure to dust.
Hygiene measures : Wash contaminated clothing before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Keep container tightly closed.
Incompatible materials : Oxidizing agent.
Storage area : Store in a well-ventilated place. Store away from heat.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Bis(pentamethylcyclopentadienyl)zirconium dichloride (54039-38-3)		
USA OSHA	OSHA PEL (TWA) (mg/m ³)	5 mg/m ³ Zr

8.2. Exposure controls

Appropriate engineering controls:

Provide local exhaust or general room ventilation.

Personal protective equipment:

Avoid all unnecessary exposure. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

Hand protection:

Neoprene or nitrile rubber gloves

Eye protection:

Chemical goggles. Contact lenses should not be worn

Skin and body protection:

Wear suitable protective clothing

Respiratory protection:

Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. NIOSH-certified dust and mist (teal cartridge) respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Solid

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE

Safety Data Sheet

Appearance	: Crystals.
Molecular mass	: 432.56 g/mol
Colour	: Pale yellow.
Odour	: No data available
Odour threshold	: No data available
Refractive index	: No additional information available
pH	: No data available
Relative evaporation rate (butylacetate=1)	: No data available
Melting point	: > 300 °C
Freezing point	: No data available
Boiling point	: No data available
Flash point	: > 110 °C
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapour pressure	: < 0.01 mm Hg @ 20°C
Relative vapour density at 20 °C	: No data available
Relative density	: > 1
% Volatiles	: < 3 %
Solubility	: Insoluble in water.
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidising properties	: No data available
Explosive limits	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable in sealed containers.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Avoid high concentrations of dust.

10.5. Incompatible materials

Oxidizing agent.

10.6. Hazardous decomposition products

Organic acid vapors. Zirconium oxide fumes.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity	: Not classified
Skin corrosion/irritation	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitisation	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
STOT-single exposure	: Not classified
STOT-repeated exposure	: Not classified

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE

Safety Data Sheet

Aspiration hazard	: Not classified
Symptoms/effects after inhalation	: May cause irritation to the respiratory tract.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: May be harmful if swallowed.
Reason for classification	: Expert judgment

SECTION 12: Ecological information

12.1. Toxicity

Acute aquatic toxicity	: Not classified
Chronic aquatic toxicity	: Not classified

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

No additional information available

12.4. Mobility in soil

No additional information available

12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Other adverse effects : This substance may be hazardous to the environment.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Sewage disposal recommendations	: Do not dispose of waste into sewer.
Product/Packaging disposal recommendations	: Dispose in a safe manner in accordance with local/national regulations. Dispose of solid materials or residues at a licensed site.
Ecology - waste materials	: Avoid release to the environment.

SECTION 14: Transport information

14.1. UN number

In accordance with ADR / RID / IMDG / IATA / ADN

14.1. UN number

UN-No. (ADR)	: Not applicable
UN-No. (IMDG)	: Not applicable
UN-No. (IATA)	: Not applicable
UN-No. (ADN)	: Not applicable
UN-No. (RID)	: Not applicable

14.2. UN proper shipping name

Proper Shipping Name (ADR)	: Not applicable
Proper Shipping Name (IMDG)	: Not applicable
Proper Shipping Name (IATA)	: Not applicable
Proper Shipping Name (ADN)	: Not applicable
Proper Shipping Name (RID)	: Not applicable

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR) : Not applicable

IMDG

Transport hazard class(es) (IMDG) : Not applicable

IATA

Transport hazard class(es) (IATA) : Not applicable

ADN

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE

Safety Data Sheet

Transport hazard class(es) (ADN) : Not applicable

RID

Transport hazard class(es) (RID) : Not applicable

14.4. Packing group

Packing group (ADR) : Not applicable
Packing group (IMDG) : Not applicable
Packing group (IATA) : Not applicable
Packing group (ADN) : Not applicable
Packing group (RID) : Not applicable

14.5. Environmental hazards

Dangerous for the environment : No
Marine pollutant : No
Other information : No supplementary information available

14.6. Special precautions for user

- Overland transport

Not applicable

- Transport by sea

Not applicable

- Air transport

Not applicable

- Inland waterway transport

Not applicable

- Rail transport

Not applicable

14.7. Transport in bulk according to Annex II of Marpol and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

15.1.1. EU-Regulations

No REACH Annex XVII restrictions

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE is not on the REACH Candidate List

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE is not on the REACH Annex XIV List

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE is not subject to REGULATION (EU) No 649/2012 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 4 July 2012 concerning the export and import of hazardous chemicals.

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE is not subject to Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC

% Volatiles : < 3 %

15.1.2. National regulations

Germany

12th Ordinance Implementing the Federal Immission Control Act - 12.BImSchV : Is not subject of the 12. BImSchV (Hazardous Incident Ordinance)

Netherlands

SZW-lijst van kankerverwekkende stoffen : The substance is not listed

SZW-lijst van mutagene stoffen : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Borstvoeding : The substance is not listed

NIET-limitatieve lijst van voor de voortplanting giftige stoffen – Vruchtbaarheid : The substance is not listed

BIS(PENTAMETHYLCYCLOPENTADIENYL)ZIRCONIUM DICHLORIDE

Safety Data Sheet

NIET-limitatieve lijst van voor de voortplanting : The substance is not listed
giftige stoffen – Ontwikkeling

15.2. Chemical safety assessment

No additional information available

SECTION 16: Other information

Abbreviations and acronyms:

Abbreviations: ND: Not Determined, No Data; NA: Not Applicable; LD: Lethal Dose; LC: Lethal Concentration; ATE: Acute Toxicity Estimates; H: hour; °: °C unless otherwise stated; mm: millimeters Hg, torr; PEL: permissible exposure level; TWA: time weighted average; TLV: threshold limit value; TG: Test Guideline; NIOSH: National Institute for Occupational Safety and Health; IARC: International Agency for Research on Cancer; NTP: National Toxicology Program; HMIS: Hazardous Material Information System; CAS No.: Chemical Abstract Service Registration Number; EC No.: European Commission Registration Number; EC Index No.: European Commission Index Number; OECD: The Organisation for Economic Co-operation and Development; GHS: The Globally Harmonized System of Classification and Labelling; APF: Assigned Protection Factor
--

Other information : Prepared by safety and environmental affairs.

Full text of H- and EUH-statements:

Eye Irrit. 2	Serious eye damage/eye irritation, Category 2
Skin Irrit. 2	Skin corrosion/irritation, Category 2
H315	Causes skin irritation.
H319	Causes serious eye irritation.

SDS EU (REACH Annex II) - Custom

The information contained in this document has been gathered from reference materials and/or Gelest, Inc. test data and is to the best knowledge and belief of Gelest, Inc. accurate and reliable. Such information is offered solely for your consideration, investigation and verification. It is not suggested or guaranteed that the hazard precautions or procedures described are the only ones which exist. Gelest, Inc. makes no warranties, express or implied, with respect to the use of such information and assumes no responsibility therefore. Information on this safety data sheet is not intended to constitute a basis for product specifications.

© 2019 Gelest Inc. Morrisville, PA 19067