

BIS(CYCLOPENTADIENYL)TITANIUM(III) CHLORIDE

Safety Data Sheet OMTI010

Date of issue: 11/01/2017 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(CYCLOPENTADIENYL)TITANIUM(III) CHLORIDE |
| Product code | : OMTI010 |
| Formula | : C ₁₀ H ₁₀ ClTi |
| Synonyms | : NUGENT'S REAGENT TITANOCENE CHLORIDE TITANOCENE MONOCHLORIDE CHLORODICYCLOPENTADIENYL TITANIUM |
| 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.

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Precautionary statements (CLP)

H319 - Causes serious eye irritation.

- : P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P264 - Wash hands thoroughly after handling.
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(CYCLOPENTADIENYL)TITANIUM(III) CHLORIDE
CAS-No. : 60955-54-6

| Name | Product identifier | % | Classification according to Regulation (EC) No. 1272/2008 [CLP] |
|---|----------------------|----------|---|
| Bis(cyclopentadienyl)titanium(III) chloride | (CAS-No.) 60955-54-6 | 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.

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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. Should be handled under argon, preferably in a glove-box.
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. Do not expose to light.
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

No additional information available

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

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| | |
|--|--|
| Appearance | : Solid. |
| Molecular mass | : 213.55 g/mol |
| Colour | : Green. |
| 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 | : > 250 °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 |
| Relative vapour density at 20 °C | : No data available |
| Relative density | : > 1 |
| % Volatiles | : < 3 % |
| Solubility | : Insoluble in water. Reacts with water. Organic solvent:Soluble: THF |
| 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

Extremely sensitive to air. Should be handled under argon, preferably in a glove-box.

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. Titanium oxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

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| | |
|--------------------------|--|
| LD50 intraperitoneal rat | 25 mg/kg related compound- TITANOCENE DICHLORIDE |
|--------------------------|--|

| | |
|-----------------------------------|----------------------------------|
| 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 |

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| | |
|---|--|
| Carcinogenicity | : Not classified None of the components in this product at concentrations >0.1% are listed by IARC, NTP, OSHA or ACGIH as a carcinogen. |
| Reproductive toxicity | : Not classified |
| STOT-single exposure | : Not classified |
| STOT-repeated exposure | : Not classified |
| Aspiration hazard | : Not classified |
| Potential adverse human health effects and symptoms | : The following data is for the related compound- TITANOCENE DICHLORIDE. Chronic Toxicity: Tumorigenic by RTECS criteria EPA GENETOX PROGRAM 1988, POSITIVE SHE-CLONAL ASSAY; CELL TRANSFORM. RLV F344 RAT EMBRYO EPA GENETOX PROGRAM 1988, NEGATIVE: HOST-MEDIATED ASSAY; S CEREVISIAE-HOMOZYGOSIS. |
| 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 | : Incinerate. 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 |

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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

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(CYCLOPENTADIENYL)TITANIUM(III) CHLORIDE is not on the REACH Candidate List

BIS(CYCLOPENTADIENYL)TITANIUM(III) CHLORIDE is not on the REACH Annex XIV List

BIS(CYCLOPENTADIENYL)TITANIUM(III) CHLORIDE 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(CYCLOPENTADIENYL)TITANIUM(III) CHLORIDE 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

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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

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

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.

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