

BIS(2,6-DIFLUORO-3-(1-HYDROXYRROL-1-YL)PHENYL)TITANOCENE

Safety Data Sheet OMTI014

Date of issue: 21/08/2015 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(2,6-DIFLUORO-3-(1-HYDROXYRROL-1-YL)PHENYL)TITANOCENE
Product code	: OMTI014
Formula	: C30H22F4N2Ti
Synonyms	: BIS(,ETA.5-2,4-CYCLOPENTADIEN-1-YL)BIS[2,6-DIFLUORO-3-(1H-PYRROL-YL)-PHENYL]TITANIUM; BIS(CYCLOPENTADIENYL)-BIS(2,6-DIFLUORO-3-(PYRROL-1-YL)-PHENYL)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.

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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]

Flammable solids, Category 1	H228
Reproductive toxicity, Category 2	H361
Specific target organ toxicity — Repeated exposure, Category 2	H373
Hazardous to the aquatic environment — Chronic Hazard, Category 2	H411
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) :



GHS02

GHS08

GHS09

Signal word (CLP) :

: Danger

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Hazard statements (CLP)	: H228 - Flammable solid. H361 - Suspected of damaging fertility or the unborn child. H373 - May cause damage to organs through prolonged or repeated exposure. H411 - Toxic to aquatic life with long lasting effects.
Precautionary statements (CLP)	: P202 - Do not handle until all safety precautions have been read and understood. P280 - Wear protective gloves/protective clothing/eye protection/face protection. P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. P240 - Ground/bond container and receiving equipment. P273 - Avoid release to the environment. P314 - Get medical advice/attention if you feel unwell.

2.3. Other hazards

No additional information available

SECTION 3: Composition/information on ingredients

3.1. Substances

Substance type	: Mono-constituent
Name	: BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE
CAS-No.	: 125051-32-3

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
Bis(cyclopentadienyl)-bis(2,6-difluoro-3-(pyrrol-1-yl)-phenyl)titanium	(CAS-No.) 125051-32-3 (EC-No.) 412-000-1 (EC Index-No.) 022-003-00-6	> 95	Flam. Sol. 1, H228 Repr. 2, H361f STOT RE 2, H373 Aquatic Chronic 2, H411

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. Get medical advice/attention if you feel unwell.
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	: Do not use straight streams.

5.2. Special hazards arising from the substance or mixture

Fire hazard	: Flammable solid. Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.
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5.3. Advice for firefighters

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

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Remove ignition sources. Use special care to avoid static electric charges.

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. Use only non-sparking tools.

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

Additional hazards when processed : Avoid high concentrations of dust.

Precautions for safe handling : Avoid contact with skin and eyes. Do not breathe dust. Provide local exhaust or general room ventilation to minimize exposure to dust. Ground/bond container and receiving equipment. Use only non-sparking tools.

Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Proper grounding procedures to avoid static electricity should be followed. Use explosion-proof electrical equipment.

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:

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

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Solid.
Molecular mass	: 534.39 g/mol
Colour	: Yellow-orange.
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	: 160 - 170 °C decomposes
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)	: Flammable solid.
Vapour pressure	: < 0.001 mm Hg
Relative vapour density at 20 °C	: No data available
Relative density	: > 1
% Volatiles	: < 3 %
Solubility	: Insoluble in water. Organic solvent: Soluble: acetone, methylethylketone, > hexanediol diacrylate, toluene
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

Decomposes on exposure to light.

10.3. Possibility of hazardous reactions

At temperatures greater than 100°C may undergo self accelerating decomposition.

10.4. Conditions to avoid

Heat. Open flame. Sparks.

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

Bis(cyclopentadienyl)-bis(2,6-difluoro-3-(pyrrol-1-yl)-phenyl)titanium (125051-32-3)

LD50 oral rat	> 2000 mg/kg
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Skin corrosion/irritation	: Not classified
Serious eye damage/irritation	: Not classified
Respiratory or skin sensitisation	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Suspected of damaging fertility or the unborn child.
STOT-single exposure	: Not classified
STOT-repeated exposure	: May cause damage to organs through prolonged or repeated exposure.
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	: Toxic to aquatic life with long lasting effects.

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.
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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 contents/container to licensed waste disposal facility.
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)	: 1325
UN-No. (IMDG)	: 1325
UN-No. (IATA)	: 1325
UN-No. (ADN)	: 1325
UN-No. (RID)	: 1325

14.2. UN proper shipping name

Proper Shipping Name (ADR)	: FLAMMABLE SOLID, ORGANIC, N.O.S.
Proper Shipping Name (IMDG)	: FLAMMABLE SOLID, ORGANIC, N.O.S.
Proper Shipping Name (IATA)	: Flammable solid, organic, n.o.s.
Proper Shipping Name (ADN)	: FLAMMABLE SOLID, ORGANIC, N.O.S.
Proper Shipping Name (RID)	: FLAMMABLE SOLID, ORGANIC, N.O.S.
Transport document description (ADR)	: UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE), 4.1, III, (E), ENVIRONMENTALLY HAZARDOUS

BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE

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Transport document description (IMDG)	: UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE), 4.1, III, MARINE POLLUTANT/ENVIRONMENTALLY HAZARDOUS
Transport document description (IATA)	: UN 1325 Flammable solid, organic, n.o.s. (BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE), 4.1, III, ENVIRONMENTALLY HAZARDOUS
Transport document description (ADN)	: UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE), 4.1, III, ENVIRONMENTALLY HAZARDOUS
Transport document description (RID)	: UN 1325 FLAMMABLE SOLID, ORGANIC, N.O.S. (BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE), 4.1, III, ENVIRONMENTALLY HAZARDOUS

14.3. Transport hazard class(es)

ADR

Transport hazard class(es) (ADR)	: 4.1
Danger labels (ADR)	: 4.1



IMDG

Transport hazard class(es) (IMDG)	: 4.1
Danger labels (IMDG)	: 4.1



IATA

Transport hazard class(es) (IATA)	: 4.1
Hazard labels (IATA)	: 4.1



ADN

Transport hazard class(es) (ADN)	: 4.1
Danger labels (ADN)	: 4.1



RID

Transport hazard class(es) (RID)	: 4.1
Danger labels (RID)	: 4.1



14.4. Packing group

Packing group (ADR)	: III
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Packing group (IMDG)	: III
Packing group (IATA)	: III
Packing group (ADN)	: III
Packing group (RID)	: III

14.5. Environmental hazards

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

14.6. Special precautions for user

- Overland transport

Classification code (ADR)	: F1		
Special provisions (ADR)	: 274		
Limited quantities (ADR)	: 5kg		
Excepted quantities (ADR)	: E1		
Packing instructions (ADR)	: P002, IBC08, LP02, R001		
Special packing provisions (ADR)	: PP40		
Mixed packing provisions (ADR)	: MP10		
Portable tank and bulk container instructions (ADR)	: T1		
Portable tank and bulk container special provisions (ADR)	: TP33		
Tank code (ADR)	: SGAV		
Vehicle for tank carriage	: AT		
Transport category (ADR)	: 3		
Special provisions for carriage - Bulk (ADR)	: VC1, VC2		
Hazard identification number (Kemler No.)	: 40		
Orange plates	: <table border="1"><tr><td>40</td></tr><tr><td>1325</td></tr></table>	40	1325
40			
1325			
Tunnel restriction code (ADR)	: E		
EAC code	: 1Z		

- Transport by sea

Special provisions (IMDG)	: 223, 274, 915
Limited quantities (IMDG)	: 5 kg
Excepted quantities (IMDG)	: E1
Packing instructions (IMDG)	: P002
IBC packing instructions (IMDG)	: IBC08
IBC special provisions (IMDG)	: B3
Tank instructions (IMDG)	: T1
Tank special provisions (IMDG)	: TP33
EmS-No. (Fire)	: F-A
EmS-No. (Spillage)	: S-G
Stowage category (IMDG)	: B

- Air transport

PCA Excepted quantities (IATA)	: E1
PCA Limited quantities (IATA)	: Y443
PCA limited quantity max net quantity (IATA)	: 10kg
PCA packing instructions (IATA)	: 446
PCA max net quantity (IATA)	: 25kg
CAO packing instructions (IATA)	: 449
CAO max net quantity (IATA)	: 100kg
Special provisions (IATA)	: A3
ERG code (IATA)	: 3L

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- Inland waterway transport

Classification code (ADN)	: F1
Special provisions (ADN)	: 274
Limited quantities (ADN)	: 5 kg
Excepted quantities (ADN)	: E1
Equipment required (ADN)	: PP
Number of blue cones/lights (ADN)	: 0

- Rail transport

Classification code (RID)	: F1
Special provisions (RID)	: 274
Limited quantities (RID)	: 5kg
Excepted quantities (RID)	: E1
Packing instructions (RID)	: P002, IBC08, LP02, R001
Special packing provisions (RID)	: B3
Mixed packing provisions (RID)	: MP10
Portable tank and bulk container instructions (RID)	: T1
Portable tank and bulk container special provisions (RID)	: TP33
Tank codes for RID tanks (RID)	: SGAV
Transport category (RID)	: 3
Special provisions for carriage – Packages (RID)	: W1
Special provisions for carriage – Bulk (RID)	: VC1, VC2
Colis express (express parcels) (RID)	: CE11
Hazard identification number (RID)	: 40

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(2,6-DIFLUORO-3-(1-HYDROPIRROL-1-YL)PHENYL)TITANOCENE is not on the REACH Candidate List

BIS(2,6-DIFLUORO-3-(1-HYDROPIRROL-1-YL)PHENYL)TITANOCENE is not on the REACH Annex XIV List

BIS(2,6-DIFLUORO-3-(1-HYDROPIRROL-1-YL)PHENYL)TITANOCENE 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(2,6-DIFLUORO-3-(1-HYDROPIRROL-1-YL)PHENYL)TITANOCENE 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 : BIS(2,6-DIFLUORO-3-(1-HYDROPIRROL-1-YL)PHENYL)TITANOCENE is listed

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

Denmark

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Danish National Regulations : Young people below the age of 18 years are not allowed to use the product
Pregnant/breastfeeding women working with the product must not be in direct contact with the product
The requirements from the Danish Working Environment Authorities regarding work with carcinogens must be followed during use and disposal

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
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Other information : Prepared by safety and environmental affairs.

Full text of H- and EUH-statements:

Aquatic Chronic 2	Hazardous to the aquatic environment — Chronic Hazard, Category 2
Flam. Sol. 1	Flammable solids, Category 1
Repr. 2	Reproductive toxicity, Category 2
Repr. 2	Reproductive toxicity, Category 2
STOT RE 2	Specific target organ toxicity — Repeated exposure, Category 2
H228	Flammable solid.
H361	Suspected of damaging fertility or the unborn child.
H361f	Suspected of damaging fertility.
H373	May cause damage to organs through prolonged or repeated exposure.
H411	Toxic to aquatic life with long lasting effects.

SDS EU (REACH Annex II) - Custom

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