



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

Safety Data Sheet OMTI014

Date of issue: 08/21/2015

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

Use of the substance/mixture	: Chemical intermediate For research and industrial use only
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### 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](mailto:info@gelest.com) - [www.gelest.com](http://www.gelest.com)

### 1.4. Emergency telephone number

Emergency number	: CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)
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## SECTION 2: Hazards identification

### 2.1. Classification of the substance or mixture

#### Classification (GHS-US)

Flam. Sol. 2 H228

Skin Irrit. 2 H315

Eye Irrit. 2A H319

Full text of H-phrases: see section 16

### 2.2. Label elements

#### GHS-US labeling

Hazard pictograms (GHS-US)



GHS02

GHS07

Signal word (GHS-US)

: Warning

Hazard statements (GHS-US)

: H228 - Flammable solid  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation

Precautionary statements (GHS-US)

: P280 - Wear protective gloves/protective clothing/eye protection/face protection  
P210 - Keep away from heat, open flames, sparks. - No smoking  
P240 - Ground/bond container and receiving equipment  
P241 - Use explosion-proof electrical equipment  
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  
P321 - Specific treatment (see first aid instructions on this label)  
P362+P364 - Take off contaminated clothing and wash it before reuse  
P370+P378 - In case of fire: Use water spray or fog, foam, carbon dioxide, dry chemical to extinguish

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### 2.3. Other hazards

No additional information available

### 2.4. Unknown acute toxicity (GHS US)

No data available

## SECTION 3: Composition/information on ingredients

### 3.1. Substance

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 (GHS-US)
Bis(cyclopentadienyl)-bis(2,6-difluoro-3-(pyrrol-1-yl)-phenyl)titanium	(CAS No) 125051-32-3	> 95	Flam. Sol. 2, H228 Skin Irrit. 2, H315 Eye Irrit. 2A, H319

### 3.2. Mixture

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 victim to fresh air and keep at rest in a position comfortable for breathing. If you feel unwell, seek medical advice.

First-aid measures after skin contact : Wash with plenty of soap and 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/injuries after inhalation : May cause irritation to the respiratory tract.

Symptoms/injuries after skin contact : Causes skin irritation.

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

Symptoms/injuries 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.

### 5.3. Advice for firefighters

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

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".

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### 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 : 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
- Color : Yellow-orange.
- Odor : No data available
- Odor threshold : No data available
- Refractive index : No data available
- pH : No data available
- Relative evaporation rate (butyl acetate=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
- Vapor pressure : < 0.001 mm Hg

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Relative vapor density at 20 °C	: No data available
Relative density	: > 1
VOC content	: < 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
Oxidizing properties	: No data available
Explosion 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	: Causes skin irritation.
Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
Specific target organ toxicity (single exposure)	: Not classified
Specific target organ toxicity (repeated exposure)	: Not classified
Aspiration hazard	: Not classified
Symptoms/injuries after inhalation	: May cause irritation to the respiratory tract.
Symptoms/injuries after skin contact	: Causes skin irritation.
Symptoms/injuries after eye contact	: Causes serious eye irritation.
Symptoms/injuries after ingestion	: May be harmful if swallowed.
Reason for classification	: Expert judgment

## SECTION 12: Ecological information

### 12.1. Toxicity

No additional information available

### 12.2. Persistence and degradability

No additional information available

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### 12.3. Bioaccumulative potential

No additional information available

### 12.4. Mobility in soil

No additional information available

### 12.5. Other adverse effects

Other adverse effects : This substance may be hazardous to the environment.  
Effect on ozone layer : No additional information available  
Effect on the global warming : No known ecological damage caused by this product.

## SECTION 13: Disposal considerations

### 13.1. Waste treatment methods

Sewage disposal recommendations : Do not dispose of waste into sewer.  
Waste 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

UN-No.(DOT) : 1325  
DOT NA no. UN1325

### 14.2. UN proper shipping name

Proper Shipping Name (DOT) : Flammable solids, organic, n.o.s.  
(BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE)  
Department of Transportation (DOT) Hazard Classes : 4.1 - Class 4.1 - Flammable Solid 49 CFR 173.124  
Hazard labels (DOT) : 4.1 - Flammable solid



DOT Symbols : G - Identifies PSN requiring a technical name  
Packing group (DOT) : III - Minor Danger  
DOT Packaging Exceptions (49 CFR 173.xxx) : 151  
DOT Packaging Non Bulk (49 CFR 173.xxx) : 213  
DOT Packaging Bulk (49 CFR 173.xxx) : 240

### 14.3. Additional information

Other information : No supplementary information available.

### Transport by sea

DOT Vessel Stowage Location : B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.

### Air transport

DOT Quantity Limitations Passenger aircraft/rail : 25 kg  
(49 CFR 173.27)  
DOT Quantity Limitations Cargo aircraft only (49 : 100 kg  
CFR 175.75)

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

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

Listed on the United States TSCA (Toxic Substances Control Act) inventory

### 15.2. International regulations

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

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

Listed on the Canadian NDSL (Non-Domestic Substances List)  
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)  
Listed on ELINCS (European List of Notified Chemical Substances)  
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory  
Listed on NZIoC (New Zealand Inventory of Chemicals)

### 15.3. US State regulations

#### BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE(125051-32-3)

U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No

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

U.S. - California - Proposition 65 - Carcinogens List	U.S. - California - Proposition 65 - Developmental Toxicity	U.S. - California - Proposition 65 - Reproductive Toxicity - Female	U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No significance risk level (NSRL)
No	No	No	No	

## 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.

### Full text of H-phrases::

Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A
Flam. Sol. 2	Flammable solids Category 2
Skin Irrit. 2	Skin corrosion/irritation Category 2
H228	Flammable solid
H315	Causes skin irritation
H319	Causes serious eye irritation

### HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur  
Flammability : 3 Serious Hazard  
Physical : 1 Slight Hazard

Prepared by safety and environmental affairs.

Date of issue: 08/21/2015 Version: 1.0

SDS US (GHS HazCom 2012) - Custom

According to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

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