



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

1.1. Identification

Product name	: BIS(2,6-DIFLUORO-3-(1-HYDROXYRROL-1-YL)PHENYL)TITANOCENE
Product code	: OMTI014
Product form	: Substance
Physical state	: Solid
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. Recommended use and restrictions on use

Recommended use : Chemical intermediate

1.3. Supplier

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

1.4. Emergency telephone number

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

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification

Flammable solids Category 2	H228	Flammable solid
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US) :



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.

2.3. Hazards not otherwise classified (HNOC)

No additional information available

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2.4. Unknown acute toxicity (GHS US)

Not applicable

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	%	GHS-US classification
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

Full text of hazard classes and 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 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 (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. Immediate medical attention and special treatment, if necessary

No additional information available

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

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

Unsuitable extinguishing media : Do not use straight streams.

5.2. Specific hazards arising from the chemical

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

5.3. Special protective equipment and precautions for fire-fighters

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".

6.2. Environmental precautions

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

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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.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Appropriate engineering controls

- Appropriate engineering controls : Provide local exhaust or general room ventilation.

8.3. Individual protection measures/Personal protective equipment

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

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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
Relative vapor 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
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
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/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

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SECTION 12: Ecological information

12.1. Toxicity

No additional information available

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. Other adverse effects

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

Effect on the ozone layer : No additional information available

SECTION 13: Disposal considerations

13.1. Disposal 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

UN-No.(DOT) : 1325

DOT NA no. : UN1325

14.2. UN proper shipping name

Transport document description : UN1325 Flammable solids, organic, n.o.s. (BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE), 4.1, III

Proper Shipping Name (DOT) : Flammable solids, organic, n.o.s.
(BIS(2,6-DIFLUORO-3-(1-HYDROPYRROL-1-YL)PHENYL)TITANOCENE)

Class (DOT) : 4.1 - Class 4.1 - Flammable Solid 49 CFR 173.124

Packing group (DOT) : III - Minor Danger

Hazard labels (DOT) : 4.1 - Flammable solid



DOT Packaging Non Bulk (49 CFR 173.xxx) : 213

DOT Packaging Bulk (49 CFR 173.xxx) : 240

DOT Packaging Exceptions (49 CFR 173.xxx) : 151

DOT Symbols : G - Identifies PSN requiring a technical name

14.3. Additional information

Emergency Response Guide (ERG) Number : 133

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 (49 CFR 173.27) : 25 kg

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 100 kg

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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

CANADA

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

Listed on the Canadian NDSL (Non-Domestic Substances List)

EU-Regulations

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

Listed on ELINCS (European List of Notified Chemical Substances)

National regulations

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

Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)

Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory

Listed on NZIoC (New Zealand Inventory of Chemicals)

15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

SECTION 16: Other information

Full text of H-phrases::

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

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.

Hazard Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 3 Serious Hazard - Materials capable of ignition under almost all normal temperature conditions. Includes flammable liquids with flash points below 73 F and boiling points above 100 F, as well as liquids with flash points between 73 F and 100 F. (Classes IB & IC)

Physical : 1 Slight Hazard - Materials that are normally stable but can become unstable (self-react) at high temperatures and pressures. Materials may react non-violently with water or undergo hazardous polymerization in the absence of inhibitors.

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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