

## Chemical Safety Data Sheet MSDS / SDS

## Pentamethylcyclopentadienyltitanium trichloride

Revision Date:2025-07-05 Revision Number:1

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

## Product identifier

Product name : Pentamethylcyclopentadienyltitanium trichloride  
CBnumber : CB7740594  
CAS : 12129-06-5  
Synonyms : (pentamethylcyclopentadienyl)titanium(IV) trichloride,Pentamethylcyclopentadienyltitanium trichloride

## Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

## Company Identification

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

## SECTION 2: Hazards identification

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

P501 Dispose of contents/container to.....  
P406 Store in corrosive resistant/... container with a resistant inner liner.  
P405 Store locked up.  
P390 Absorb spillage to prevent material damage.  
P310 Immediately call a POISON CENTER or doctor/physician.  
P308+P313 IF exposed or concerned: 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.  
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.  
P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.

P264 Wash skin thoroughly after handling.  
P264 Wash hands thoroughly after handling.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.  
P234 Keep only in original container.  
P202 Do not handle until all safety precautions have been read and understood.  
P201 Obtain special instructions before use.

#### **Hazard statements**

H341 Suspected of causing genetic defects  
H318 Causes serious eye damage  
H314 Causes severe skin burns and eye damage  
H290 May be corrosive to metals

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: Pentamethylcyclopentadienyltitanium trichloride
Synonyms	: (pentamethylcyclopentadienyl)titanium(IV) trichloride, Pentamethylcyclopentadienyltitanium trichloride
CAS	: 12129-06-5
MF	: C <sub>10</sub> H <sub>15</sub> Cl <sub>3</sub> Ti
MW	: 289.45

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **General advice**

First aider needs to protect himself. Show this material safety data sheet to the doctor in attendance.

#### **If inhaled**

After inhalation: fresh air. Call in physician.

#### **In case of skin contact**

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

#### **In case of eye contact**

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

#### **If swallowed**

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

### **Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### **Indication of any immediate medical attention and special treatment needed**

No data available

## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

### Special hazards arising from the substance or mixture

Carbon oxides, Hydrogen chloride gas, Titanium/titanium oxides Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

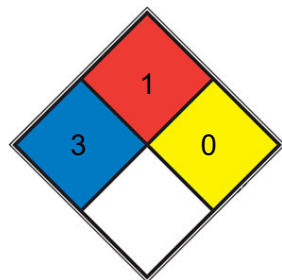
### Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

### NFPA 704



**HEALTH 3** Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

**FIRE 1** Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

☐ SPEC.

☐ HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### **Environmental precautions**

Do not let product enter drains.

### **Methods and materials for containment and cleaning up**

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### **Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **Precautions for safe handling**

For precautions see section 2.2.

### **Conditions for safe storage, including any incompatibilities**

Tightly closed. Dry.

Handle and store under inert gas.

### **Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **SECTION 8: Exposure controls/personal protection**

### **control parameter**

#### **Hazard composition and occupational exposure limits**

Does not contain substances with occupational exposure limits.

### **Exposure controls**

#### **Appropriate engineering controls**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

#### **Personal protective equipment**

##### **Eye/face protection**

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

##### **Skin protection**

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:KCL 741 Dermatil? L

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:KCL 741 Dermatil? L

#### Body Protection

protective clothing

#### Respiratory protection

required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

#### Control of environmental exposure

Do not let product enter drains.

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	red powder
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 200 °C - dec.
Initial boiling point and boiling range	190 - 220 °C at 5,33 - 9,33 hPa
Flash point	Not applicable
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	No data available
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

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## SECTION 10: Stability and reactivity

### Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### Possibility of hazardous reactions

No data available

### Conditions to avoid

no information available

### Incompatible materials

Strong oxidizing agents

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Hydrogen chloride gas, Titanium/titanium oxides

Other decomposition products - No data available In the event of fire: see section 5

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

No data available

#### Skin corrosion/irritation

No data available

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

No data available

#### Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

#### Reproductive toxicity

No data available

#### Specific target organ toxicity - single exposure

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 12: Ecological information

**Toxicity**

No data available

**Persistence and degradability**

No data available

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

**Waste treatment methods****Product**

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

**UN number**

ADR/RID: 3261 IMDG: 3261 IATA: 3261

### UN proper shipping name

ADR/RID: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.

(Trichloro(pentamethylcyclopentadienyl)titanium(IV)) IMDG: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.

(Trichloro(pentamethylcyclopentadienyl)titanium(IV)) IATA: Corrosive solid, acidic, organic, n.o.s.

(Trichloro(pentamethylcyclopentadienyl)titanium(IV))

### Transport hazard class(es)

ADR/RID: 8 IMDG: 8 IATA: 8

### Packaging group

ADR/RID: II IMDG: II IATA: II

### Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

### Special precautions for user

No data available

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## SECTION 15: Regulatory information

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Not Listed.

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## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

## References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.