

## Chemical Safety Data Sheet MSDS / SDS

**(R,R)-DUTHALER-HAFNER REAGENT**Revision Date:2026-05-31 Revision Number:1

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : (R,R)-DUTHALER-HAFNER REAGENT  
CBnumber : CB9195367  
CAS : 132068-98-5  
Synonyms : Duthaler-Hafner Reagent;Chloro(h5-cyclopentadienyl)[(4R,trans)-2,2-dimethyl-a,a,a

**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

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**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P363 Wash contaminated clothing before reuse.

**Hazard statements**H314 Causes severe skin burns and eye damage

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**SECTION 3: Composition/information on ingredients**

## Substance

Product name	: (R,R)-DUTHALER-HAFNER REAGENT
Synonyms	: Duthaler-Hafner Reagent;Chloro(h5-cyclopentadienyl)[(4R,trans)-2,2-dimethyl-a,a,a
CAS	: 132068-98-5
MF	: C36H35ClO4Ti5*
MW	: 614.98

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

No data available

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

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

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

No data available

### 4.4 Notes to physician

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

No data available

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen chloride gas

Titanium/titanium oxides

Combustible.

### 5.3 Advice for firefighters

No data available

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

For personal protection see section 8.

### 6.2 Environmental precautions

No data available

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

No data available

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

For precautions see section 2.2.

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

Store under inert gas. Moisture sensitive.

#### Storage class

Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

No data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

a) Physical state	powder
b) Color	light yellow
c) Odor	No data available
d) Melting point/freezing point	Melting point/ range: 209 - 213 °C
e) Initial boiling point and boiling range	No data available
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	No data available
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available

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k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available
	Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	No data available
p) Density	No data available
Relative density	No data available
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available
Solubility	sol toluene (ca. 370 mg mL <sup>-1</sup> ), THF (ca. 470 mg mL <sup>-1</sup> ), diethyl ether (ca. 150 mg mL <sup>-1</sup> )

## 9.2 Other safety information

No data available

## SECTION 10: Stability and reactivity

### 10.1 Chemical stability

No data available

### 10.2 Possibility of hazardous reactions

No data available

### 10.3 Conditions to avoid

No data available

### 10.4 Incompatible materials

Strong oxidizing agents

### 10.5 Hazardous decomposition products

In the event of fire: see section 5

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

Remarks: No data available

**Serious eye damage/eye irritation**

Remarks: No data available

**Respiratory or skin sensitization**

Classified based on available data. For more details, see section 2

**Germ cell mutagenicity**

Classified based on available data. For more details, see section 2

**Carcinogenicity**

Classified based on available data. For more details, see section 2

**Reproductive toxicity**

Classified based on available data. For more details, see section 2

**Specific target organ toxicity - single exposure**

Classified based on available data. For more details, see section 2

**Specific target organ toxicity - repeated exposure**

Classified based on available data. For more details, see section 2

**Aspiration hazard**

Classified based on available data. For more details, see section 2

**11.2 Additional Information**

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, Vomiting, 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

**12.1 Toxicity**

No data available

**12.2 Persistence and degradability**

No data available

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

**12.6 Endocrine disrupting properties**

No data available

## 12.7 Other adverse effects

No data available

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# SECTION 13: Disposal considerations

## 13.1 Waste treatment methods

No data available

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# SECTION 14: Transport information

## 14.1 UN number

ADR/RID: 3261

IMDG: 3261

IATA-DGR: 3261

## 14.2 UN proper shipping name

ADR/RID: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. ((4R,5R)-Chloro- cyclopentadienyl-[2,2-dimethyl-1,3-dioxolan-4,5-bis(diphenylmethoxy)]titanium)

IMDG: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. ((4R,5R)-Chloro- cyclopentadienyl-[2,2-dimethyl-1,3-dioxolan-4,5-bis(diphenylmethoxy)]titanium)

IATA-DGR: Corrosive solid, acidic, organic, n.o.s. ((4R,5R)-Chloro-cyclopentadienyl-[2,2- dimethyl-1,3-dioxolan-4,5-bis(diphenylmethoxy)]titanium)

## 14.3 Transport hazard class(es)

ADR/RID: 8

IMDG: 8

IATA-DGR: 8

## 14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

## 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

## 14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

## 14.7 Incompatible materials

Strong oxidizing agents

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## SECTION 15: Regulatory information

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

National regulatory information

Measures on the Environmental Administration of New Chemical Substances Registration

Registration/Notification number : B1A222232634

Downstream users need to comply with the conditions of safe use of the chemical, understand the environmental and health hazard and risk management measures identified on the SDS as well as the local/national regulations concerning the chemical.

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

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## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

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

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

#### 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.