

## Chemical Safety Data Sheet MSDS / SDS

**(3S-CIS)-(+)-TETRAHYDRO-3,7A-DIPHENYLPYRROLO[2,1-B]OXAZOL-5(6H)-ONE**

Revision Date:2026-03-21 Revision Number:1

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

Product name : (3S-CIS)-(+)-TETRAHYDRO-3,7A-DIPHENYLPYRROLO[2,1-B]OXAZOL-5(6H)-ONE  
CBnumber : CB3256369  
CAS : 161970-71-4  
Synonyms : (3S,7aS)-3,7a-Diphenyltetrahydropyrrolo[2,1-b]oxazol-5(6H)-one;(3S-CIS)-(+)-3,7A-DIPHENYLTETRAHYDROPYRROLO-[2,1-B]-OXAZOL-5(6H)-ONE

**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

Warning

**Precautionary statements**

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

Continuerinsing.

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

P264 Wash skin thoroughly after handling.

P362 Take off contaminated clothing and wash before reuse.

P332+P313 IF SKIN irritation occurs: Get medical advice/attention.

P321 Specific treatment (see ... on this label).

P302+P352 IF ON SKIN: wash with plenty of soap and water.

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

P264 Wash skin thoroughly after handling.

#### **Hazard statements**

H335 May cause respiratory irritation

H319 Causes serious eye irritation

H315 Causes skin irritation

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name : (3S-CIS)-(+)-TETRAHYDRO-3,7A-DIPHENYLPYRROLO[2,1-B]OXAZOL-5(6H)-ONE  
Synonyms : (3S,7aS)-3,7a-Diphenyltetrahydropyrrolo[2,1-b]oxazol-5(6H)-one;(3S-CIS)-(+)-3,7A-DIPHENYLTETRAHYDROPYRROLO-[2,1-B]-OXAZOL-5(6H)-ONE  
CAS : 161970-71-4  
MF : C18H17NO2  
MW : 279.33

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## SECTION 4: First aid measures

### **4.1 Description of first-aid measures**

#### **General advice**

Consult a physician. Show this material safety data sheet to the doctor in attendance.

#### **If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration.

Consult a physician.

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

Wash off with soap and plenty of water. Consult a physician.

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

Flush eyes with water as a precaution.

#### **If swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### **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

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## SECTION 5: Firefighting measures

### **5.1 Extinguishing media**

#### **Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Nature of decomposition products not known.

## **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

## **5.4 Further information**

No data available

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# **SECTION 6: Accidental release measures**

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

Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

For personal protection see section 8.

## **6.2 Environmental precautions**

Do not let product enter drains.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

## **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**

### **Advice on safe handling**

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.

### **Advice on protection against fire and explosion**

Provide appropriate exhaust ventilation at places where dust is formed.

### **Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

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

### **Storage conditions**

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.

### **Storage class**

Storage class (TRGS 510): 11: Combustible Solids

### 7.3 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

### 8.1 Control parameters

#### Ingredients with workplace control parameters

### 8.2 Exposure controls

#### Personal protective equipment

##### Eye/face protection

Safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as

NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

##### Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU

EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### 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

a) Physical state	solid
b) Color	No data available
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	422.1°C (rough estimate)
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available

limits

h) Flash point	No data available
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
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	1.1441 (rough estimate)
Relative density	1.1441 (rough estimate)
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

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## 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**

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

**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****Endocrine disrupting properties**

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

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.

## 12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission

Delegated regulation (EU) 2017/2100 or Commission

Regulation (EU) 2018/605 at levels of 0.1% or higher.

## 12.7 Other adverse effects

No data available

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# SECTION 13: Disposal considerations

## 13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

### Contaminated packaging

Dispose of as unused product.

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# SECTION 14: Transport information

## 14.1 UN number

ADR/RID: -

IMDG: -

IATA: -

## 14.2 UN proper shipping name

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

## 14.3 Transport hazard class(es)

ADR/RID: -

IMDG: -

IATA: -

## 14.4 Packaging group

ADR/RID: -

IMDG: -

IATA: -

#### **14.5 Environmental hazards**

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

#### **14.6 Special precautions for user**

No data available

Further information: Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15: Regulatory information

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

This material safety data sheet complies with the requirements of Regulation (EC) No.

1907/2006.

### **15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

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## SECTION 16: Other information

### **Full text of other abbreviations**

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways

ADR - Agreement concerning the International Carriage of Dangerous Goods by Road

AIIIC - Australian Inventory of Industrial Chemicals

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC<sub>x</sub> - Concentration associated with x% response

EL<sub>x</sub> - Loading rate associated with x% response

EmS - Emergency Schedule

ENCS - Existing and New Chemical Substances (Japan)

ErC<sub>x</sub> - Concentration associated with x% growth rate response

GHS - Globally Harmonized System

GLP - Good Laboratory Practice

IARC - International Agency for Research on Cancer

IATA - International Air Transport Association

IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk

IC50 - Half maximal inhibitory concentration  
ICAO - International Civil Aviation Organization  
IECSC - Inventory of Existing Chemical Substances in China  
IMDG - International Maritime Dangerous Goods  
IMO - International Maritime Organization  
ISHL - Industrial Safety and Health Law (Japan)  
ISO - International Organisation for Standardization  
KECI - Korea Existing Chemicals Inventory  
LC50 - Lethal Concentration to 50 % of a test population  
LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose)  
MARPOL - International Convention for the Prevention of Pollution from Ships  
n.o.s. - Not Otherwise Specified  
NO(A)EC - No Observed (Adverse) Effect Concentration  
NO(A)EL - No Observed (Adverse) Effect Level  
NOELR - No Observable Effect Loading Rate  
NZIoC - New Zealand Inventory of Chemicals  
OECD - Organization for Economic Co-operation and Development  
OPPTS - Office of Chemical Safety and Pollution Prevention  
PBT - Persistent, Bioaccumulative and Toxic substance  
PICCS - Philippines Inventory of Chemicals and Chemical Substances  
(Q)SAR - (Quantitative) Structure Activity Relationship  
REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals  
RID - Regulations concerning the International Carriage of Dangerous Goods by Rail  
SADT - Self-Accelerating Decomposition Temperature  
SDS - Safety Data Sheet  
TCSI - Taiwan Chemical Substance Inventory  
TECI - Thailand Existing Chemicals Inventory  
TSCA - Toxic Substances Control Act (United States)  
UN - United Nations  
UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods  
vPvB - Very Persistent and Very Bioaccumulative

**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.