

## Chemical Safety Data Sheet MSDS / SDS

**(5R,6S)-2-Mesityl-5,6-diphenyl-6,8-dihydro-5H-[1,2,4]triazolo[3,4-c][1,4]oxazin-2-ium tetrafluoroborate 97%**Revision Date:2023-11-29 Revision Number:1

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

**Product identifier**

Product name : (5R,6S)-2-Mesityl-5,6-diphenyl-6,8-dihydro-5H-[1,2,4]triazolo[3,4-c][1,4]oxazin-2-ium tetrafluoroborate 97%

CBnumber : CB32730179

CAS : 950842-71-4

**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 : 400-158-6606

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## SECTION 2: Hazards identification

**GHS Label elements, including precautionary statements**

Signal word : no data available

**Hazard statement(s)**

no data available

**Prevention**

no data available

**Response**

no data available

**Storage**

no data available

**Disposal**

no data available

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## SECTION 3: Composition/information on ingredients

## Substance

Product name	: (5R,6S)-2-Mesityl-5,6-diphenyl-6,8-dihydro-5H-[1,2,4]triazolo[3,4-c][1,4]oxazin-2-ium tetrafluoroborate 97%
CAS	: 950842-71-4
MF	: C <sub>26</sub> H <sub>26</sub> BF <sub>4</sub> N <sub>3</sub> O
MW	: 483.32

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of HF. After decontamination with water, further damage can occur due to penetration/absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or Milk of Magnesia to conscious victims. Conditions such as hypocalcemia, hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure.

#### If inhaled

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

#### In case of skin contact

Wash off with soap and plenty of water. First treatment with calcium gluconate paste.

#### 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.

### 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

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing media

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

### Special hazards arising from the substance or mixture

Carbon oxides, Nitrogen oxides (NOx), Hydrogen fluoride, Borane/boron oxides

### **Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

### **Further information**

No data available

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## **SECTION 6: Accidental release measures**

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

Avoid dust formation. Avoid breathing vapors, mist or gas. For personal protection see section 8.

### **Environmental precautions**

Do not let product enter drains.

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

Sweep up and shovel. Keep in suitable, closed containers for disposal.

### **Reference to other sections**

For disposal see section 13.

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

### **Precautions for safe handling**

Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection.

For precautions see section 2.2.

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

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Moisture sensitive. Store under nitrogen.

### **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**

General industrial hygiene practice.

### 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).

#### 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

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. 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

Appearance	solid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 187 - 193 °C
Initial boiling point and boiling range	No data available
Flash point	No data available
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

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### Other safety information

No data available

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## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under recommended storage conditions.

### Possibility of hazardous reactions

No data available

### Conditions to avoid

No data available

### Incompatible materials

Strong oxidizing agents

### Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen fluoride, Borane/boron 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

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

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**

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

**Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

**Waste treatment methods**

**Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

**Contaminated packaging**

Dispose of as unused product.

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## SECTION 14: Transport information

### UN number

ADR/RID: - IMDG: - IATA: -

### 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: -

Packaging group

#### 14.4

ADR/RID: - IMDG: - IATA: -

Environmental hazards

#### 14.5

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

### 14.6 Special precautions for user

### Further information

Not classified as dangerous in the meaning of transport regulations.

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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

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

EC Inventory:Not Listed.

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

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

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/>

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

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

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## SECTION 16: Other information

### Abbreviations and acronyms

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

## 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.