

## Chemical Safety Data Sheet MSDS / SDS

**Tetrabutylammonium bis(3,4,6-trichloro-1,2-benzene-dithiolato)nickelate**

Revision Date:2026-05-31 Revision Number:1

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

Product name : Tetrabutylammonium bis(3,4,6-trichloro-1,2-benzene-dithiolato)nickelate  
CBnumber : CB41500907  
CAS : 87314-12-3  
Synonyms : Tetrabutylammonium Bis(3,4,6-trichloro-1,2-benzenedithiolato)nickel(III) Complex

**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**

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P272 Contaminated work clothing should not be allowed out of the workplace.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P302+P352 IF ON SKIN: wash with plenty of soap and water.  
P333+P313 IF SKIN irritation or rash occurs: Get medical advice/attention.  
P321 Specific treatment (see ... on this label).  
P363 Wash contaminated clothing before reuse.  
P501 Dispose of contents/container to....  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P285 In case of inadequate ventilation wear respiratory protection.  
P304+P341 IF INHALED: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.

P342+P311 IF experiencing respiratory symptoms: call a POISON CENTER or doctor/physician.

P501 Dispose of contents/container to.....

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

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P314 Get medical advice/attention if you feel unwell.

P501 Dispose of contents/container to.....

#### **Hazard statements**

H334 May cause allergy or asthma symptoms or breathing difficulties if inhaled

H350 May cause cancer

H317 May cause an allergic skin reaction

H372 Causes damage to organs through prolonged or repeated exposure

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: Tetrabutylammonium bis(3,4,6-trichloro-1,2-benzene-dithiolato)nickelate
Synonyms	: Tetrabutylammonium Bis(3,4,6-trichloro-1,2-benzenedithiolato)nickel(III) Complex
CAS	: 87314-12-3
MF	: C <sub>28</sub> H <sub>42</sub> Cl <sub>6</sub> NNiS <sub>4</sub>
MW	: 792.28

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## SECTION 4: First aid measures

### **If inhaled**

Remove person to fresh air and keep comfortable for breathing. Get medical advice/ attention.

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

Take off all contaminated clothing immediately. Wash off with plenty of water. Get medical advice/ attention.

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

Rinse with plenty of water. If easy to do, remove contact lens, if worn. Get medical advice/ attention.

### **If swallowed**

Get medical advice/ attention. Rinse mouth.

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

None known.

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## SECTION 5: Firefighting measures

### **Suitable extinguishing media**

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

### **Specific hazards during fire fighting**

No information available.

### **Specific extinguishing methods**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment. Immediately evacuate personnel to safe areas. Remove undamaged containers from fire area if it is safe to do so.

### **Special protective equipment for fire-fighters**

Use personal protective equipment.

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

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

Wear suitable protective equipment. Keep people away from and upwind of spill/leak. Entry to non-involved personnel should be controlled around the leakage area by roping off, etc.

### **Environmental precautions**

Prevent product from entering drains.

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

Pick up and arrange disposal without creating dust.

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

### **Handling**

#### **Technical measures**

Prevent dispersion of dust.

#### **Local/Total ventilation**

Ensure adequate ventilation. Handle product only in closed system or provide appropriate exhaust ventilation at machinery. Use a local exhaust ventilation.

#### **Advice on safe handling**

Avoid contact with skin, eyes and clothing. Wear personal protective equipment. Wash hands and face thoroughly after handling.

#### **Avoidance of contact**

Oxidizing agents

### **Storage**

#### **Conditions for safe storage**

Keep container tightly closed. Store in a cool and shaded area. Store locked up.

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

### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **Engineering measures**

Install a closed system or local exhaust.

Also install safety shower and eye bath.

### **Personal protective equipment**

#### **Respiratory protection**

Dustproof gas mask

Self-contained breathing apparatus

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

Safety glasses

Safety goggles

Face-shield

#### **Skin and body protection**

Impervious protective clothing

#### **Hand protection**

Impervious gloves \*Use personal protective equipment(PPE) approved under appropriate government standards and follow local and national regulations.

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## SECTION 9: Physical and chemical properties

### **Information on basic physicochemical properties**

solid

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#### **Color**

green

#### **Odor**

No data available

#### **Odor Threshold**

No data available

#### **pH**

No data available

#### **Melting point/freezing point**

No data available

#### **Boiling point/boiling range**

No data available

**Flash point**

No data available

**Evaporation rate**

No data available

**Flammability**

No data available

**Upper explosion limit / Upper flammability limit**

No data available

**Lower explosion limit / Lower flammability limit**

No data available

**Vapor pressure**

No data available

**Solubility(ies)****Water solubility**

No data available

**Solubility in other solvents**

No data available

**Partition coefficient: n-octanol/water (log value)**

No data available

**Autoignition temperature**

No data available

**Decomposition temperature**

No data available

**Viscosity****Viscosity, dynamic**

No data available

**Viscosity, kinematic**

No data available

**Molecular weight**

788.25 g/mol

## Physical state

powder to crystal

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## SECTION 10: Stability and reactivity

### Reactivity

No data available

### Chemical stability

Stable under normal conditions.

### Possibility of hazardous reactions

None under normal processing.

### Incompatible materials

Oxidizing agents

### Hazardous decomposition products

Carbon monoxide, Carbon dioxide (CO<sub>2</sub>), Nitrogen oxides (NO<sub>x</sub>), Sulfur oxides, Hydrogen chloride gas, Metal oxides

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## SECTION 11: Toxicological information

### Acute toxicity

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

### Skin corrosion/irritation

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

### Serious eye damage/eye irritation

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

### Respiratory or skin sensitization

### Product

### Assessment

May cause sensitization by inhalation.

### Components

### Tetrabutylammonium Bis(3,4,6-trichloro-1,2-benzenedithiolato)nickelate

### Assessment

May cause sensitization by inhalation.

## **Assessment**

May cause sensitization by skin contact.

## **Germ cell mutagenicity**

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

## **Carcinogenicity**

## **Product**

## **Carcinogenicity - Assessment**

Human carcinogen.

## **Components**

## **Tetrabutylammonium Bis(3,4,6-trichloro-1,2-benzenedithiolato)nickelate**

## **Carcinogenicity - Assessment**

Human carcinogen.

## **Reproductive toxicity**

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

## **STOT-single exposure**

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

## **STOT-repeated exposure**

## **Product**

## **Target Organs**

Respiratory system

## **Assessment**

Causes damage to organs through prolonged or repeated exposure.

## **Components**

## **Tetrabutylammonium Bis(3,4,6-trichloro-1,2-benzenedithiolato)nickelate**

## **Target Organs**

Respiratory system

## **Assessment**

Causes damage to organs through prolonged or repeated exposure.

## **Repeated dose toxicity**

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

### **Aspiration toxicity**

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

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## SECTION 12: Ecological information

### **Ecotoxicity**

No data available

### **Persistence and degradability**

No data available

### **Bioaccumulative potential**

No data available

### **Mobility in soil**

No data available

### **Other adverse effects**

No data available

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## SECTION 13: Disposal considerations

### **Disposal methods**

#### **Waste from residues**

Disposal in accordance with local and national regulations. Entrust disposal to a licensed waste disposal company.

#### **Contaminated packaging**

Disposal in accordance with local and national regulations. Before disposal of used container, remove contents completely.

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## SECTION 14: Transport information

### **International Regulations**

#### **IATA-DGR**

##### **UN/ID No.**

Not applicable

##### **Proper shipping name**

Not applicable

##### **Class**

Not applicable

**Subsidiary risk**

Not applicable

**Packing group**

Not applicable

**IMDG-Code****UN number**

Not applicable

**Proper shipping name**

Not applicable

**Class**

Not applicable

**Subsidiary risk**

Not applicable

**Packing group**

Not applicable

**EmS Code**

Not applicable

**Domestic regulation****GB 6944/12268****UN number**

Not applicable

**Proper shipping name**

Not applicable

**Class**

Not applicable

**Subsidiary risk**

Not applicable

**Packing group**

Not applicable

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## SECTION 15: Regulatory information

**Measures on the Environmental Administration of New Chemical Substances Registration****Registration/Notification number**

B1A232216159

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.

**The ingredients of this product are reported in the following inventories****CH BAGREG**

Not in compliance with the inventory

**TSCA**

Substance(s) not listed on TSCA inventory

**AICS**

Not in compliance with the inventory

**DSL**

This product contains the following components that are not on the Canadian DSL nor NDSL.

Tetrabutylammonium Bis(3,4,6-trichloro-1,2benzenedithiolato)nickelate

**ENCS**

Not in compliance with the inventory

**ISHL**

Not in compliance with the inventory

**KECI**

Not in compliance with the inventory

**PICCS**

Not in compliance with the inventory

**IECSC**

Not in compliance with the inventory

**NZIoC**

Not in compliance with the inventory

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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.