

## Chemical Safety Data Sheet MSDS / SDS

**5-oxo-1,3,3-trimethyl-cyclohexanecarbonitril**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 : 5-oxo-1,3,3-trimethyl-cyclohexanecarbonitril  
CBnumber : CB6857604  
CAS : 7027-11-4  
EINECS Number : 411-490-4  
Synonyms : 3-cyano-3,5,5-trimethylcyclohexanone,5-oxo-1,3,3-trimethyl-cyclohexanecarbonitril

**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

Warning

**Precautionary statements**

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

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

**Hazard statements**

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

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

|              |   |
|--------------|---|
| Product name | : 5-oxo-1,3,3-trimethyl-cyclohexanecarbonitril                                      |
| Synonyms     | : 3-cyano-3,5,5-trimethylcyclohexanone,5-oxo-1,3,3-trimethyl-cyclohexanecarbonitril |
| CAS          | : 7027-11-4   |
| EC number    | : 411-490-4   |
| MF           | : C10H15NO  |
| MW           | : 165.23  |

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## SECTION 4: First aid measures

### Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

#### 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

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

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

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

The most important known symptoms and effects are described in the labelling (see section 2 or 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 bromide gas

### Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

## Further information

no data available

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## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. For personal protection see section 8.

### Environmental precautions

Do not let product enter drains.

### 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.

### Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### Precautions for safe handling

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

Provide appropriate exhaust ventilation at places where dust is formed.

Normal measures for preventive fire protection.

For precautions see section 2.

### Conditions for safe storage, including any incompatibilities

### Specific end use(s)

Apart from the uses mentioned in section 1, no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### Appropriate engineering controls

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

### Personal protective equipment

#### Eye/face protection

Face shield and safety glasses 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.

### 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

|                           |  |
|---------------------------|--|
| Appearance / Form         | no data available                      |
| Odor                      | no data available                      |
| Odor Threshold            | no data available                      |
| pH                        | no data available                      |
| Melting point             | no data available                      |
| Boiling point/range       | 105-110 °C(Press: 0.075 Torr)          |
| Flash point               | no data available                      |
| Evaporation rate          | no data available                      |
| Flammability              | no data available                      |
| Upper/lower flammability  | no data available                      |
| explosive limits          | no data available                      |
| Vapor pressure            | 0.16Pa at 20°C                         |
| Vapour density            | no data available                      |
| Relative density          | 0.98±0.1 g/cm <sup>3</sup> (Predicted) |
| Water solubility          | 4.76g/L at 20°C                        |
| Partition coefficient     | no data available                      |
| Auto-ignition temperature | no data available                      |
| Decomposition Temp        | no data available                      |
| log Pow                   | no data available                      |
| Viscosity                 | no data available                      |

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|                      |                   |
|----------------------|-------------------|
| Explosive properties | no data available |
| Oxidizing properties | no data available |
| Physical state       | solid             |
| Colour               | Faint yellow      |

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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**

no data available

#### **Hazardous decomposition products**

no data available

#### **Other decomposition products**

no data available

#### **In the event of fire**

see section 5

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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/irritation**

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

### **Respiratory or skin sensitisation**

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**

#### **IARC**

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

#### **ACGIH**

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

#### **NTP**

No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

#### **OSHA**

No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

### **Reproductive toxicity**

#### **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

#### **Additional Information**

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

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**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

### **Contaminated packaging**

Dispose of as unused product.

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## **SECTION 14: Transport information**

### **UN number**

ADR/RID:

IMDG:

IATA-DGR:

### **UN proper shipping name**

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

### **Transport hazard class(es)**

ADR/RID:

IMDG:

IATA-DGR:

### **Packaging group**

ADR/RID:

IMDG:

IATA-DGR:

## Environmental hazards

ADR/RID: -

IMDG: -

IATA-DGR: -

## Special precautions for user

Further information : No data available

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## SECTION 15: Regulatory information

### SARA 302

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

### SARA 311/312 Hazards

Acute Health Hazard

### Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

### Pennsylvania Right To Know Components

### New Jersey Right To Know Components

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## SECTION 16: Other information

### Full text of H-Statements referred to under sections 2 and 3.

Acute Tox. Acute toxicity

Eye Irrit. Eye irritation

Skin Irrit. Skin irritation

H302 Harmful if swallowed

H315 Causes skin irritation

H319 Causes serious eye irritation

H335 May cause respiratory irritation

#### 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.