

## Chemical Safety Data Sheet MSDS / SDS

**3,5,5-Trimethylhexanoyl chloride**Revision Date:2025-07-05 Revision Number:1

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

Product name : 3,5,5-Trimethylhexanoyl chloride  
CBnumber : CB4278902  
CAS : 36727-29-4  
EINECS Number : 253-168-4  
Synonyms : incl,Isononanoyl chloride

**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****Classification of the substance or mixture**

Corrosive to metals, Category 1  
Acute toxicity - Category 4, Oral  
Skin corrosion, Sub-category 1A  
Skin sensitization, Category 1  
Acute toxicity - Category 1, Inhalation  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

**Label elements****Pictogram(s)**

Signal word : Danger

**Hazard statement(s)**

H290 May be corrosive to metals  
H302 Harmful if swallowed  
H314 Causes severe skin burns and eye damage

H317 May cause an allergic skin reaction

H330 Fatal if inhaled

H412 Harmful to aquatic life with long lasting effects

#### **Precautionary statement(s)**

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

P273 Avoid release to the environment.

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

P284 Wear respiratory protection.

P310 Immediately call a POISON CENTER or doctor/physician.

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

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#### **Prevention**

P234 Keep only in original packaging.

P264 Wash ... thoroughly after handling.

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

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

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

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P272 Contaminated work clothing should not be allowed out of the workplace.

P271 Use only outdoors or in a well-ventilated area.

P284 [In case of inadequate ventilation] wear respiratory protection.

P273 Avoid release to the environment.

#### **Response**

P390 Absorb spillage to prevent material damage.

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P363 Wash contaminated clothing before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

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

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

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P320 Specific treatment is urgent (see ... on this label).

#### **Storage**

P406 Store in a corrosion resistant/...container with a resistant inner liner.

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

#### **Disposal**

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and

product characteristics at time of disposal.

#### Other hazards

no data available

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 3,5,5-Trimethylhexanoyl chloride
Synonyms	: incl,Isononanoyl chloride
CAS	: 36727-29-4
EC number	: 253-168-4
MF	: C <sub>9</sub> H <sub>17</sub> ClO
MW	: 176.68

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## SECTION 4: First aid measures

### Description of first aid measures

#### If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

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

no data available

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

no data available

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## SECTION 5: Firefighting measures

### Extinguishing media

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

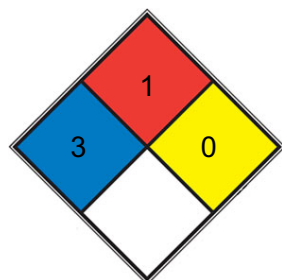
### Specific Hazards Arising from the Chemical

no data available

## Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

## NFPA 704



☒ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

☒ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

☒ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

☐ SPEC.

☐ HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

### Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

## SECTION 7: Handling and storage

### Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

## Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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## SECTION 8: Exposure controls/personal protection

### Control parameters

#### Occupational Exposure limit values

no data available

#### Biological limit values

no data available

### Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### Individual protection measures

#### Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### Skin protection

Wear fire/flamm resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

#### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

#### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Physical state	Liquid.
Colour	no data available
Odour	no data available
Melting point/freezing point	< -50 °C.
Boiling point or initial boiling point and boiling range	190.3 °C. Atm. press.:1 013.25 hPa. Remarks:Extrapolated.
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	74 °C. Atm. press.:1 013 hPa.
Auto-ignition temperature	372 °C. Atm. press.:1 012 - 1 016 hPa.
Decomposition temperature	no data available

pH	no data available
Kinematic viscosity	no data available
Solubility	no data available
Partition coefficient n-octanol/water	no data available
Vapour pressure	0.68 hPa. Temperature:20 °C. Remarks:Extrapolated based on experimental data.;4.98 hPa. Temperature:50 °C. Remarks:Extrapolated based on experimental data.
Density and/or relative density	0.940
Relative vapour density	0.940
Particle characteristics	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

### Conditions to avoid

no data available

### Incompatible materials

no data available

### Hazardous decomposition products

no data available

## SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD50 - rat (male/female) - ca. 1 700 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - ca. 0.24 mg/L air.
- Dermal: no data available

### Skin corrosion/irritation

no data available

### Serious eye damage/irritation

no data available

### **Respiratory or skin sensitization**

no data available

### **Germ cell mutagenicity**

no data available

### **Carcinogenicity**

no data available

### **Reproductive toxicity**

no data available

### **STOT-single exposure**

no data available

### **STOT-repeated exposure**

no data available

### **Aspiration hazard**

no data available

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## **SECTION 12: Ecological information**

### **Toxicity**

Toxicity to fish: LC50 - *Cyprinus carpio* - 4.3 pH - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 26.9 mg/L - 48 h.

Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - 40.8 mg/L - 72 h.

Toxicity to microorganisms: EC20 - activated sludge, domestic - 650 mg/L - 30 min. Remarks: Respiration rate.

### **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**

**Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

**Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

**UN Number**

ADR/RID: no data available

IMDG: no data available

IATA: no data available

**UN Proper Shipping Name**

ADR/RID: no data available

IMDG: no data available

IATA: no data available

**Transport hazard class(es)**

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

**Packing group, if applicable**

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

**Environmental hazards**

ADR/RID: No

IMDG: No

IATA: No

**Special precautions for user**

no data available

**Transport in bulk according to IMO instruments**

no data available

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## SECTION 15: Regulatory information



## **Safety, health and environmental regulations specific for the product in question**

### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

### **EC Inventory**

Listed.

### **United States Toxic Substances Control Act (TSCA) Inventory**

Listed.

### **China Catalog of Hazardous chemicals 2015**

Not Listed.

### **New Zealand Inventory of Chemicals (NZIoC)**

Not Listed.

### **PICCS**

Not Listed.

### **Vietnam National Chemical Inventory**

Listed.

### **IECSC**

Listed.

### **Korea Existing Chemicals List (KECL)**

Listed.

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## **SECTION 16: Other information**

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

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

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

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### **References**

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

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)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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