

## Chemical Safety Data Sheet MSDS / SDS

**3,5,5-Trimethylcyclohexane-1,2-dione**

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

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

Product name : 3,5,5-Trimethylcyclohexane-1,2-dione  
CBnumber : CB4459648  
CAS : 57696-89-6  
EINECS Number : 640-099-3  
Synonyms : 3,5,5-trimethylcyclohexane-1,2-dione,FEMA 3459

**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.

**Hazard statements**

H319 Causes serious eye irritation

H317 May cause an allergic skin reaction

H302 Harmful if swallowed

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

## Substance

|              |  |
|--------------|--|
| Product name | : 3,5,5-Trimethylcyclohexane-1,2-dione           |
| Synonyms     | : 3,5,5-trimethylcyclohexane-1,2-dione,FEMA 3459 |
| CAS          | : 57696-89-6                                     |
| EC number    | : 640-099-3                                      |
| MF           | : C9H14O2  |
| MW           | : 154.21   |

---

## 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

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.

### 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

---

## 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

Carbon oxides

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

No data available

## NFPA 704



HEALTH 0 Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials

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, [N<sub>2</sub>](#))

SPEC.  
 HAZ.

---

## 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.

---

## 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

---

# 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**

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.

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.

---

# 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      | 214.6±9.0 °C(Predicted)  |
| f) Flammability (solid, gas)                    | No data available  |
| g) Upper/lower flammability or explosive limits | No data available  |
| h) Flash point                                  | >100°(212°F)   |
| i) Autoignition temperature                     | No data available  |
| j) Decomposition temperature                    | No data available  |
| k) pH   | No data available  |
| l) Viscosity                                    | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                             | No data available  |
| n) Partition coefficient n-octanol/water        | log Pow: 0,111   |
| o) Vapor pressure                               | No data available  |
| p) Density                                      | 0.976±0.06 g/cm <sup>3</sup> (Predicted)   |
| Relative density                                | 0.976±0.06 g/cm <sup>3</sup> (Predicted)   |
| 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  |
| Appearance                                      | White to off-white Solid   |

## 9.2 Other safety information

No data available

---

## 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

---

# SECTION 11: Toxicological information

## 11.1 Information on toxicological effects

### Acute toxicity

LD50 Oral - 500,01 mg/kg

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

The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

### 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.

---

# 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

---

## **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.

---

## **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.

---

## **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.

International Chemical Weapons Convention : (CWC) Schedules of Toxic Chemicals and Precursors

Restrictions on the marketing and use of certain : dangerous substances and preparations

Regulation (EU) No 649/2012 of the European : Parliament and the Council concerning the export and import of dangerous chemicals

REACH - Candidate List of Substances of Very : High Concern for Authorisation (Article 59).

### **15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

---

## **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

AllC - 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  
IC<sub>50</sub> - 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  
LC<sub>50</sub> - Lethal Concentration to 50 % of a test population  
LD<sub>50</sub> - 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.