
1. Identification

1.1 GHS Product identifier

Product name 1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile

1.2 Other means of identification

Product number -

Other names 5-Oxo-1,3,3-trimethylcyclohexanecarbonitrile;3-Cyano-3,5,5-trimethylcyclohexanone;Cyclohexanecarbonitrile,1,3,3-trimethyl-5-oxo

1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research uses.

Uses advised against no data available

1.4 Supplier's details

Company -

Address -

Telephone -

Fax -

1.5 Emergency phone number

Emergency phone number -

Service hours Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

2. Hazard identification

2.1 Classification of the substance or mixture

Acute toxicity - Oral, Category 4

Skin sensitization, Category 1

Specific target organ toxicity "repeated exposure, Category 2

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 3

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word Warning

Hazard statement(s) H302 Harmful if swallowed
H317 May cause an allergic skin reaction
H412 Harmful to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
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.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P273 Avoid release to the environment.
P301+P312 IF SWALLOWED: Call a POISON CENTER/doctor/ if you feel unwell.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P333+P313 If skin irritation or rash occurs: Get medical advice/attention.
P321 Specific treatment (see ... on this label).
P362+P364 Take off contaminated clothing and wash it before reuse.
P314 Get medical advice/attention if you feel unwell.

Storage none

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.

2.3 Other hazards which do not result in classification

no data available

3. Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile	1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile	7027-11-4	-	100%

4. First-aid measures

4.1 Description of necessary first-aid measures

General advice

Medical attention is required. Consult a doctor. Show this safety data sheet (SDS) to the doctor in attendance.

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.

4.2 Most important symptoms/effects, acute and delayed

no data available

4.3 Indication of immediate medical attention and special treatment needed, if necessary

no data available

5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

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

5.2 Specific hazards arising from the chemical

no data available

5.3 Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

6. Accidental release measures

6.1 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.

6.2 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.

6.3 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.

7. Handling and storage

7.1 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.

7.2 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.

8. Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

no data available

8.2 Appropriate engineering controls

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

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

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

Skin protection

Wear fire/flammable 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

9. Physical and chemical properties

Physical state	Solid. Melt.
Colour	no data available
Odour	no data available
Melting point/ freezing point	62 Â°C.
Boiling point or initial boiling point and boiling range	279.88 Â°C. Atm. press.:1 013.25 hPa. Remarks:Boiling temperature extrapolated.;Ca. 145 - 150 Â°C. Atm. press.:16 hPa. Remarks:Value reasonably corresponds with Beilstein.
Flammability	no data available
Lower and upper explosion limit / flammability limit	no data available
Flash point	157 Â°C. Atm. press.:1 013.25 hPa.
Auto-ignition temperature	465 Â°C. Atm. press.:1 013.25 hPa.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water: 4.91 g/L. Temperature:20 Â°C. pH:8 - 8.1.
Partition coefficient n-octanol/water	log Pow = 1.6. Temperature:23 Â°C. Remarks:Main component.;log Pow = 1.8. Temperature:23 Â°C. Remarks:Isophorone.
Vapour pressure	0.001 hPa. Temperature:20 Â°C.;0.038 hPa. Temperature:50 Â°C.
Density and/or relative density	943.1 g/L. Temperature:80 Â°C.
Relative vapour density	no data available
Particle characteristics	no data available

10. Stability and reactivity

10.1 Reactivity

no data available

10.2 Chemical stability

no data available

10.3 Possibility of hazardous reactions

no data available

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

no data available

11. Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - 365 mg/kg bw.
- Inhalation: no data available
- 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

12. Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - Danio rerio (previous name: Brachydanio rerio) - > 10 - 22 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - > 100 mg/L - 48 h.
- Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 350 mg/L - 72 h.
- Toxicity to microorganisms: TT = toxic threshold concentration - Pseudomonas putida - 1 380 mg/L - 17 h.

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 Other adverse effects

no data available

13. Disposal considerations

13.1 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.

14. Transport information

14.1 UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

no data available

15. Regulatory information

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

Chemical name	Common names and synonyms	CAS number	EC number
1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile	1,3,3-trimethyl-5-oxocyclohexane-1-carbonitrile	7027-11-4	-
European Inventory of Existing Commercial Chemical Substances (EINECS)			Not Listed.
EC Inventory			Not 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.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Not Listed.
Korea Existing Chemicals List (KECL)			Listed.

16. Other information

Information on revision

Creation Date July 15, 2019

Revision Date July 15, 2019

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
- 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/>