Chemical Safety Data Sheet MSDS / SDS

1,1-Di-(tert-butylperoxy)-3,3,5-trimethylcyclohexane

Revision Date:2023-04-29 Revision Number:1

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

Product identifier

Product name	: 1,1-Di-(tert-butylperoxy)-3,3,5-trimethylcyclohexane	
CBnumber	: CB9369425	
CAS	: 6731-36-8	
EINECS Number	: 229-782-3	
Synonyms	: TMCH,1,1-Di-(tert-butylperoxy)-3,3,5-trimethylcyclohexane	
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	: 400-158-6606	

SECTION 2: Hazards identification

Classification of the substance or mixture

Organic peroxides, Type B

Label elements

Pictogram(s)

Signal word

Danger

Hazard statement(s)

H241 Heating may cause a fire or explosion

H413 May cause long lasting harmful effects to aquatic life

Precautionary statement(s)

P220 Keep/Store away from clothing/.../combustible materials.

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

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

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

Continuerinsing.

P410+P412 Protect from sunlight. Do not expose to temperatures exceeding 50 oC/122oF.

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P234 Keep only in original packaging.

P235 Keep cool.

P240 Ground and bond container and receiving equipment.

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

Response

none

Storage

P403 Store in a well-ventilated place.

P410 Protect from sunlight.

P411 Store at temperatures not exceeding ...°C/...°F.

P420 Store separately.

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

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1,1-Di-(tert-butylperoxy)-3,3,5-trimethylcyclohexane
Synonyms	: TMCH,1,1-Di-(tert-butylperoxy)-3,3,5-trimethylcyclohexane
CAS	: 6731-36-8
EC number	: 229-782-3
MF	: C17H34O4
MW	: 302.46

SECTION 4: First aid measures

Description of first aid measures

lf 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

Excerpt from ERG Guide 146 [Organic Peroxides (Heat, Contamination and Friction Sensitive)]: Fire may produce irritating, corrosive and/or toxic gases. Ingestion or contact (skin, eyes) with substance may cause severe injury or burns. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

Excerpt from ERG Guide 145 [Organic Peroxides (Heat and Contamination Sensitive)]: Fire may produce irritating, corrosive and/or toxic gases. Ingestion or contact (skin, eyes) with substance may cause severe injury or burns. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

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Indication of any immediate medical attention and special treatment needed

no data available

SECTION 5: Firefighting measures

Extinguishing media

Excerpt from ERG Guide 146 [Organic Peroxides (Heat, Contamination and Friction Sensitive)]: SMALL FIRE: Water spray or fog is preferred; if water not available use dry chemical, CO2 or regular foam. LARGE FIRE: Flood fire area with water from a distance. Use water spray or fog; do not use straight streams. Do not move cargo or vehicle if cargo has been exposed to heat. Move containers from fire area if you can do it without risk. FIRE INVOLVING TANKS OR CAR/TRAILER LOADS: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2016)

Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 146 [Organic Peroxides (Heat, Contamination and Friction Sensitive)]: May explode from heat, shock, friction or contamination. May ignite combustibles (wood, paper, oil, clothing, etc.). May be ignited by heat, sparks or flames. May burn rapidly with flareburning effect. Containers may explode when heated. Runoff may create fire or explosion hazard. (ERG, 2016) Excerpt from ERG Guide 145 [Organic Peroxides (Heat and Contamination Sensitive)]: May explode from heat or contamination. May ignite combustibles (wood, paper, oil, clothing, etc.). May be ignited by heat, sparks or flames. May burn rapidly with flare-burning effect. Containers may explode when heated. Runoff may create fire or explosion hazard. (ERG, 2016) Excerpt from ERG Guide 145 [Organic Peroxides (Heat, sparks or flames. May burn rapidly with flare-burning effect. Containers may explode when heated. Runoff may create fire or explosion hazard. (ERG, 2016) Excerpt from ERG Guide 146 [Organic Peroxides (Heat, Contamination and Friction Sensitive)]: May explode from heat, shock, friction or

contamination. May ignite combustibles (wood, paper, oil, clothing, etc.). May be ignited by heat, sparks or flames. May burn rapidly with flareburning effect. Containers may explode when heated. Runoff may create fire or explosion hazard. (ERG, 2016)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

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 sparkproof 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.

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 riskelimination 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/flame 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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Solution
Colour	Clear
Odour	no data available
Melting point/freezing point	-20°C
Boiling point or initial boiling point and	312.2°C at 760 mmHg
boiling range	
Flammability	no data available
Lower and upper explosion	no data available
limit/flammability limit	
Flash point	45°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	Acetonitrile (Slightly), Chloroform (Sparingly)
Partition coefficient n-octanol/water	no data available
Vapour pressure	no data available
Density and/or relative density	0.904g/mLat 25°C
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

No rapid reaction with air. No rapid reaction with water.

Chemical stability

no data available

Possibility of hazardous reactions

Peroxides, such as 1,1-DI-(TERT-BUTYLPEROXY)-3,3,5-TRIMETHYL CYCLOHEXANE, are good oxidizing agents. Organic compounds can ignite on contact with concentrated peroxides. Strongly reduced material such as sulfides, nitrides, and hydrides may react explosively with peroxides. There are few chemical classes that do not at least produce heat when mixed with peroxides. Many produce explosions or generate gases (toxic and nontoxic). Generally, dilute solutions of peroxides (<70%) are safe, but the presence of a catalyst (often a transition metal such as cobalt, iron, manganese, nickel, or vanadium) as an impurity may even then cause rapid decomposition, a buildup of heat, and even Chemical Book

an explosion. Solutions of peroxides often become explosive when evaporated to dryness or near-dryness. May explode from heat or contamination.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available
- 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

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available Toxicity to daphnia and other aquatic invertebrates: no data available Toxicity to algae: no data available Toxicity to microorganisms: 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

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.

SECTION 14: Transport information

UN Number

ADR/RID: UN3103 (For reference only, please check.) IMDG: UN3103 (For reference only, please check.) IATA: UN3103 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ORGANIC PEROXIDE TYPE C, LIQUID (For reference only, please check.)

IMDG: ORGANIC PEROXIDE TYPE C, LIQUID (For reference only, please check.) IATA: ORGANIC PEROXIDE TYPE C, LIQUID (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 5.2 (For reference only, please check.) IMDG: 5.2 (For reference only, please check.) IATA: 5.2 (For reference only, please check.)

Packing group, if applicable

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

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
Listed.
New Zealand Inventory of Chemicals (NZIoC)
Listed.
PICCS
Listed.
Vietnam National Chemical Inventory
Listed.
IECSC
Listed.
Korea Existing Chemicals List (KECL)

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

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

ChemlDplus, 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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