

Chemical Safety Data Sheet MSDS / SDS

1,1-Di(tert-butylperoxy)cyclohexaneRevision Date:2025-01-11 Revision Number:1

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

Product name : 1,1-Di(tert-butylperoxy)cyclohexane
CBnumber : CB7451603
CAS : 3006-86-8
EINECS Number : 221-111-2
Synonyms : 1,1-DI(TERT-BUTYLPEROXY)CYCLOHEXANE,1,1-Bis(tert-butylperoxy)cyclohexane

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 C
Aspiration hazard, Category 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 4

Label elements**Pictogram(s)**

☐☐☐

Signal word : Danger

Hazard statement(s)

H242 Heating may cause a fire
H304 May be fatal if swallowed and enters airways
H315 Causes skin irritation
H319 Causes serious eye irritation
H332 Harmful if inhaled
H335 May cause respiratory irritation

H340 May cause genetic defects

H350 May cause cancer

Precautionary statement(s)

P201 Obtain special instructions before use.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P234 Keep only in original container.

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

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

P308+P313 IF exposed or concerned: Get medical advice/attention.

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/...

P273 Avoid release to the environment.

Response

P370+P378 In case of fire: Use ... to extinguish.

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P331 Do NOT induce vomiting.

Storage

P403 Store in a well-ventilated place.

P410 Protect from sunlight.

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

P420 Store separately.

P405 Store locked up.

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)cyclohexane
Synonyms	: 1,1-DI(TERT-BUTYLPEROXY)CYCLOHEXANE, 1,1-Bis(tert-butylperoxy)cyclohexane
CAS	: 3006-86-8
EC number	: 221-111-2
MF	: C14H28O4
MW	: 260.37

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

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)

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 145 [Organic Peroxides (Heat and Contamination 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 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 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 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 flare-burning effect. Containers may explode when heated. Runoff may create fire or explosion hazard. (ERG, 2016)

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Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

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.

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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Liquid
Colour	Clear
Odour	no data available
Melting point/freezing point	65°C
Boiling point or initial boiling point and boiling range	52-54°C (0.1 mmHg)
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	68°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water: miscible
Partition coefficient n-octanol/water	no data available
Vapour pressure	no data available
Density and/or relative density	0.891g/mL at 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

The explosive instability of the lower dialkyl peroxides (e.g., dimethyl peroxide) and 1,1-bis-peroxides decreases rapidly with increasing chain length and degree of branching, the di-tert-alkyl derivatives being amongst the most stable class of peroxides. Though many 1,1-bis-peroxides have been reported, few have been purified because of the higher explosion hazards compared with the monofunctional peroxides. It is unlikely that this derivative would be particularly unstable compared to other peroxides in its class. [Bretherick 2nd ed., p 44 1979.]

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

Toxics Screening Level

The initial threshold screening level (ITSL) for 1,1-Di-(tert-butylperoxy)cyclohexane is set at trace, 0.1 µg/m³ based on an annual averaging time.

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: UN3105 (For reference only, please check.)

IMDG: UN3105 (For reference only, please check.)

IATA: UN3105 (For reference only, please check.)

UN Proper Shipping Name

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

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

IATA: ORGANIC PEROXIDE TYPE D, 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)

Listed.

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>

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>
Chemical Book

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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