

## Chemical Safety Data Sheet MSDS / SDS

**2,5-Di(tert-butylperoxy)-2,5-dimethyl-3-hexyne**Revision Date:2023-05-19 Revision Number:1

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

Product name : 2,5-Di(tert-butylperoxy)-2,5-dimethyl-3-hexyne  
CBnumber : CB9346307  
CAS : 1068-27-5  
EINECS Number : 213-944-5  
Synonyms : trigonox 145,2,5-di(tert-butylperoxy)-2,5-dimethyl-3-hexyne

**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

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**SECTION 2: Hazards identification****Classification of the substance or mixture**

Organic peroxides, Type C  
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

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

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Signal word : Danger

**Hazard statement(s)**

H241 Heating may cause a fire or explosion  
H242 Heating may cause a fire  
H315 Causes skin irritation  
H319 Causes serious eye irritation  
H332 Harmful if inhaled  
H335 May cause respiratory irritation

**Precautionary statement(s)**

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

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

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.

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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P370+P380+P375 in case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

P410 Protect from sunlight.

P412 Do not expose to temperatures exceeding 50 oC/ 122 oF.

#### **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.

P391 Collect spillage.

#### **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

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 2,5-Di(tert-butylperoxy)-2,5-dimethyl-3-hexyne
Synonyms	: trigonox 145,2,5-di(tert-butylperoxy)-2,5-dimethyl-3-hexyne
CAS	: 1068-27-5
EC number	: 213-944-5
MF	: C16H30O4
MW	: 286.41

## 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 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)

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

no data available

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## 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, CO<sub>2</sub> 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 flare-burning 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.

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## 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.

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# 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/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

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## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Physical state	This liquid peroxide is particularly sensitive to temperature rises and contamination. Above a given "Control Temperature" they decompose violently. It is generally stored or transported as a mixture, with an inert solid.
Colour	no data available
Odour	no data available
Melting point/freezing point	88°C
Boiling point or initial boiling point and boiling range	304.8°C at 760 mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	87°C
Auto-ignition temperature	no data available
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	0.00154mmHg at 25°C
Density and/or relative density	1.26g/mL at 25°C(lit.)
Relative vapour density	no data available
Particle characteristics	no data available

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## 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 2,5-BIS(TERT-BUTYLPEROXY)-2,5-DIMETHYL-3-HEXYNE, 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 an explosion. Solutions of peroxides often become explosive when evaporated to dryness or near-dryness. Danger of explosion when dry. May explode from heat, shock, friction or contamination. May ignite combustibles (wood, paper, oil, clothing, etc.). May be ignited by heat, sparks or flames.

#### **Conditions to avoid**

no data available

#### **Incompatible materials**

no data available

#### **Hazardous decomposition products**

no data available

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## 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

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## **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

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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: UN3106 (For reference only, please check.)

IMDG: UN3106 (For reference only, please check.)

IATA: UN3106 (For reference only, please check.)

### **UN Proper Shipping Name**

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

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

IATA: ORGANIC PEROXIDE TYPE D, SOLID (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: Yes

IMDG: Yes

IATA: Yes

### **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**

Listed.

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

Listed.

#### **PICCS**

Listed.

#### **Vietnam National Chemical Inventory**

Not 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/>

#### **Disclaimer:**

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