SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: Luperox® 101, 2,5-Bis(tert-butylperoxy)-2,5-dimethylhexane

Product Number: 388092
Brand: Aldrich
CAS-No.: 78-63-7

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Flammable liquids (Category 4), H227
Organic peroxides (Type C), H242
Skin irritation (Category 2), H315
Germ cell mutagenicity (Category 2), H341

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram

Signal Word: Danger
### Hazard statement(s)
- **H227**: Combustible liquid.
- **H242**: Heating may cause a fire.
- **H315**: Causes skin irritation.
- **H341**: Suspected of causing genetic defects.

### Precautionary statement(s)
- **P201**: Obtain special instructions before use.
- **P202**: Do not handle until all safety precautions have been read and understood.
- **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.
- **P264**: Wash skin thoroughly after handling.
- **P280**: Wear protective gloves/ protective clothing/ eye protection/ face protection.
- **P302 + P352**: IF ON SKIN: Wash with plenty of soap and water.
- **P308 + P313**: IF exposed or concerned: Get medical advice/ attention.
- **P332 + P313**: If skin irritation occurs: Get medical advice/ attention.
- **P362**: Take off contaminated clothing and wash before reuse.
- **P403 + P405**: In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
- **P405**: Store locked up.
- **P410**: Protect from sunlight.
- **P420**: Store away from other materials.
- **P501**: Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

### SECTION 3: Composition/information on ingredients

#### 3.2 Mixtures

**Synonyms**: 2,5-Bis(tert-butyldioxy)-2,5-dimethylhexane

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,5-Bis(tert-butyldioxy)-2,5-dimethylhexane</td>
<td>Flam. Liq. 4; Org. Perox. C; Skin Irrit. 2; H227, H242, H315</td>
<td>&gt;= 90 - &lt;= 100 %</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>EC-No.</td>
<td></td>
</tr>
<tr>
<td>78-63-7</td>
<td>201-128-1</td>
<td></td>
</tr>
</tbody>
</table>

| 3,3,6,6-Tetramethyl-1,2-dioxacyclohexane | Flam. Liq. 3; Org. Perox. D; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H226, H242, H315, H319, H335 | >= 5 - < 10 % |
| CAS-No. | 22431-89-6 |
| di-tert-butyl peroxide | Flam. Liq. 2; Org. Perox. E; Muta. 2; Aquatic Acute | >= 1 - < 5 % |
| CAS-No. | EC-No. | |
| 110-05-4 | 203-733-6 |
SECTION 4: First aid measures

4.1 Description of first-aid measures

**General advice**
Show this material safety data sheet to the doctor in attendance.

**If inhaled**
After inhalation: fresh air. Call in physician.

**In case of skin contact**
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Consult a physician.

**In case of eye contact**
After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

**If swallowed**
After swallowing: immediately make victim drink water (two glasses at most). 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 2.2) 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**
Foam Carbon dioxide (CO2) Dry powder

**Unsuitable extinguishing media**
For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture
Carbon oxides
Combustible.
Avoid shock and friction.
In the event of decomposition: danger of explosion!
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

For the full text of the H-Statements mentioned in this Section, see Section 16.
5.4 Further information
Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. 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
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Tightly closed and away from sources of ignition and heat. Observe national regulations.

Storage stability
Recommended storage temperature
2 - 8 °C

Storage class
Storage class (TRGS 510): 4.1A: Other explosive hazardous materials

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
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

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.

Full contact
Material: Fluorinated rubber
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 30 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374
If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

protective clothing

Respiratory protection
required when vapours/aerosols are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure
Do not let product enter drains.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: liquid

b) Odor
   No data available

c) Odor Threshold
   No data available

d) pH
   No data available

e) Melting point/freezing point
   (No data available)

f) Initial boiling point and boiling range
   55 - 57 °C (131 - 135 °F) at 9 hPa - lit.

g) Flash point
   65 °C (149 °F) - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   No data available

k) Vapor pressure
   No data available

l) Vapor density
   No data available

m) Density
   0.877 g/cm³ at 25 °C (77 °F) - lit.
   Relative density
   No data available

n) Water solubility
   No data available

o) Partition coefficient: n-octanol/water
   No data available

p) Autoignition temperature
   No data available

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   Not classified as explosive.

t) Oxidizing properties
   none

9.2 Other safety information
   No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
   Forms explosive mixtures with air on intense heating.
   A range from approx. 15 Kelvin below the flash point is to be rated as critical.
10.2 **Chemical stability**
The product is chemically stable under standard ambient conditions (room temperature).

10.3 **Possibility of hazardous reactions**
Violent reactions possible with:
- Strong bases
- Powdered metals
- Strong oxidizing agents
- Reducing agents
- Acids

10.4 **Conditions to avoid**
Strong heating.

10.5 **Incompatible materials**
No data available

10.6 **Hazardous decomposition products**
In the event of fire: see section 5

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**SECTION 11: Toxicological information**

11.1 **Information on toxicological effects**

**Mixture**

**Acute toxicity**
- Oral: No data available
- Inhalation: No data available
- Dermal: No data available

Acute toxicity estimate Dermal - 4,316 mg/kg
(Calculation method)

**Skin corrosion/irritation**
Mixture causes skin irritation.

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
Evidence of genetic defects.

**Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**  
No data available

**Aspiration hazard**  
No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Other dangerous properties cannot be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

**Components**

2,5-Bis(tert-butyldioxy)-2,5-dimethylhexane

**Acute toxicity**

- **LD50 Oral - Rat** - male and female - > 2,000 mg/kg  
  (OECD Test Guideline 401)
- **Inhalation**: No data available
- **LD50 Dermal - Rabbit** - male - 4,100 mg/kg  
  (OECD Test Guideline 402)

**Skin corrosion/irritation**

- **Skin - Rabbit**
  Result: Irritating to skin. - 4 h  
  (OECD Test Guideline 404)

**Serious eye damage/eye irritation**

- **Eyes - Rabbit**
  Result: No eye irritation  
  (OECD Test Guideline 405)

**Respiratory or skin sensitization**

- **Maximization Test - Guinea pig**
  Result: negative  
  (OECD Test Guideline 406)

**Germ cell mutagenicity**

- **Test Type**: In vitro mammalian cell gene mutation test
- **Test system**: mouse lymphoma cells
  Result: negative
- **Method**: OECD Test Guideline 474
- **Species**: Mouse - male and female - Red blood cells (erythrocytes)
  Result: negative

**Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available
Specific target organ toxicity - repeated exposure

Aspiration hazard
No data available

3,3,6,6-Tetramethyl-1,2-dioxacyclohexane

Acute toxicity
Oral: No data available
Inhalation: No data available
Dermal: No data available
No data available

Skin corrosion/irritation
No data available

Serious eye damage/eye 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
No data available

Specific target organ toxicity - single exposure
May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

di-tert-butyl peroxide

Acute toxicity
LD50 Oral - Rat - > 2,000 mg/kg
(OECD Test Guideline 423)
LC50 Inhalation - Rat - male and female - 4 h - > 22 mg/l - vapor
(OECD Test Guideline 436)
LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
(OECD Test Guideline 405)

**Respiratory or skin sensitization**
Buehler Test - Guinea pig
Result: Does not cause skin sensitization.
(OECD Test Guideline 406)

**Germ cell mutagenicity**
Suspected of causing genetic defects.
In vitro tests showed mutagenic effects
Test Type: Ames test
Test system: TA1535
Result: negative
Remarks: (National Toxicology Program)
Test Type: gene mutation test
Test system: mouse lymphoma cells
Result: negative
Method: OECD Test Guideline 474
Species: Rat - male
Result: negative
Remarks: DNA damage

**Carcinogenicity**
No data available

**Reproductive toxicity**
No data available

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**
Aspiration hazard
No data available

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**SECTION 12: Ecological information**

12.1 Toxicity

**Mixture**
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
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties
No data available
12.7 Other adverse effects

No data available

Components

**2,5-Bis(tert-butyldioxy)-2,5-dimethylhexane**

Toxicity to fish
semi-static test LC50 - Oryzias latipes (Orange-red killifish) - ca. 4.5 mg/l - 96 h
(OECD Test Guideline 203)

Toxicity to algae
static test ErC50 - Pseudokirchneriella subcapitata (green algae) - >= 0.236 mg/l - 72 h
(OECD Test Guideline 201)

Toxicity to bacteria

**3,3,6,6-Tetramethyl-1,2-dioxacycloclohexane**

No data available

**di-tert-butyl peroxide**

No data available

Toxicity to daphnia and other aquatic invertebrates
static test EC50 - Daphnia magna (Water flea) - > 73.1 mg/l - 48 h
(OECD Test Guideline 202)

Toxicity to algae
static test ErC50 - Pseudokirchneriella subcapitata (algae) - ca. 36 mg/l - 72 h
(OECD Test Guideline 201)

Toxicity to bacteria
static test EC50 - activated sludge - > 1,000 mg/l - 30 min
(OECD Test Guideline 209)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

**Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

**DOT (US)**

UN number: 3103    Class: 5.2    Packing group: II
Proper shipping name: Organic peroxide type C, liquid (2,5-Dimethyl-2,5-di-(tert-buty1peroxy)hexane, > 90-100%)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

**IMDG**

UN number: 3103    Class: 5.2    EMS-No: F-J, S-R

Aldrich - 388092
Proper shipping name: ORGANIC PEROXIDE TYPE C, LIQUID (2,5-DIMETHYL-2,5-DI-(tert-BUTYLPEROXY)HEXANE)

IATA

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Fire Hazard, Reactivity Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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