1. PRODUCT AND COMPANY IDENTIFICATION

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
3050 Spruce Street
SAINT LOUIS MO  63103
USA

Telephone: +1 800-325-5832
Fax: +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone #: +1-703-527-3887 (CHEMTREC)

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
Eye irritation (Category 2A), H319
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.
H319: Causes serious eye 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.
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.

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

P321
Specific treatment (see supplemental first aid instructions on this label).

P322 + P333
If skin irritation occurs: Get medical advice/ attention.

P337 + P338
If eye irritation persists: Get medical advice/ attention.

P370 + P378
In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.

P410
Protect from sunlight.

P411 + P235
Store at temperatures not exceeding 30°C/ 86 °F. Keep cool.

P420
Store away from other materials.

P501
Dispose of contents/ container to an approved waste disposal plant.

Signal word: Danger

Hazard statement(s)
H227
Combustible liquid.

H242
Heating may cause a fire.

H315
Causes skin irritation.

H319
Causes serious eye 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.

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

P308 + P333
IF exposed or concerned: Get medical advice/ attention.

P322 + P333
If skin irritation occurs: Get medical advice/ attention.

P337 + P338
If eye irritation persists: Get medical advice/ attention.

P370 + P378
In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P405
Store locked up.

P410
Protect from sunlight.

P411 + P235
Store at temperatures not exceeding 30°C/ 86 °F. Keep cool.

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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.2 Mixtures
Synonyms: 2,5-Bis(tert-butylperoxy)-2,5-dimethylhexane

Formula: \( \text{C}_{16}\text{H}_{34}\text{O}_{4} \)

Molecular weight: 290.44 g/mol

Hazardous components

Aldrich - 388092
### Component Classification Concentration

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide</td>
<td>Flam. Liq. 3; Org. Perox. D; Skin Irrit. 2; Eye Irrit. 2A; H226, H242, H315, H319</td>
<td>90 - 100 %</td>
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<tr>
<td>CAS-No.</td>
<td>78-63-7</td>
<td></td>
</tr>
<tr>
<td>EC-No.</td>
<td>201-128-1</td>
<td></td>
</tr>
<tr>
<td>3,3,6,6-Tetramethyl-1,2-dioxacyclohexane</td>
<td>Flam. Liq. 3; Org. Perox. D; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H226, H242, H315, H319, H335</td>
<td>5 - 10 %</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>22431-89-6</td>
<td></td>
</tr>
<tr>
<td>Di-tert-butyl peroxide</td>
<td>Flam. Liq. 2; Org. Perox. E; Muta. 2; Aquatic Acute 3; Aquatic Chronic 3; H225, H242, H341, H412</td>
<td>1 - 5 %</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>110-05-4</td>
<td></td>
</tr>
<tr>
<td>EC-No.</td>
<td>203-73-6</td>
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<tr>
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<td>617-001-00-2</td>
<td></td>
</tr>
</tbody>
</table>

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

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### 4. FIRST AID MEASURES

#### 4.1 Description of first aid measures

**General advice**
Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**If inhaled**
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**
Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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.

---

### 5. FIREFIGHTING MEASURES

#### 5.1 Extinguishing media

**Suitable extinguishing media**
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

#### 5.2 Special hazards arising from the substance or mixture
No data available.

#### 5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

#### 5.4 Further information
Use water spray to cool unopened containers.
6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.

6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections
For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge. Keep away from heat and sources of ignition.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Store in original container. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Recommended storage temperature 2 - 8 °C
Storage class (TRGS 510): 5.2: Organic peroxides and self-reacting hazardous materials

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters
Components with workplace control parameters
Contains no substances with occupational exposure limit values.
Hazardous components without workplace control parameters

8.2 Exposure controls
Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

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

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 CE 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  
Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection  
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure  
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance  
Form: liquid

b) Odour  
No data available

c) Odour 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 (7 mmHg) - 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) Vapour pressure  
No data available

l) Vapour density  
No data available

m) Relative density  
0.877 g/cm³ at 25 °C (77 °F)

n) Water solubility  
No data available

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

p) Auto-ignition temperature  
No data available

q) Decomposition temperature  
No data available

r) Viscosity  
No data available

s) Explosive properties  
No data available
9.2 Other safety information
No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
No data available

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatible materials
Strong bases, Powdered metals, Strong oxidizing agents, Reducing agents, Organic materials, acids, Strong reducing agents

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides
Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
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 sensitisation
No data available

Germ cell mutagenicity
No data available

Carcinogenicity

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

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

No component 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 identified as a carcinogen or potential carcinogen by OSHA.

No component of this product present at levels greater than or equal to 0.1% is identified as a
carcinogen or potential carcinogen by OSHA.

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

Additional Information
RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

12. ECOLOGICAL INFORMATION

12.1 Toxicity
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 Other adverse effects
No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging
Dispose of as unused product.

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-butylperoxy)hexane, > 90-100%)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 3103  Class: 5.2  EMS-No: F-J, S-R
Proper shipping name: ORGANIC PEROXIDE TYPE C, LIQUID (2,5-DIMETHYL-2,5-DI-(tert-BUTYLPEROXY)HEXANE)

IATA
UN number: 3103    Class: 5.2 (HEAT)
Proper shipping name: Organic peroxide type C, liquid (2,5-Dimethyl-2,5-di-(tert-butylperoxy)-hexane)

15. REGULATORY INFORMATION

SARA 302 Components
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

<table>
<thead>
<tr>
<th>CAS-No.</th>
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<tr>
<td>110-05-4</td>
<td>1993-04-24</td>
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Pennsylvania Right To Know Components

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New Jersey Right To Know Components

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<td>22431-89-6</td>
<td>1993-04-24</td>
</tr>
</tbody>
</table>

California Prop. 65 Components
This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Aquatic Acute    Acute aquatic toxicity
Aquatic Chronic  Chronic aquatic toxicity
Eye Irrit.      Eye irritation
Flam. Liq.     Flammable liquids
H225          Highly flammable liquid and vapour.
H226          Flammable liquid and vapour.
H227          Combustible liquid.
H242          Heating may cause a fire.
H315          Causes skin irritation.
H319          Causes serious eye irritation.
H335          May cause respiratory irritation.
H341          Suspected of causing genetic defects.
H412          Harmful to aquatic life with long lasting effects.
Muta.         Germ cell mutagenicity
Org. Perox.   Organic peroxides
Skin Irrit.   Skin irritation
STOT SE       Specific target organ toxicity - single exposure

HMIS Rating
Health hazard:  2
Chronic Health Hazard:  *
Flammability:  2
Physical Hazard:  1

NFPA Rating
Health hazard:  2
Fire Hazard:  2
Reactivity Hazard:  1
Special hazard:I:  OX

Further information
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slip for additional terms and conditions of sale.

Preparation Information
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

Version: 5.8    Revision Date: 11/06/2017    Print Date: 11/10/2018