SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: Luperox® DI, tert-Butyl peroxide

Product Number: 168521
Brand: Aldrich
Index-No.: 617-001-00-2
CAS-No.: 110-05-4

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 2), H225
- Organic peroxides (Type E), H242
- Germ cell mutagenicity (Category 2), H341
- Short-term (acute) aquatic hazard (Category 3), H402
- Long-term (chronic) aquatic hazard (Category 3), H412

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

2.2 GHS Label elements, including precautionary statements

Signal Word: Danger

Aldrich - 168521
Hazard statement(s)

H225 Highly flammable liquid and vapor.
H242 Heating may cause a fire.
H341 Suspected of causing genetic defects.
H412 Harmful to aquatic life with long lasting effects.

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.
P233 Keep container tightly closed.
P234 Keep only in original container.
P240 Ground/bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 Use only non-sparking tools.
P243 Take precautionary measures against static discharge.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235 Store in a well-ventilated place. Keep cool.
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

3.1 Substances

<table>
<thead>
<tr>
<th>Synonyms</th>
<th>Di-tert-butyl peroxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>C₈H₁₈O₂</td>
</tr>
<tr>
<td>Molecular weight</td>
<td>146.23 g/mol</td>
</tr>
<tr>
<td>CAS-No.</td>
<td>110-05-4</td>
</tr>
<tr>
<td>EC-No.</td>
<td>203-733-6</td>
</tr>
<tr>
<td>Index-No.</td>
<td>617-001-00-2</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>di-tert-butyl peroxide</td>
<td>Flam. Liq. 2; Org. Perox. E; Muta. 2; Aquatic Acute 3; Aquatic Chronic 3;</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>
For the full text of the H-Statements mentioned in this Section, see Section 16.

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
Carbon dioxide (CO2) Foam 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.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

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.
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. Risk of explosion.

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
Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities
Storage conditions
Tightly closed. Separately or together with other organic peroxides only and away from sources of ignition and heat.

Storage stability
Recommended storage temperature
2 - 8 °C

Storage class
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
**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**
Change contaminated clothing. Preventive skin protection recommended. Wash hands 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**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

- **Full contact**
  - Material: Nitrile rubber
  - Minimum layer thickness: 0.4 mm
  - Break through time: 480 min
  - Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

- **Splash contact**
  - Material: Nitrile rubber
  - Minimum layer thickness: 0.11 mm
  - Break through time: 30 min
  - Material tested: KCL 741 Dermatril® L

**Body Protection**
Flame retardant antistatic 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. Risk of explosion.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: clear, liquid
   Color: colorless

b) Odor
   very faint

c) Odor Threshold
   No data available

d) pH
   No data available

e) Melting point/range/Freezing point
   Melting point/range: < -29 °C (< -20 °F) - OECD Test Guideline 102

f) Initial boiling point
   and boiling range
   109 - 110 °C 228 - 230 °F - lit.

g) Flash point
   6 °C (43 °F) at ca.1,013 hPa - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   Upper explosion limit: > 99 %(V)

k) Vapor pressure
   53 hPa at 20 °C (68 °F)

l) Vapor density
   No data available

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

n) Water solubility
   0.171 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - soluble

o) Partition coefficient: n-octanol/water
   log Pow: 3.2 at 22 °C (72 °F)

p) Autoignition temperature
   No data available

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   none

9.2 Other safety information

   No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

   Vapors may form explosive mixture with air.
10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
Risk of explosion with:
- Amines
- Alkalines
- Heavy metal salts
- Strong reducing agents
- Boron compounds
- Acids
- Impurities
- Halogen-halogen compounds
- Rust
- Heavy metals
- Sulfur
- Sulfur compounds
Risk of ignition or formation of inflammable gases or vapours with:
- Highly flammable solvents

10.4 Conditions to avoid
Warming.

10.5 Incompatible materials
No data available

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

SECTION 11: Toxicological information

11.1 Information on toxicological effects

**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  
Metabolic activation: with and without metabolic activation  
**Method:** OECD Test Guideline 471  
**Result:** negative  
**Remarks:** (National Toxicology Program)  
**Test Type:** gene mutation test  
**Test system:** mouse lymphoma cells  
Metabolic activation: with and without metabolic activation  
**Method:** OECD Test Guideline 476  
**Result:** negative

**Test Type:** In vivo micronucleus test  
**Species:** Rat  
**Application Route:** inhalation (vapor)  
**Method:** OECD Test Guideline 474  
**Result:** negative  
**Remarks:** DNA damage

**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**
Repeated dose toxicity - Rat - male and female - Oral - NOAEL (No observed adverse effect level) - 100 mg/kg - LOAEL (Lowest observed adverse effect level) - 300 mg/kg

**RTECS:** ER2450000
Cough, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption of large quantities:

Nausea

Aldrich - 168521
Organic peroxides generally show a more or less strongly pronounced irritant effect on skin and mucous membranes. In some cases it has displayed a sensitisising effect with allergic manifestations in predisposed persons. Mutagenic properties are associated with some compounds. The product should be handled with the care due when dealing with chemicals. Handle in accordance with good industrial hygiene and safety practice.

SECTION 12: Ecological information

12.1 Toxicity
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)

12.2 Persistence and degradability

- Biodegradability
  aerobic - Exposure time 28 d
  Result: 6 % - Not readily biodegradable.
  (OECD Test Guideline 301D)

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
Discharge into the environment must be avoided.

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.
SECTION 14: Transport information

DOT (US)
- UN number: 3107  Class: 5.2
- Proper shipping name: Organic peroxide type E, liquid (Di-tert-butyl peroxide, >52-100%)
- Reportable Quantity (RQ):
  Poison Inhalation Hazard: No

IMDG
- UN number: 3107  Class: 5.2
- Proper shipping name: ORGANIC PEROXIDE TYPE E, LIQUID (DI-tert-BUTYL PEROXIDE)
- EMS-No: F-J, S-R

IATA
- UN number: 3107  Class: 5.2 (HEAT)
- Proper shipping name: Organic peroxide type E, liquid (Di-tert-Butyl peroxide)
- Special Provisions: "Keep away from heat" label required.

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, 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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