

## SAFETY DATA SHEET

Version 6.1

Revision Date 07/24/2018

Print Date 11/16/2018

---

1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : Luperox® 331M80, 1,1-Bis(<|>tert</>-  
butylperoxy)cyclohexane solution

Product Number : 531758

Brand : Aldrich

CAS-No. : 3006-86-8

## 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 Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765

Fax : +1 800 325-5052

## 1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

---

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

Acute toxicity, Inhalation (Category 4), H332

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

Skin sensitisation (Category 1), H317

Germ cell mutagenicity (Category 1B), H340

Carcinogenicity (Category 2), H351

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

Aspiration hazard (Category 1), H304

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.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H350	May cause cancer.

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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing should not be allowed out of the workplace.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
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 + P313	IF exposed or concerned: Get medical advice/ attention.
P321	Specific treatment (see supplemental first aid instructions on this label).
P331	Do NOT induce vomiting.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
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.

Sensitising components:

tert-Butyl hydroperoxide

May produce an allergic reaction.

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

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

#### 3.2 Mixtures

Synonyms : 1,1-Bis(<I>tert</I>-butylperoxy)cyclohexane

Formula : C<sub>14</sub>H<sub>28</sub>O<sub>4</sub>

Molecular weight : 260.37 g/mol

#### Hazardous components

Component		Classification	Concentration
<b>Cyclohexylidenebis[tert-butyl] peroxide</b>			
CAS-No.	3006-86-8	Flam. Liq. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H227, H315, H319, H335	>= 70 - < 90 %
EC-No.	221-111-2		
<b>Low boiling point modified naphtha</b>			
CAS-No.	64741-65-7	Flam. Liq. 3; Acute Tox. 3; Carc. 1B; Asp. Tox. 1; H226, H304, H331, H350	>= 10 - < 20 %
<b>Naphtha (petroleum), hydrotreated heavy</b>			
CAS-No.	64742-48-9	Flam. Liq. 4; Muta. 1B; Carc. 1B; Asp. Tox. 1; H227, H304, H340, H350	>= 10 - < 20 %
EC-No.	265-150-3		
Index-No.	649-327-00-6		
<b>tert-Butyl hydroperoxide</b>			
CAS-No.	75-91-2	Flam. Liq. 3; Org. Perox. F; Acute Tox. 4; Acute Tox. 2; Acute Tox. 3; Skin Corr. 1C; Eye Dam. 1; Skin Sens. 1; Muta. 2; Aquatic Acute 2; Aquatic Chronic 2; H226, H242, H302, H311, H314, H317, H330, H341, H411, H226, H242, H302, H311, H314, H317, H318, H330, H341, H411	>= 0.1 - < 1 %
EC-No.	200-915-7		

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

### 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**

Carbon oxides

#### **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

Component	CAS-No.	Value	Control parameters	Basis
Low boiling point modified naphtha	64741-65-7	TWA	500.000000 ppm 2,000.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
	Remarks	The value in mg/m3 is approximate.		
Naphtha (petroleum), hydrotreated heavy	64742-48-9	TWA	500.000000 ppm 2,000.000000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		The value in mg/m3 is approximate.		

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.

#### 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      | No data available               |
| g) Flash point                                  | 68.3 °C (154.9 °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	0.891 g/cm <sup>3</sup> 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
t) Oxidizing 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, Oxidizing agents, Alkali metals, Powdered metals, Strong oxidizing agents, Copper, Strong acids, Organic materials, Aluminum, Plastics

### 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

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: 2B - Group 2B: Possibly carcinogenic to humans (Low boiling point modified naphtha)
- 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 on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available  
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

Proper shipping name: Organic peroxide type C, liquid (1,1-Di-(tert-butylperoxy)cyclohexane, >52-80%)

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 (1,1-DI-(tert-BUTYLPEROXY)CYCLOHEXANE)

**IATA**

UN number: 3103 Class: 5.2 (HEAT)

Proper shipping name: Organic peroxide type C, liquid (1,1-Di-(tert-butylperoxy) cyclohexane)Special Provisions: "Keep away from heat" label required.

A20WITH ABSORBENT MATERIAL IN OUTER PACKAGING.

---

**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, Chronic Health Hazard

**Massachusetts Right To Know Components**

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

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
Cyclohexylidenebis[tert-butyl] peroxide	3006-86-8	1994-07-31
Low boiling point modified naphtha	64741-65-7	1989-08-11
Naphtha (petroleum), hydrotreated heavy	64742-48-9	2009-07-17
tert-Butyl alcohol	75-65-0	2007-03-01
Cyclohexanone	108-94-1	1993-04-24

	CAS-No.	Revision Date
Cyclohexylidenebis[tert-butyl] peroxide	3006-86-8	1994-07-31
Low boiling point modified naphtha	64741-65-7	1989-08-11
Naphtha (petroleum), hydrotreated heavy	64742-48-9	2009-07-17
tert-Butyl alcohol	75-65-0	2007-03-01
Cyclohexanone	108-94-1	1993-04-24

**New Jersey Right To Know Components**

	CAS-No.	Revision Date
Cyclohexylidenebis[tert-butyl] peroxide	3006-86-8	1994-07-31
Low boiling point modified naphtha	64741-65-7	1989-08-11
Naphtha (petroleum), hydrotreated heavy	64742-48-9	2009-07-17
tert-Butyl hydroperoxide	75-91-2	1991-07-01

**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.**

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity



Asp. Tox.	Aspiration hazard
Carc.	Carcinogenicity
Eye Dam.	Serious eye damage
Eye Irrit.	Eye irritation
Flam. Liq.	Flammable liquids
H226	Flammable liquid and vapour.
H227	Combustible liquid.
H242	Heating may cause a fire.
H302	Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H331	Toxic if inhaled.
H332	Harmful if inhaled.
H335	May cause respiratory irritation.
H340	May cause genetic defects.
H341	Suspected of causing genetic defects.
H350	May cause cancer.
H351	Suspected of causing cancer.
H411	Toxic to aquatic life with long lasting effects.
Muta.	Germ cell mutagenicity
Org. Perox.	Organic peroxides
Skin Corr.	Skin corrosion
Skin Irrit.	Skin irritation
Skin Sens.	Skin sensitisation
STOT SE	Specific target organ toxicity - single exposure

#### Further information

Copyright 2016 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.  
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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

#### Preparation Information

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

Version: 6.1

Revision Date: 07/24/2018

Print Date: 11/16/2018