SAFETY DATA SHEET

Version 6.6
Revision Date 10/01/2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

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 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
Eye irritation (Category 2A), H319
Germ cell mutagenicity (Category 1B), H340
Carcinogenicity (Category 1B), H350
Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336
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/ vapors/ 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.

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.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H340	May cause genetic defects.
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/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P271	Use only outdoors or in a well-ventilated area.
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 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
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.
P331	Do NOT induce vomiting.
P332 + P313	If skin irritation 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 to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
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.

Sensitizing components:
tert-Butyl hydroperoxide
May produce an allergic reaction.

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

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : 1,1-Bis(tert-butylperoxy)cyclohexane

Formula : $C_{14}H_{28}O_4$

Molecular weight : 260.37 g/mol

Component		Classification	Concentration
Cyclohexylidenebis[tert-butyl] peroxide			
CAS-No. EC-No.	3006-86-8 221-111-2	Flam. Liq. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H227, H315, H319, H335	>= 70 - < 90 %
Low boiling point modified naphtha			
CAS-No. EC-No. Index-No.	64741-65-7 265-067-2 649-275-00-4	Flam. Liq. 3; Skin Irrit. 2; Muta. 1B; Carc. 1B; STOT SE 3; Asp. Tox. 1; Aquatic Acute 3; H226, H315, H340, H350, H336, H304, H402	>= 10 - < 20 %
Naphtha (petroleum), hydrotreated heavy			
CAS-No. EC-No. Index-No.	64742-48-9 265-150-3 649-327-00-6	Flam. Liq. 4; Muta. 1B; Carc. 1B; Asp. Tox. 1; H227, H340, H350, H304	>= 10 - < 20 %
tert-Butyl hydroperoxide			
CAS-No. EC-No.	75-91-2 200-915-7	Flam. Liq. 3; Org. Perox. A; Acute Tox. 4; Acute Tox. 3; Skin Corr. 1C; Eye Dam. 1; Muta. 2; Aquatic Acute 2; Aquatic Chronic 2; H226, H240, H302, H332, H311, H314, H318, H341, H401, H411	>= 0.1 - < 1 %

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: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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
Mixture with combustible ingredients.
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.

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 safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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. Keep locked up or in an area accessible only to qualified or authorized persons. 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

Component	CAS-No.	Value	Control parameters	Basis
Low boiling point modified naphtha	64741-65-7	TWA	500 ppm 2,000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	400 ppm 1,600 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
Naphtha (petroleum), hydrotreated heavy	64742-48-9	TWA	500 ppm 2,000 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	400 ppm 1,600 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
tert-Butyl hydroperoxide	75-91-2	TWA	0.1 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		

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
required

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	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)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Density	0.891 g/cm3 at 25 °C (77 °F)
	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
No data available

10.4 Conditions to avoid
Strong heating.

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

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity
Acute toxicity estimate Oral - > 5,000 mg/kg
(Calculation method)
Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Inhalation: No data available

Acute toxicity estimate Inhalation - 4 h - 26.25 mg/l
(Calculation method)
Symptoms: Possible symptoms:, mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
Dermal: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)

Skin corrosion/irritation
Mixture causes skin irritation.

Serious eye damage/eye irritation
Mixture causes serious eye irritation.

Respiratory or skin sensitization
Mixture may cause an allergic skin reaction.

Germ cell mutagenicity
Possible mutagen

Carcinogenicity
Possible carcinogen.

IARC:	2B - Group 2B: Possibly carcinogenic to humans (Low boiling point modified naphtha)
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
Mixture may cause respiratory irritation.
Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

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

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components

Cyclohexylidenebis[tert-butyl] peroxide

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
Inhalation - May cause respiratory irritation.

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Low boiling point modified naphtha

Acute toxicity
LD50 Oral - Rat - > 7,500 mg/kg
Remarks: (IUCLID)
LD50 Oral - Rat - > 2,000 mg/kg
Remarks: (External MSDS)
LC50 Inhalation - Rat - 4 h - > 5 mg/l
Remarks: (IUCLID)

LD50 Dermal - Rabbit - > 2,000 mg/kg
Remarks: (IUCLID)

Skin corrosion/irritation
Skin - Rabbit
Result: Irritating to skin.
Remarks: (in analogy to similar products)
(ECHA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: No eye irritation
Remarks: (IUCLID)

Respiratory or skin sensitization
No data available

Germ cell mutagenicity
May cause genetic defects.

Carcinogenicity
Presumed to have carcinogenic potential for humans

Reproductive toxicity
No data available

Specific target organ toxicity - single exposure
Inhalation - May cause drowsiness or dizziness. - Central nervous system

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
Aspiration may cause pulmonary edema and pneumonitis.

Naphtha (petroleum), hydrotreated heavy

Acute toxicity
LD50 Oral - Rat - male and female - > 5,000 mg/kg
(OECD Test Guideline 401)
LC50 Inhalation - Rat - male and female - 4 h - > 7,630 mg/l
(OECD Test Guideline 403)
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)
No data available

Skin corrosion/irritation
No data available

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

Respiratory or skin sensitization
Buehler Test - Guinea pig

Did not cause sensitization on laboratory animals.
(OECD Test Guideline 406)

Germ cell mutagenicity
Test Type: reverse mutation assay
Test system: S. typhimurium
Result: negative
Species: Rat - male and female
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
No data available

Aspiration hazard
No data available

tert-Butyl hydroperoxide

Acute toxicity
LD50 Oral - Rat - male and female - 560 mg/kg
Remarks: Aqueous solution
(ECHA)
LC50 Inhalation - Rat - male and female - 4 h - 1.85 mg/l
(OECD Test Guideline 403)
Remarks: (in analogy to similar products)
LD50 Dermal - Rabbit - male and female - 440 mg/kg
(OECD Test Guideline 402)
Remarks: Aqueous solution
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Corrosive, category 1C - where responses occur after exposures between 1 hour and 4 hours and observations up to 14 days. - 24 h
Remarks: Aqueous solution

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Corrosive - 21 d
Remarks: Aqueous solution

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: positive
(OECD Test Guideline 406)
Remarks: Aqueous solution

Germ cell mutagenicity
Suspected of causing genetic defects.

Test Type: Mutagenicity (mammal cell test): chromosome aberration.
Test system: Chinese hamster cells
Result: positive
Remarks: (in analogy to similar products)
Test Type: In vitro mammalian cell gene mutation test
Test system: Mouse lymphoma test
Result: positive
Remarks: (in analogy to similar products)
Test Type: Ames test
Test system: S. typhimurium
Result: positive
Remarks: (in analogy to similar products)
Method: Regulation (EC) No. 440/2008, Annex, B.12
Species: Mouse - male and female
Result: negative
Remarks: (in analogy to similar products)
Method: Regulation (EC) No. 440/2008, Annex, B.12
Species: Mouse - male
Result: positive
Remarks: (in analogy to similar products)
Species: Rat - male
Result: negative
Remarks: (in analogy to similar products)
(ECHA)

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

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 Other adverse effects

No data available

Components

Cyclohexylidenebis[tert-butyl] peroxide

No data available

Low boiling point modified naphtha

Toxicity to algae	IC50 - Pseudokirchneriella subcapitata (green algae) - 13 mg/l - 72 h (OECD Test Guideline 201)

Naphtha (petroleum), hydrotreated heavy

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 2,200 mg/l - 96 h

tert-Butyl hydroperoxide

Toxicity to fish	semi-static test LC50 - Pimephales promelas (fathead minnow) - 29.61 mg/l - 96 h (OECD Test Guideline 203) Remarks: Aqueous solution
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 14.1 mg/l - 48 h (OECD Test Guideline 202) Remarks: Aqueous solution
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 1.5 mg/l - 72 h (OECD Test Guideline 201) Remarks: Aqueous solution
Toxicity to bacteria	Growth inhibition EC50 - activated sludge - 17 mg/l - 30 h (OECD Test Guideline 209) Remarks: Aqueous solution

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
Proper shipping name: Organic peroxide type C, liquid (1,1-Di-(tert-butylperoxy)cyclohexane, >52-80%)
Reportable Quantity (RQ): 100 lbs
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 (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.

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

Reportable Quantity : F003 lbs

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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