

SAFETY DATA SHEET

Version 6.3
Revision Date 09/14/2020
Print Date 02/05/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Luperox® 231, 1,1-Bis(*tert*-butylperoxy)-
3,3,5-trimethylcyclohexane

Product Number : 479896
Brand : Aldrich
CAS-No. : 6731-36-8

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)**

Organic peroxides (Type B), H241

Long-term (chronic) aquatic hazard (Category 4), H413

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)
H241

Heating may cause a fire or explosion.

H413	May cause long lasting harmful effects to aquatic life.
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.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P410	Protect from sunlight.
P411 + P235	Store at temperatures not exceeding .? °C/ .? °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

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	: 1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane
Formula	: C ₁₇ H ₃₄ O ₄
Molecular weight	: 302.45 g/mol
CAS-No.	: 6731-36-8
EC-No.	: 229-782-3

Component	Classification	Concentration
1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox™ 1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox 231)		
	Org. Perox. B; Aquatic Chronic 4; H241, H413	<= 100 %

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

Consult a physician. Show this material 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

Flush eyes with water as a precaution.

If swallowed

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

SECTION 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.

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe 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.
Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage**7.1 Precautions for safe handling**

Keep away from sources of ignition - No smoking. Keep away from heat and sources of ignition.
For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

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): 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

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. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---------------|------------------|
| a) Appearance | Form: liquid |
| | Color: colorless |

b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Freezing point/ range: < -29 °C (< -20 °F) at 1,013 hPa
f) Initial boiling point and boiling range	No data available
g) Flash point	No data available
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	0.00009 hPa at 20 °C (68 °F)
l) Vapor density	No data available
m) Relative density	0.904 g/cm ³ at 25 °C (77 °F)
n) Water solubility	0.004 g/l at 20 °C (68 °F) - insoluble
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	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 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

Organic materials, Powdered metals Strong oxidizing agents, Strong acids, Strong bases, Reducing agents, Organic materials, Powdered metals

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

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 5.6 mg/l

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

Maximization Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

Germ cell mutagenicity

Mouse

lymphocyte

Result: negative

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

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: SD8600000

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

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	semi-static test LC50 - Danio rerio (zebra fish) - > 0.043 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - > 1 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	Growth inhibition NOEC - Pseudokirchneriella subcapitata (algae) - 1 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	Respiration inhibition EC50 - Sludge Treatment - > 1,000 mg/l - 3 h (OECD Test Guideline 209)

12.2 Persistence and degradability

Biodegradability Result: - Not biodegradable.
(OECD Test Guideline 301C)

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

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

SECTION 13: Disposal considerations**13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in

igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 3101 Class: 5.2 (1)

Proper shipping name: Organic peroxide type B, liquid (1,1-Di-(tert-butylperoxy)-3,3,5-trimethylcyclohexane, >90-100%)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

IMDG

UN number: 3101 Class: 5.2 (1)

EMS-No: F-J, S-R

Proper shipping name: ORGANIC PEROXIDE TYPE B, LIQUID (1,1-DI-(tert-BUTYLPEROXY)-3,3,5-TRIMETHYLCYCLOHEXANE)

IATA

UN number: 3101 Class: 5.2 (1)

Proper shipping name: Organic peroxide type B, liquid (1,1-Di-(tert-butylperoxy)-3,3,5-trimethylcyclohexane, >90-100%)

IATA Passenger: Not permitted for transport

IATA Cargo: Not permitted for transport

SECTION 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

Reactivity Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

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

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

Pennsylvania Right To Know Components

1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox™ 1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox 231)	CAS-No. 6731-36-8	Revision Date 1994-07-31
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1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox™ 1-Bis(tert-butylperoxy)-3,3,5-	CAS-No. 6731-36-8	Revision Date 1994-07-31
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trimethylcyclohexane (Luperox 231)

New Jersey Right To Know Components

1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox™ 1-Bis(tert-butylperoxy)-3,3,5- trimethylcyclohexane (Luperox 231)	CAS-No. 6731-36-8	Revision Date 1994-07-31
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SECTION 16: Other information

Further information

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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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