

SAFETY DATA SHEET

Version 5.6
Revision Date 10/08/2017
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION**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
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)**

Organic peroxides (Type B), H241

Chronic aquatic toxicity (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/ protective clothing/ 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.

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

Hazardous components

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	90 - 100 %

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

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. Discharge into the environment must be avoided.

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): 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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components 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, Flame retardant antistatic protective clothing., 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.

9. PHYSICAL AND CHEMICAL PROPERTIES**9.1 Information on basic physical and chemical properties**

a) Appearance	Form: liquid Colour: colourless
b) Odour	No data available
c) Odour 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 (760 mmHg)
f) Initial boiling point and boiling range	No data available
g) Flash point	45.6 °C (114.1 °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	0.00009 hPa (0.00007 mmHg) at 20 °C (68 °F)
l) Vapour 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) 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

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

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 sensitisation

Maximisation Test - Guinea pig

Result: Does not cause skin sensitisation.
(OECD Test Guideline 406)

Germ cell mutagenicity

Mouse

lymphocyte

Result: negative

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.

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

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.

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

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.

13. DISPOSAL CONSIDERATIONS**13.1 Waste treatment methods****Product**

Contact a licensed professional waste disposal service to dispose of this material. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

IMDG

IATA

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.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox™ 1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox 231)	6731-36-8	2009-07-17

New Jersey Right To Know Components

	CAS-No.	Revision Date
1,1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox™ 1-Bis(tert-butylperoxy)-3,3,5-trimethylcyclohexane (Luperox 231)	6731-36-8	2009-07-17

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 Chronic	Chronic aquatic toxicity
H241	Heating may cause a fire or explosion.
H413	May cause long lasting harmful effects to aquatic life.
Org. Perox.	Organic peroxides

HMIS Rating

Health hazard:	1
Chronic Health Hazard:	*
Flammability:	0
Physical Hazard	1

NFPA Rating

Health hazard:	0
Fire Hazard:	0
Reactivity Hazard:	1
Special hazard.I:	OX

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 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: 5.6

Revision Date: 10/08/2017

Print Date: 11/10/2018