

SAFETY DATA SHEET

Version 7.1
Revision Date 03/02/2024
Print Date 04/27/2024

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

Product name : Luperox® P, *tert*-Butyl peroxybenzoate

Product Number : 159042
Brand : Aldrich
CAS-No. : 614-45-9

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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 C), H242
Acute toxicity, Inhalation (Category 4), H332
Skin irritation (Category 2), H315
Skin sensitization (Category 1), H317

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Short-term (acute) aquatic hazard (Category 1), H400
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

Pictogram



Signal Word

Danger

Hazard Statements

H242	Heating may cause a fire.
H315	Causes skin irritation.
H317	May cause an allergic skin reaction.
H332	Harmful if inhaled.
H400	Very toxic to aquatic life.
H412	Harmful to aquatic life with long lasting effects.

Precautionary Statements

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 must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
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.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P391	Collect spillage.
P403 + P235	Store in a well-ventilated place. Keep cool.
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

Synonyms : tert-Butyl perbenzoate
tert-Butyl peroxybenzoate

Formula : C₁₁H₁₄O₃

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Molecular weight : 194.23 g/mol
CAS-No. : 614-45-9
EC-No. : 210-382-2

Component	Classification	Concentration
Tert-Butyl perbenzoate		
	Org. Perox. C; Acute Tox. 4; Skin Irrit. 2; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 3; H242, H332, H315, H317, H400, H412 M-Factor - Aquatic Acute: 1	<= 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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately 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. 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

Water Foam Carbon dioxide (CO2) Dry powder

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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.

Has a fire-promoting effect due to release of oxygen.

Explosive decomposition possible on heating.

Avoid shock and friction.

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.

In the event of decomposition: danger of explosion!

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. 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 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.

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

Store at temperatures not exceeding 38 °C/ 100 °F. Keep cool.

Storage class

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

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

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter B-(P2)

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

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: clear, liquid Color: light yellow
b) Odor	weakly aromatic
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 9 - 11 °C (48 - 52 °F) at 1,013 hPa - OECD Test Guideline 102
f) Initial boiling point and boiling range	75 - 76 °C 167 - 169 °F at 0.3 hPa - lit.
g) Flash point	93.4 °C (200.1 °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) Vapor pressure	< 0.003 hPa at 20 °C (68 °F)
l) Vapor density	6.71 - (Air = 1.0)
m) Density	1.021 g/cm ³ at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	1.18 g/l - soluble
o) Partition coefficient: n-octanol/water	log Pow: 3 at 25 °C (77 °F) - Bioaccumulation is not expected.

- | | |
|------------------------------|----------------------|
| p) Autoignition temperature | No data available |
| q) Decomposition temperature | > 60 °C (> 140 °F) - |
| r) Viscosity | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

Relative vapor density	6.71 - (Air = 1.0)
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SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
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

Sensitivity to light
The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Risk of explosion with:
Risk of ignition or formation of inflammable gases or vapours with:
Heavy metal salts
Strong acids
alkalines
Reducing agents
combustible substances
Metals
Organic Substances

10.4 Conditions to avoid

Heating may cause a fire.
Strong heating.

10.5 Incompatible materials

Lead, rubber, Copper, brass, Polyvinyl chloride, Mild steel

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 - female - > 2,000 mg/kg
(OECD Test Guideline 423)

LC50 Inhalation - Rat - male and female - 4 h - 1.01 - 4.9 mg/l - dust/mist

(OECD Test Guideline 436)

LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 72 h
(OECD Test Guideline 405)

Respiratory or skin sensitization

Sensitisation test: - Mouse

Result: positive
(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: In vivo micronucleus test
Species: Mouse

Application Route: Oral

Result: negative
Remarks: (ECHA)

Test Type: in vivo assay
Species: Rat

Application Route: Oral
Method: OECD Test Guideline 489
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

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 - 90 d - NOAEL (No observed adverse effect level) - 30 mg/kg

Remarks: (ECHA)

Subchronic toxicity

RTECS: SD9450000

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

SECTION 12: Ecological information**12.1 Toxicity**

Toxicity to fish	semi-static test LC50 - Danio rerio (zebra fish) - 1.6 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 11 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 0.4 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 43 mg/l - 0.5 h (OECD Test Guideline 209)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test EC10 - Daphnia magna (Water flea) - 0.49 mg/l - 21 d (OECD Test Guideline 211)

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 28 d Result: 70 % - Readily biodegradable. (OECD Test Guideline 301D)
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12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

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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

No data available

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: 3103 Class: 5.2

Proper shipping name: Organic peroxide type C, liquid (tert-Butyl peroxybenzoate)

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 (tert-BUTYL PEROXYBENZOATE)

IATA

UN number: 3103 Class: 5.2 (HEAT)

Proper shipping name: Organic peroxide type C, liquid (tert-Butyl peroxybenzoate)

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.

Massachusetts Right To Know Components

tert-Butyl peroxybenzoate	CAS-No. 614-45-9	Revision Date 2007-03-01
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Pennsylvania Right To Know Components

tert-Butyl peroxybenzoate	CAS-No. 614-45-9	Revision Date 2007-03-01
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SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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