

1. PRODUCT AND COMPANY IDENTIFICATION**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

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 C), H242
Acute toxicity, Inhalation (Category 4), H332
Skin irritation (Category 2), H315
Skin sensitisation (Category 1), H317
Acute aquatic toxicity (Category 1), H400

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)

H242 Heating may cause a fire.
H315 Causes skin irritation.
H317 May cause an allergic skin reaction.
H400 Very toxic 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.
P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
P264 Wash skin thoroughly after handling.

P272 Contaminated work clothing should not be allowed out of the workplace.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P235 Keep cool.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P321 Specific treatment (see supplemental first aid instructions on this label).
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P391 Collect spillage.
P410 Protect from sunlight.
P420 Store away from other materials.
P501 Dispose of contents/ container to an approved waste disposal plant.

Pictogram



Signal word

Danger

Hazard statement(s)

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.

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.
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.
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.
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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : tert-Butyl perbenzoate
tert-Butyl peroxybenzoate

Formula : C₁₁H₁₄O₃
Molecular weight : 194.23 g/mol
CAS-No. : 614-45-9
EC-No. : 210-382-2

Hazardous components

Component	Classification	Concentration
tert-Butyl perbenzoate	Org. Perox. C; Acute Tox. 4;	90 - 100 %

	Skin Irrit. 2; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 3; H242, H315, H317, H400, H242, H315, H317, H332, H400, H412	
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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

Move out of dangerous area. Consult a physician. Show this safety data sheet to the doctor in attendance.

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

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. 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.

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. 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.

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

Full contact

Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 480 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact

Material: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 30 min
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

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.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance	Form: clear, liquid Colour: light yellow
b) Odour	pungent, unpleasant
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 9 - 11 °C (48 - 52 °F) - OECD Test Guideline 102
f) Initial boiling point and boiling range	75 - 76 °C (167 - 169 °F) at 0.3 hPa (0.2 mmHg) - 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) Vapour pressure	4.48 hPa (3.36 mmHg) at 50 °C (122 °F)
l) Vapour density	6.71 - (Air = 1.0)
m) Relative density	1.021 g/cm ³ at 25 °C (77 °F)
n) Water solubility	1.18 g/l - soluble
o) Partition coefficient: n-octanol/water	log Pow: 3.0 at 25 °C (77 °F)
p) Auto-ignition 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	No data available

9.2 Other safety information

Relative vapour density	6.71 - (Air = 1.0)
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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

Reacts violently with: Strong acids, Bases, Reducing agents, Oxidizing agents, Amines, Brass, Copper

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 - female - > 2,000 mg/kg

(OECD Test Guideline 423)

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

(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 sensitisation

Sensitisation test: - Mouse

Result: positive

(OECD Test Guideline 429)

Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: positive

(ECHA)

In vitro mammalian cell gene mutation test

Mouse lymphoma test

Result: positive

(ECHA)

Mouse - male and female

Result: negative

(ECHA)

Carcinogenicity

Carcinogenicity - Mouse - Unreported

Tumorigenic: Equivocal tumorigenic agent by RTECS criteria. Blood: Lymphomas including Hodgkin's disease.

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.

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

Specific target organ toxicity - single exposure

Specific target organ toxicity - repeated exposure

Aspiration hazard

Additional Information

Repeated dose toxicity Rat - male and female - Oral - 90 d - NOAEL : 30 mg/kg -(ECHA) Subchronic toxicity

RTECS: SD9450000

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish	semi-static test LC50 - Brachydanio rerio (zebrafish) - 1.6 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 16 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)

12.2 Persistence and degradability

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

12.4 Mobility in soil

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. Very toxic to aquatic life.

No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Contact a licensed professional waste disposal service to dispose of this material. 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.

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 (tert-Butyl peroxybenzoate, >77-100%)

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.

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, Acute Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
tert-Butyl perbenzoate	614-45-9	2007-03-01

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
tert-Butyl perbenzoate	614-45-9	2007-03-01

	CAS-No.	Revision Date
tert-Butyl perbenzoate	614-45-9	2007-03-01

New Jersey Right To Know Components

	CAS-No.	Revision Date
tert-Butyl perbenzoate	614-45-9	2007-03-01

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
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.
Org. Perox.	Organic peroxides
Skin Irrit.	Skin irritation
Skin Sens.	Skin sensitisation

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.

Preparation Information

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

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