

SAFETY DATA SHEET

Version 7.6
Revision Date 05/06/2025
Print Date 05/07/2025

SECTION 1. 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

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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Organic peroxides : Type C

Acute toxicity (Inhalation) : Category 4

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Skin irritation : Category 2

Skin sensitization : Category 1

Short-term (acute) aquatic hazard : Category 1

Long-term (chronic) aquatic hazard : Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :



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 :

Prevention:

- 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 mist or vapors.
- 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.

Response:

- 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.

Storage:

P403 + P235 Store in a well-ventilated place. Keep cool.
P410 Protect from sunlight.
P420 Store away from other materials.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Tert-Butyl perbenzoate	614-45-9*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. 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.

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

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available

SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media : Water
Foam
Carbon dioxide (CO₂)
Dry powder

Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting : 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!

Hazardous combustion products : Carbon oxides

Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

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. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	: Do not let product enter drains.
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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	: Keep away from open flames, hot surfaces and sources of ignition.
Advice on safe handling	: Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Storage class	: 4.1A, Other explosive hazardous materials
Recommended storage temperature	: Recommended storage temperature see product label.

Further information on storage stability : Store at temperatures not exceeding 38 °C/ 100 °F.
Keep cool.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

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.

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.

Hand protection

Material : butyl-rubber
Break through time : 480 min
Glove thickness : 0.7 mm
Protective index : Full contact
Manufacturer : Butoject® (KCL 898)

Material : Nitrile rubber
Break through time : 30 min
Glove thickness : 0.4 mm
Protective index : Splash contact
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Remarks : 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).

Eye protection : Use equipment for eye protection tested and
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approved under appropriate government standards
such as NIOSH (US) or EN 166(EU).
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply
preventive skin protection. Wash hands and face
after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : clear, liquid

Color : light yellow

Odor : weakly aromatic

Odor Threshold : No data available

pH : No data available

Melting point/ range : 48 - 52 °F / 9 - 11 °C
(1,013 hPa)
Method: OECD Test Guideline 102

Boiling point/boiling range : 167 - 169 °F / 75 - 76 °C (0.3 hPa)
Method: lit.

Flash point : 200.1 °F / 93.4 °C
Method: closed cup

Evaporation rate : No data available

Flammability (solid, gas) : No data available

Flammability (liquids) : No data available

Burning rate : No data available

Upper explosion limit /
Upper flammability limit : No data available

Lower explosion limit /
Lower flammability limit : No data available

Vapor pressure : < 0.003 hPa (68 °F / 20 °C)

Relative vapor density	: 6.71 (Air = 1.0)
Relative density	: No data available
Density	: 1.021 g/cm ³ (77 °F / 25 °C) Method: lit.
Solubility(ies)	
Water solubility	: 1.18 g/l soluble
Partition coefficient: n-octanol/water	: log Pow: 3 (77 °F / 25 °C) pH: 6.5 Method: OECD Test Guideline 117 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	: No data available
Decomposition temperature	: > 140 °F / > 60 °C
Self-Accelerating decomposition temperature (SADT)	: 140 °F / 60 °C
Viscosity	
Viscosity, dynamic	: 7.5 mPa.s (68 °F / 20 °C) Method: OECD Test Guideline 114
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 194.23 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

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
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is to be rated as critical.

Chemical stability	: Sensitivity to light The product is chemically stable under standard ambient conditions (room temperature) .
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
Conditions to avoid	: Heating may cause a fire. Strong heating.
Incompatible materials	: Lead rubber Copper brass Polyvinyl chloride Mild steel
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

Ecotoxicity

Components:

Tert-Butyl perbenzoate:

Toxicity to fish	: LC50 (Danio rerio (zebra fish)): 1.6 mg/l End point: mortality Exposure time: 96 h Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): 11 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes
Toxicity to algae/aquatic plants	: ErC50 (Pseudokirchneriella subcapitata (green algae)): 0.4 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes
M-Factor (Acute aquatic toxicity)	: 1
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	: EC10 (Daphnia magna (Water flea)): 0.49 mg/l End point: reproduction rate Exposure time: 21 d Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 211 GLP: yes
Toxicity to microorganisms	: EC50 (activated sludge): 43 mg/l Exposure time: 0.5 h Test Type: static test Method: OECD Test Guideline 209 GLP: yes

Persistence and degradability

Components:

Tert-Butyl perbenzoate:

Biodegradability : aerobic
Concentration: 1 mg/l
Result: Readily biodegradable.
Biodegradation: 70 %
Exposure time: 28 d
Method: OECD Test Guideline 301D
GLP: yes

Bioaccumulative potential

Components:

Tert-Butyl perbenzoate:

Partition coefficient: n-octanol/water : log Pow: 3 (77 °F / 25 °C)
pH: 6.5
Method: OECD Test Guideline 117
GLP: yes
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances
Remarks: This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

UN/ID No. : UN 3103
Proper shipping name : Organic peroxide type C, liquid (tert-Butyl peroxybenzoate)
(tert-Butyl peroxybenzoate)
Class : 5.2
Packing group : Not assigned by regulation
Labels : Division 5.2 - Organic peroxides, Handling Label - Keep Away From Heat
Packing instruction (cargo : 570
aircraft)
Packing instruction : 570
(passenger aircraft)

IMDG-Code

UN number : UN 3103
Proper shipping name : ORGANIC PEROXIDE TYPE C, LIQUID (tert-BUTYL PEROXYBENZOATE)

Class : 5.2
Packing group : Not assigned by regulation
Labels : 5.2
EmS Code : F-J, S-R
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National regulation**49 CFR Road**

UN/ID/NA number : UN 3103
Proper shipping name : Organic peroxide type C, liquid (tert-Butyl peroxybenzoate, >77-100%)
(tert-Butyl peroxybenzoate)
Class : 5.2
Packing group : Not assigned by regulation
Labels : Division 5.2 - Organic peroxides
ERG Code : 146
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 313

: 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.

Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCM Intermediate or Final VOC's (40 CFR 60.489).

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

US State Regulations

Massachusetts Right To Know

Tert-Butyl perbenzoate	614-45-9
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Pennsylvania Right To Know

Tert-Butyl perbenzoate	614-45-9
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Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

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TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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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Revision Date : 05/06/2025

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