

ALFAAA13997

## 4-tert-Butylbenzoic acid

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

**产品说明:**  
**Product Description:** 4-叔丁基苯甲酸, 99+%  
 4-tert-Butylbenzoic acid

**Cat No. :** A13997  
**Synonyms** PTBBA  
**CAS No** 98-73-7  
**Molecular Formula** C11 H14 O2

**Supplier** Avocado Research Chemicals Ltd.  
 (Part of Thermo Fisher Scientific)  
 Shore Road, Heysham  
 Lancashire, LA3 2XY,  
 United Kingdom  
 Office Tel: +44 (0) 1524 850506  
 Office Fax: +44 (0) 1524 850608

**Emergency Telephone Number** For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

**E-mail address** begel.sdsdesk@thermofisher.com

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
 Solid

**Appearance**  
 Light yellow

**Odor**  
 Odorless

#### Emergency Overview

Harmful if swallowed. May damage fertility or the unborn child. Causes damage to organs through prolonged or repeated exposure. May form combustible dust concentrations in air.

#### Classification of the substance or mixture

Acute Oral Toxicity	Category 4
Reproductive Toxicity	Category 1A
Specific target organ toxicity - (repeated exposure)	Category 1

#### Label Elements



**Signal Word**

**Danger**

## 4-tert-Butylbenzoic acid

**Hazard Statements**

H302 - Harmful if swallowed  
H372 - Causes damage to organs through prolonged or repeated exposure  
H360 - May damage fertility or the unborn child

**Precautionary Statements****Prevention**

P201 - Obtain special instructions before use  
P202 - Do not handle until all safety precautions have been read and understood  
P260 - Do not breathe dust/fume/gas/mist/vapors/spray  
P264 - Wash face, hands and any exposed skin thoroughly after handling  
P270 - Do not eat, drink or smoke when using this product  
P271 - Use only outdoors or in a well-ventilated area  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

**Response**

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P330 - Rinse mouth  
P361 + P364 - Take off immediately all contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

**Disposal**

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

**Physical and Chemical Hazards**

None identified. May form combustible dust concentrations in air.

**Health Hazards**

Harmful if swallowed. May damage fertility or the unborn child. Causes damage to organs through prolonged or repeated exposure.

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. . Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil.

May form explosible dust-air mixture if dispersed. Toxic to terrestrial vertebrates. This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
p-tert-Butylbenzoic acid	98-73-7	99

**SECTION 4. FIRST AID MEASURES****General Advice**

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

**Skin Contact**

Immediate medical attention is required. Wash off immediately with plenty of water for at least 15 minutes.

**Inhalation**

Remove to fresh air. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required. If not breathing, give artificial respiration.

**Ingestion**

## 4-tert-Butylbenzoic acid

Do NOT induce vomiting. Call a physician or poison control center immediately.

**Most important symptoms and effects**

No information available.

**Self-Protection of the First Aider**

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES****Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Dust can form an explosive mixture with air. Fine dust dispersed in air may ignite.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Avoid dust formation.

**Environmental Precautions**

Should not be released into the environment. Do not flush into surface water or sanitary sewer system. See Section 12 for additional Ecological Information.

**Methods for Containment and Clean Up**

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Do not get in eyes, on skin, or on clothing. Do not ingest. If swallowed then seek immediate medical assistance. Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not breathe (dust, vapor, mist, gas). Avoid dust formation.

**Storage**

Keep containers tightly closed in a dry, cool and well-ventilated place.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

## 4-tert-Butylbenzoic acid

## Control Parameters

Component	ACGIH TLV	OSHA PEL	NIOSH	The United Kingdom	European Union
p-tert-Butylbenzoic acid	TWA: 0.1 mg/m <sup>3</sup> Skin			-	

## Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

## Exposure Controls

## Engineering Measures

Ensure adequate ventilation, especially in confined areas. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

## Personal protective equipment

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Nitrile rubber	recommendations			
Neoprene				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Skin and body protection** Long sleeved clothing

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Particulates filter conforming to EN 143

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Particle filtering: EN149:2001  
When RPE is used a face piece Fit Test should be conducted

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** Prevent product from entering drains.

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

## 4-tert-Butylbenzoic acid

<b>Appearance</b>	Light yellow	
<b>Physical State</b>	Solid	
<b>Odor</b>	Odorless	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	3.5	0.06g/L aq. sol
<b>Melting Point/Range</b>	164 - 167 °C / 327.2 - 332.6 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flash Point</b>	> 180 °C / > 356 °F	<b>Method -</b> No information available
<b>Evaporation Rate</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	<0.1 hPa @ 20 °C	
<b>Vapor Density</b>	Not applicable	Solid
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Water Solubility</b>	0.07g/L (20°C)	practically insoluble
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Component</b>	<b>log Pow</b>	
p-tert-Butylbenzoic acid	3.4	
<b>Autoignition Temperature</b>	510 - °C / 950 - °F	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid
<b>Explosive Properties</b>	No information available	
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C11 H14 O2	
<b>Molecular Weight</b>	178.23	

## SECTION 10. STABILITY AND REACTIVITY

<b>Stability</b>	Stable under normal conditions.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Conditions to Avoid</b>	Incompatible products. Excess heat.
<b>Materials to avoid</b>	Strong oxidizing agents. Strong bases.

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
p-tert-Butylbenzoic acid	LD50 = 473 mg/kg ( Rat )	LD50 > 2000 mg/kg ( Rabbit )	LC50 > 1.802 mg/L ( Rat ) 4 h

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

## 4-tert-Butylbenzoic acid

## (d) respiratory or skin sensitization;

Respiratory	No data available
Skin	No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; Category 1A

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; Category 1

Target Organs	Kidney, Reproductive System, Brain, Peripheral Nervous System (PNS), Hematopoietic System.
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(j) aspiration hazard;	Not applicable
	Solid

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed No information available

## SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Do not empty into drains. Contains a substance which is: Harmful to aquatic organisms. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
p-tert-Butylbenzoic acid				EC50 = 1000 mg/L 48 h

## Persistence and Degradability

Persistence	Persistence is unlikely.
Degradation in sewage treatment plant	Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Bioaccumulative Potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)
p-tert-Butylbenzoic acid	3.4	No data available

Mobility in soil	Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility
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Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant	This product does not contain any known or suspected substance
Ozone Depletion Potential	This product does not contain any known or suspected substance

## SECTION 13. DISPOSAL CONSIDERATIONS

## 4-tert-Butylbenzoic acid

**Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point.

**Other Information**

Do not flush to sewer. Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

**SECTION 14. TRANSPORT INFORMATION****Road and Rail Transport**

**UN-No** UN2811  
**Proper Shipping Name** Toxic solid, organic, n.o.s.  
**Hazard Class** 6.1  
**Packing Group** III

**IMDG/IMO**

**UN-No** UN2811  
**Proper Shipping Name** Toxic solid, organic, n.o.s.  
**Hazard Class** 6.1  
**Packing Group** III

**IATA**

**UN-No** UN2811  
**Proper Shipping Name** TOXIC SOLID, ORGANIC, N.O.S.\*  
**Hazard Class** 6.1  
**Packing Group** III

**Special Precautions for User** No special precautions required

**SECTION 15. REGULATORY INFORMATION****International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
p-tert-Butylbenzoic acid	-	-	X	X	202-696-3	X	X	X	X	X	X	KE-11369

**National Regulations****SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department

## 4-tert-Butylbenzoic acid

**Revision Date** 07-Mar-2024  
**Revision Summary** New emergency telephone response service provider.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

**Legend**

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Disclaimer**

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**End of Safety Data Sheet**