

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
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)
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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 (CO₂), 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 ³ 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 recommendations	-	EN 374	(minimum requirement)
Nitrile rubber				
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

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

SECTION 10. STABILITY AND REACTIVITY

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

Hazardous Decomposition Products Carbon monoxide (CO). Carbon dioxide (CO₂).

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.

(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

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/NDL - 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

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet