

1 Identification

Product identifier

Product name: 4-tert-Butylbenzoic acid

Stock number: A13997

CAS Number:

98-73-7

EC number:

202-696-3

Index number:

607-698-00-1

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

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar
Thermo Fisher Scientific Chemicals, Inc.

30 Bond Street

Ward Hill, MA 01835-8099

Tel: 800-343-0660

Fax: 800-322-4757

Email: tech@alfa.com

www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS06 Skull and crossbones

Acute Tox. 3 H311 Toxic in contact with skin.



GHS08 Health hazard

Repr. 1A H360 May damage fertility or the unborn child.

STOT RE 1 H372 Causes damage to the kidneys and the liver through prolonged or repeated exposure. Route of exposure: Inhalative and Dermal.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS06 GHS08

Signal word

Danger

Hazard statements

H302 Harmful if swallowed.

H311 Toxic in contact with skin.

H360 May damage fertility or the unborn child.

H372 Causes damage to the kidneys and the liver through prolonged or repeated exposure. Route of exposure: Inhalative and Dermal.

Precautionary statements

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P281 Use personal protective equipment as required.

P361 Remove/Take off immediately all contaminated clothing.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

D1B - Toxic material causing immediate and serious toxic effects

D2A - Very toxic material causing other toxic effects



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 2 Health (acute effects) = 2

FIRE 1 Flammability = 1

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

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3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

98-73-7 4-tert-Butylbenzoic acid

Identification number(s):

EC number: 202-696-3

Index number: 607-698-00-1

4 First-aid measures

Description of first aid measures

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm.

Seek immediate medical advice.

After skin contact

Immediately wash with water and soap and rinse thoroughly.

Seek immediate medical advice.

After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.

After swallowing Seek medical treatment.

Information for doctor

Most important symptoms and effects, both acute and delayed

Harmful if swallowed.

Toxic in contact with skin.

May damage fertility or the unborn child.

Causes damage to the kidneys and the liver through prolonged or repeated exposure. Route of exposure: Inhalative and Dermal.

Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media

Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

Special hazards arising from the substance or mixture

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Advice for firefighters

Protective equipment:

Wear self-contained respirator.

Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Environmental precautions: Do not allow product to reach sewage system or any water course.

Methods and material for containment and cleaning up: Dispose of contaminated material as waste according to section 13.

Prevention of secondary hazards: No special measures required.

Reference to other sections

See Section 7 for information on safe handling

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

7 Handling and storage

Handling

Precautions for safe handling

Keep container tightly sealed.

Store in cool, dry place in tightly closed containers.

Ensure good ventilation at the workplace.

Open and handle container with care.

Information about protection against explosions and fires: No information known.

Conditions for safe storage, including any incompatibilities

Storage

Requirements to be met by storerooms and receptacles: No special requirements.

Information about storage in one common storage facility:

Store away from strong bases.

Store away from oxidizing agents.

Further information about storage conditions:

Keep container tightly sealed.

Store in cool, dry conditions in well sealed containers.

Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Control parameters

Components with limit values that require monitoring at the workplace:

The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.

Additional information: No data

Exposure controls

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures for handling chemicals should be followed.

Keep away from foodstuffs, beverages and feed.

Remove all soiled and contaminated clothing immediately.

Wash hands before breaks and at the end of work.

Store protective clothing separately.

Maintain an ergonomically appropriate working environment.

Breathing equipment: Use suitable respirator when high concentrations are present.

Recommended filter device for short term use:

Use a respirator with type P100 (USA) or P3 (EN 143) cartridges as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards.

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Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.
Material of gloves Nitrile rubber, NBR
Penetration time of glove material (in minutes) 480
Glove thickness 0.11 mm
Eye protection: Safety glasses
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form: Crystals/flakes
Color: White to cream
Odor: Not determined
Odor threshold: Not determined.

pH-value: Not applicable.

Change in condition

Melting point/Melting range: 164-168 °C (327-334 °F)
Boiling point/Boiling range: 280 °C (536 °F) (dec)
Sublimation temperature / start: Not determined

Flash point: 180 °C (356 °F)
Flammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined.

Danger of explosion: Not determined.
Explosion limits:

Lower: Not determined
Upper: Not determined
Vapor pressure: Not applicable.
Density: Not determined
Relative density Not determined.
Vapor density Not applicable.
Evaporation rate Not applicable.

Solubility in / Miscibility with
Water: Insoluble
Partition coefficient (n-octanol/water): Not determined.

Viscosity:
dynamic: Not applicable.
kinematic: Not applicable.
Other information No further relevant information available.

10 Stability and reactivity

Reactivity No information known.
Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.
Possibility of hazardous reactions Reacts with strong oxidizing agents
Conditions to avoid No further relevant information available.
Incompatible materials:
Oxidizing agents
Bases
Hazardous decomposition products: Carbon monoxide and carbon dioxide

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful if swallowed.
Toxic in contact with skin.
The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for this substance.

LD/LC50 values that are relevant for classification:

Oral	LD50	473 mg/kg (rat)
Dermal	LD50	300 mg/kg (rat)

Skin irritation or corrosion: May cause irritation

Eye irritation or corrosion: May cause irritation

Sensitization: No sensitizing effects known.

Germ cell mutagenicity: No effects known.

Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

Reproductive toxicity:

May damage fertility or the unborn child.

The Registry of Toxic Effects of Chemical Substances (RTECS) contains reproductive data for this substance.

Specific target organ system toxicity - repeated exposure:

Causes damage to the kidneys and the liver through prolonged or repeated exposure. Route of exposure: Inhalative and Dermal.

Specific target organ system toxicity - single exposure: No effects known.

Aspiration hazard: No effects known.

Subacute to chronic toxicity: The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for this substance.

Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

Carcinogenic categories

OSHA-Ca (Occupational Safety & Health Administration) Substance is not listed.

12 Ecological information

Toxicity

Aquatic toxicity: No further relevant information available.

Persistence and degradability No further relevant information available.

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Product name: 4-tert-Butylbenzoic acid

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Bioaccumulative potential No further relevant information available.
Mobility in soil No further relevant information available.
Additional ecological information:
General notes:
Do not allow product to reach ground water, water course or sewage system, even in small quantities.
Danger to drinking water if even extremely small quantities leak into the ground.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations

Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, IMDG, IATA	UN2811
UN proper shipping name DOT IMDG, IATA	Toxic solids, organic, n.o.s. (4-tert-Butylbenzoic acid) TOXIC SOLID, ORGANIC, N.O.S. (4-tert-Butylbenzoic acid)
Transport hazard class(es) DOT  Class Label Class Label IMDG, IATA  Class Label	6.1 Toxic substances. 6.1 6.1 (T2) Toxic substances 6.1 6.1 Toxic substances. 6.1
Packing group DOT, IMDG, IATA	III
Environmental hazards:	Not applicable.
Special precautions for user EMS Number:	Warning: Toxic substances F-A,S-A
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information: DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	UN2811, Toxic solids, organic, n.o.s. (4-tert-Butylbenzoic acid), 6.1, III

15 Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms



GHS06 GHS08
Signal word Danger
Hazard statements
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National regulations
All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.
All components of this product are listed on the Canadian Domestic Substances List (DSL).
SARA Section 313 (specific toxic chemical listings) Substance is not listed.
California Proposition 65
Prop 65 - Chemicals known to cause cancer Substance is not listed.
Prop 65 - Developmental toxicity Substance is not listed.
Prop 65 - Developmental toxicity, female Substance is not listed.
Prop 65 - Developmental toxicity, male Substance is not listed.
Information about limitation of use: For use only by technically qualified individuals.

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Product name: 4-tert-Butylbenzoic acid

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Other regulations, limitations and prohibitive regulations
Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.
The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.
Substance is not listed.
Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.
Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information
Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department
Date of preparation / last revision 03/24/2016 / -
Abbreviations and acronyms:
ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
EINECS: European Inventory of Existing Commercial Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMIS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
vPvB: very Persistent and very Bioaccumulative
ACGIH: American Conference of Governmental Industrial Hygienists (USA)
OSHA: Occupational Safety and Health Administration (USA)
NTP: National Toxicology Program (USA)
IARC: International Agency for Research on Cancer
EPA: Environmental Protection Agency (USA)
Acute Tox. 4: Acute toxicity, Hazard Category 4
Acute Tox. 3: Acute toxicity, Hazard Category 3
Repr. 1A: Reproductive toxicity, Hazard Category 1A
STOT RE 1: Specific target organ toxicity - Repeated exposure, Hazard Category 1

USA