

4-*tert*-Butylbenzoic-d₁₃ Acid

Section 1. Chemical product and company identifications

Product code: D-7697
Chemical formula: C₁₁H₁₃O₂
CAS: N/A
CAS (unlabelled): 98-73-7
Synonyms: *p-tert*-Butylbenzoic Acid

Supplier / Manufacturer:

C/D/N Isotopes Inc.
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In case of emergency:

TOXYSKAN HOTLINE: 1-855-780-0599

Section 2. Hazards identifications



Physical state: Solid
Warning: Harmful if swallowed or inhaled. Toxic in contact with skin.
Routes of entry: Inhalation, ingestion, skin and eyes

GHS (Globally Harmonized System of Classification and Labelling of Chemicals):

GHS Classification:

- Acute toxicity, Oral (Category 4)
- Acute toxicity, Dermal (Category 3)
- Acute toxicity, Inhalation (Category 4)

GHS Label elements:

- Pictograms:  
- Signal word: Danger

Hazards statement:

- H302 + H332 Harmful if swallowed or inhaled.
- H311 Toxic in contact with skin.

Precautionary statement:

- P261 Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.
- P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
- P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
- P302 + P350 IF ON SKIN: Wash with plenty of soap and water.
- P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
- P316 Get emergency medical help immediately.

Section 3. Composition and information on ingredients

<u>Name</u>	<u>CAS</u>	<u>Concentration %</u>
4- <i>tert</i> -Butylbenzoic-d ₁₃ Acid	N/A	> 98

Section 4. First aid measures

Eye contact: Flush eyes with water as a precaution.
Skin contact: Wash off with soap and plenty of water. Consult a physician.
Inhalation: If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.
Ingestion: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.
General advice: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

Section 5. Firefighting measures

Flammability of the product: Not flammable or combustible.

Lower explosion limit: No data available.

Upper explosion limit: No data available.

Auto-ignition temperature: 510 °C (950 °F)

Flash point: No data available.

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.

Firefighting media and instructions: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special protective equipment for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Section 6. Accidental release measures

Personal precautions: Use personal protective equipment. Avoid dust formation. Ensure adequate ventilation. Avoid breathing dust.

Environmental precautions: Do not let product enter drains. Discharge into the environment must be avoided.

Methods for cleaning up: Pick up and arrange disposal without creating dust. Keep in suitable, closed containers for disposal.

Section 7. Handling and storage

Handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation.

Storage: Store at room temperature. Adequate ventilation.

Section 8. Exposure Controls, Personal Protections

Engineering controls: Use mechanical exhaust or laboratory fumehood to avoid exposure.

Eyes: Safety glasses with side-shields conforming to NIOSH (US) or EN 166 (EU).

Respiratory: 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).

Hands: Handle with gloves. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Skin/body: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Section 9. Physical and chemical properties (unlabelled)

Molecular weight: 178.23 g/mol

Physical status: Solid

Color: White to off-white

Odour: No data available

Density: No data available

Melting point: 162 - 165 °C (324 - 329 °F)

Boiling point: No data available

Vapour pressure: No data available

Vapour density: No data available

Partition coefficient (octanol/water): log Pow: 3.85

Water solubility: 28 mg/L

Section 10. Stability and reactivity

Stability and reactivity: Stable under recommended storage conditions.

Incompatibility: Strong oxidizing agents.

Products of combustion: Hazardous decomposition products formed under fire conditions: Carbon oxides.

Reactivity conditions: No data available.

Section 11. Toxicological information (unlabelled)

Toxicological data: 4-*tert*-Butylbenzoic Acid

Information on ingredients:

<u>Name</u>	<u>CAS</u>	<u>LD₅₀</u>	<u>LC₅₀</u>
4- <i>tert</i> -Butylbenzoic Acid	98-73-7	Oral - Rat - 473 mg/kg Dermal - Rat - 300 mg/kg	Inhalation - Rat - 4 h - > 1,900 mg/m ³

Potential acute effects

- **Eyes:** May cause eye irritation.
- **Skin:** Toxic if absorbed through skin. May cause skin irritation.
- **Inhalation:** Harmful if inhaled. May cause respiratory tract irritation.
- **Ingestion:** Harmful if swallowed.

Potential chronic effects

- **Carcinogenic effects:** 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. ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- **Mutagenic effects:** No data available.
- **Teratogenic effects:** No data available.
- **Medical conditions aggravated by overexposure:** No data available.

Section 12. Ecological information

Ecological data:

<u>Name</u>	<u>Results</u>	<u>Species</u>	<u>Period</u>
4- <i>tert</i> -Butylbenzoic Acid	33 mg/l LC50	Carassius auratus	96 h
	70 mg/l LC50	Oryzias latipes	96 h
	24 mg/l EC50	Daphnia magna	48 h
	> 90 mg/l EC50	Pseudokirchneriella subcapitata	72 h

Effects on environment: An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Mobility: No data available.

Environmental precautions: No data available.

Persistence and degradability: No data available.

Bioaccumulative potential: No data available.

Section 13. Disposal considerations

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

Section 14. Transportation information

Classification DOT/IMDG/IATA label:

Shipping name: Toxic solid, organic, n.o.s. (4-*tert*-Butylbenzoic Acid)

UN number: UN2811

Class: 6.1

Packaging group: III

Additional information: None

Section 15. Regulatory information

UNITED STATES: NFPA classification



Health: 3
Flammable: 0
Reactivity: 0
Special conditions: None

Legend: 4: Severe, 3: High, 2: Moderate, 1: Slightly, 0: Not hazardous

U.S. Federal regulations:

TSCA 8(b) inventory: 4-*tert*-Butylbenzoic Acid
SARA 302/304/311/312 extremely hazardous substances: Not Listed
SARA 302/304 emergency planning and notification: Not Listed
SARA 302/304/311/312 hazardous chemicals: Not Listed
SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard: Not Listed
CWA (Clean Water Act) 307: Not Listed
CWA (Clean Water Act) 311: Not Listed
CAA (Clean Air Act) 112 accidental release prevention: Not Listed
CAA (Clean Air Act) 112 regulated flammable substances: Not Listed
CAA (Clean Air Act) 112 regulated toxic substances: Not Listed

State regulations:

DEA List I Chemicals (Precursor Chemicals): Not Listed
DEA List II Chemicals (Essential Chemicals): Not Listed
Substances in Massachusetts: Not Listed
Dangerous substances in New Jersey: Not Listed
New York – Dangerous substances with acute effects: Not Listed
Dangerous substances in Pennsylvania – right to know: Not Listed

WHMIS (Canada):



D1B - Toxic material causing immediate and serious toxic effects

Section 16. Additional information

References:

- ANSI Z400.1, MSDS Standard, 2001.
- Manufacturer's Material Safety Data Sheet.
- 29CFR Part1910.1200 OSHA MSDS Requirements.
- 49CFR Table List of Hazardous Materials, UN#, Proper Shipping Names, PG. -Canada
- Gazette Part II, Vol. 122, No. 2 Registration SOR/88-64 31 December, 1987 Hazardous Products Act "Ingredient Disclosure List".
- Federal act on the controlled products
- Canadian Transport of Dangerous Goods, Regulations and Schedules, Clear Language version 2002.
- Toxicological repertory, HSC.
- Material safety data sheet from the components.

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Elaborated by: Toxyscan Inc., 1-866-780-0599

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