

## SAFETY DATA SHEET

Version 6.9  
Revision Date 08/27/2023  
Print Date 04/13/2024

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 4-*tert*-Butylbenzoic acid

Product Number : 150355  
Brand : Aldrich  
CAS-No. : 98-73-7

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

**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**

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

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Acute toxicity, Oral (Category 4), H302  
Reproductive toxicity (Category 1B), H360  
Specific target organ toxicity - repeated exposure (Category 1), H372  
Short-term (acute) aquatic hazard (Category 3), H402  
Long-term (chronic) aquatic hazard (Category 3), H412

For the full text of the H-Statements mentioned in this Section, see Section 16.

**2.2 GHS Label elements, including precautionary statements**

Pictogram



Signal Word	Danger
Hazard statement(s)	
H302	Harmful if swallowed.
H360	May damage fertility or the unborn child.
H372	Causes damage to organs through prolonged or repeated exposure.
H412	Harmful to aquatic life with long lasting effects.
Precautionary statement(s)	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P260	Do not breathe dust.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula	: $C_{11}H_{14}O_2$
Molecular weight	: 178.23 g/mol
CAS-No.	: 98-73-7
EC-No.	: 202-696-3

Component	Classification	Concentration
<b>4-tert-Butylbenzoic acid</b>		
	Acute Tox. 4; Repr. 1B; STOT RE 1; Aquatic Acute 3; Aquatic Chronic 3; H302, H360, H372, H402, H412	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. 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. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

### 4.2 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

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

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

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### 5.4 Further information

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.  
For personal protection see section 8.

### **6.2 Environmental precautions**

Do not let product enter drains.

### **6.3 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 carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

### **6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

#### **Advice on safe handling**

Work under hood. Do not inhale substance/mixture.

#### **Hygiene measures**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.  
For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

#### **Storage conditions**

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

#### **Storage class**

Storage class (TRGS 510): 6.1D: Non-combustible, acute toxic Cat.3 / toxic hazardous materials or hazardous materials causing chronic effects

### **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Component	CAS-No.	Value	Control parameters	Basis
4-tert-Butylbenzoic acid	98-73-7	TWA	0.1 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		

## 8.2 Exposure controls

### Appropriate engineering controls

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

### Personal protective equipment

#### Eye/face protection

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

#### Skin protection

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](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

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](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: KCL 741 Dermatril® L

#### Body Protection

protective clothing

#### Respiratory protection

Recommended Filter type: Filter type P3

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.  
required when dusts 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.

## Control of environmental exposure

Do not let product enter drains.

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### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: solid Color: white
b) Odor	weakly aromatic
c) Odor Threshold	No data available
d) pH	3.9 at 20 °C (68 °F) - (saturated solution)
e) Melting point/freezing point	Melting point/range: 162 - 165 °C (324 - 329 °F) - lit.
f) Initial boiling point and boiling range	280 °C 536 °F at 1,013 hPa - (decomposition)
g) Flash point	No data available
h) Evaporation rate	No data available
i) Flammability (solid, gas)	does not ignite - Flammability (solids)
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	< 0.01 hPa at 20 °C (68 °F)
l) Vapor density	No data available
m) Density	0.6 g/cm <sup>3</sup> at 20 °C (68 °F)
Relative density	No data available
n) Water solubility	12.6 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	log Pow: 3.4 at 21 °C (70 °F) - Bioaccumulation is not expected., (ECHA)
p) Autoignition temperature	No data available
q) Decomposition temperature	> 280 °C (> 536 °F) -
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	none

#### 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
Oxidizing agents  
bases

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 473 - 735 mg/kg

Remarks: (External MSDS)

Symptoms: Cough, Shortness of breath

Dermal: No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

#### Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Result: negative

Remarks: (ECHA)

Aldrich - 150355

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Test Type: Mutagenicity (mammal cell test): micronucleus.  
Test system: Chinese hamster lung cells  
Metabolic activation: Metabolic activation  
Method: OECD Test Guideline 487  
Result: positive

Test Type: In vivo micronucleus test  
Species: Rat  
Cell type: Bone marrow  
Application Route: Oral  
Method: OECD Test Guideline 475  
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**

May damage fertility.

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

Causes damage to organs through prolonged or repeated exposure.

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

RTECS: DG4708000

Liver injury may occur., Kidney injury may occur., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

ataxia (impaired locomotor coordination)

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence



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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish	semi-static test LC50 - <i>Oryzias latipes</i> (Orange-red killifish) - 70 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 24 mg/l - 48 h (US-EPA)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - > 94 mg/l - 72 h (OECD Test Guideline 201)  static test NOEC - <i>Pseudokirchneriella subcapitata</i> (green algae) - 21 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test NOEC - activated sludge - 319 mg/l - 3 h (OECD Test Guideline 209)

### 12.2 Persistence and degradability

Biodegradability	Result: 41 - 46 % - Not readily biodegradable. (OECD Test Guideline 301B)
Biochemical Oxygen Demand (BOD)	260 mg/g Remarks: (External MSDS)
Chemical Oxygen Demand (COD)	2,370 mg/g Remarks: (External MSDS)

### 12.3 Bioaccumulative potential

No data available

### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

### 12.6 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

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.

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## SECTION 14: Transport information

### **DOT (US)**

Not dangerous goods

### **IMDG**

Not dangerous goods

### **IATA**

Not dangerous goods

### **Further information**

Not classified as dangerous in the meaning of transport regulations.

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## SECTION 15: Regulatory information

### **SARA 302 Components**

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

### **SARA 313 Components**

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.

### **SARA 311/312 Hazards**

Acute Health Hazard, Chronic Health Hazard

### **Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

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## SECTION 16: Other information

### **Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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](http://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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