

## SAFETY DATA SHEET

Version 6.1  
Revision Date 07/17/2018  
Print Date 11/12/2018

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : **tert-Butylbenzene**

Product Number : 19640  
Brand : Sigma-Aldrich

CAS-No. : 98-06-6

#### 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 Street  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

#### 1.4 Emergency telephone number

Emergency Phone # : (314) 776-6555

### 2. HAZARDS IDENTIFICATION

#### 2.1 Classification of the substance or mixture

**GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226

Eye irritation (Category 2A), H319

Acute aquatic toxicity (Category 2), H401

Chronic aquatic toxicity (Category 2), H411

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 : Warning

Hazard statement(s)

H226

H319

H411

Flammable liquid and vapour.

Causes serious eye irritation.

Toxic to aquatic life with long lasting effects.

**Precautionary statement(s)**

P210	Keep away from heat/sparks/open flames/hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P391	Collect spillage.
P403 + P235	Store in a well-ventilated place. Keep cool.
P501	Dispose of contents/ container to an approved waste disposal plant.

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

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**3. COMPOSITION/INFORMATION ON INGREDIENTS****3.1 Substances**

Synonyms	: 2-Methyl-2-phenylpropane
Formula	: C<SB>10</SB>H<SB>14</SB>
Molecular weight	: 134.22 g/mol
CAS-No.	: 98-06-6
EC-No.	: 202-632-4

**Hazardous components**

Component	Classification	Concentration
<b>tert-Butylbenzene</b>		
	Flam. Liq. 3; Eye Irrit. 2A; Aquatic Acute 2; Aquatic Chronic 2; H226, H319, H411	<= 100 %

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

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**4. FIRST AID MEASURES****4.1 Description of first aid measures****General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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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### **5. FIREFIGHTING MEASURES**

#### **5.1 Extinguishing media**

##### **Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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

Carbon oxides

#### **5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

#### **5.4 Further information**

Use water spray to cool unopened containers.

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### **6. ACCIDENTAL RELEASE MEASURES**

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

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

#### **6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

#### **6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

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

For disposal see section 13.

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### **7. HANDLING AND STORAGE**

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

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

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

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Storage class (TRGS 510): 3: Flammable liquids

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

#### **8.1 Control parameters**

##### **Components with workplace control parameters**

Contains no substances with occupational exposure limit values.

#### **8.2 Exposure controls**

##### **Appropriate engineering controls**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

## Personal protective equipment

### Eye/face protection

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

### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Full contact

Material: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

#### Splash contact

Material: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

Impervious clothing, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

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) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |  |   |
|--|---|
| a) Appearance                              | Form: liquid, clear<br>Colour: colourless   |
| b) Odour                                   | No data available                           |
| c) Odour Threshold                         | No data available                           |
| d) pH                                      | No data available                           |
| e) Melting point/freezing point            | Melting point/range: -58 °C (-72 °F) - lit. |
| f) Initial boiling point and boiling range | 169 °C (336 °F) - lit.                      |
| g) Flash point                             | 34.0 °C (93.2 °F) - closed cup              |
| h) Evaporation rate                        | No data available                           |
| i) Flammability (solid, gas)               | No data available                           |
| j) Upper/lower flammability or             | Lower explosion limit: 0.8 %(V)             |

explosive limits

- |   |                             |
|---|-----------------------------|
| k) Vapour pressure                        | No data available           |
| l) Vapour density                         | No data available           |
| m) Relative density                       | 0.867 g/mL at 25 °C (77 °F) |
| n) Water solubility                       | No data available           |
| o) Partition coefficient: n-octanol/water | log Pow: 3.80               |
| p) Auto-ignition temperature              | 450.0 °C (842.0 °F)         |
| q) Decomposition temperature              | No data available           |
| r) Viscosity                              | No data available           |
| s) Explosive properties                   | No data available           |
| t) Oxidizing properties                   | No data available           |

## 9.2 Other safety information

No data available

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## 10. STABILITY AND REACTIVITY

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Strong oxidizing agents

### 10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides

Other decomposition products - No data available

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 3,045 mg/kg

Remarks: (RTECS)

LC50 Inhalation - Rat - 4 h - 4.6 mg/l

Remarks: (External MSDS)

#### Skin corrosion/irritation

Skin - Rabbit

Result: Severe irritations

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

#### **Respiratory or skin sensitisation**

Sensitisation test (Magnusson and Kligman):

Result: negative

Remarks: (External MSDS)

#### **Germ cell mutagenicity**

#### **Carcinogenicity**

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.

NTP: No component 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**

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

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

#### **Aspiration hazard**

Aspiration hazard, Aspiration may cause pulmonary oedema and pneumonitis.

#### **Additional Information**

RTECS: CY9120000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Nausea, Unconsciousness, Headache

In high concentrations:

narcosis

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## **12. ECOLOGICAL INFORMATION**

### **12.1 Toxicity**

Toxicity to fish LC50 - Leuciscus idus (Golden orfe) - 65 mg/l (tert-Butylbenzene)  
Remarks: (Lit.)

Toxicity to daphnia and other aquatic EC50 - Daphnia magna (Water flea) - 41 mg/l (tert-Butylbenzene)  
invertebrates Remarks: (Lit.)

### **12.2 Persistence and degradability**

### **12.3 Bioaccumulative potential**

### **12.4 Mobility in soil**

### **12.5 Results of PBT and vPvB assessment**

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

### **12.6 Other adverse effects**

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.  
Toxic to aquatic life.

Formation of health-hazardous mixtures possible with water.

Discharge into the environment must be avoided.

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## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

#### Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

### DOT (US)

UN number: 2709      Class: 3      Packing group: III  
Proper shipping name: Butyl benzenesMarine pollutant: no  
Poison Inhalation Hazard: No

### IMDG

UN number: 2709      Class: 3      Packing group: III      EMS-No: F-E, S-D  
Proper shipping name: BUTYLBENZENES  
Marine pollutant : yesMarine pollutant : yes

### IATA

UN number: 2709      Class: 3      Packing group: III  
Proper shipping name: Butylbenzenes

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## 15. REGULATORY INFORMATION

### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### 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

Fire Hazard, Acute Health Hazard

### Massachusetts Right To Know Components

	CAS-No.	Revision Date
tert-Butylbenzene	98-06-6	1993-04-24

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
tert-Butylbenzene	98-06-6	1993-04-24

### New Jersey Right To Know Components

	CAS-No.	Revision Date
tert-Butylbenzene	98-06-6	1993-04-24

### California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

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## 16. OTHER INFORMATION

### Full text of H-Statements referred to under sections 2 and 3.

H226      Flammable liquid and vapour.

H319	Causes serious eye irritation.
H401	Toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

**Further information**

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**Preparation Information**

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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