SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : tert-Butylbenzene
Product Number : B90602
Brand : 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 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)

- Flammable liquids (Category 3), H226
- Skin irritation (Category 2), H315

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 : Flammable liquid and vapor.
H315 : Causes skin irritation.
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.
P280 Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
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

SECTION 3: Composition/information on ingredients

3.1 Substances
Synonyms : 2-Methyl-2-phenylpropane

Formula : C_{10}H_{14}
Molecular weight : 134.22 g/mol
CAS-No. : 98-06-6
EC-No. : 202-632-4

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>tert-Butylbenzene</td>
<td>Flam. Liq. 3; Skin Irrit. 2; H226, H315</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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

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.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.
In case of eye contact
After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed
After swallowing: make victim drink water (two glasses at most). Consult doctor if feeling unwell.

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Foam Carbon dioxide (CO2) 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.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air at elevated temperatures.
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
Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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. Risk of explosion.

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 with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.
SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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
Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class
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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters
Contains no substances with occupational exposure limit values.

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).
Full contact
Material: Viton®
Minimum layer thickness: 0.7 mm
Break through time: 480 min
Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)
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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 10 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

**Body Protection**
Flame retardant antistatic protective clothing.

**Respiratory protection**
required when vapours/aerosols 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. Risk of explosion.

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**SECTION 9: Physical and chemical properties**

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

a) Appearance
   Form: liquid
b) Odor
   No data available
c) Odor 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
   47 °C (117 °F) - closed cup - closed cup
h) Evaporation rate
   No data available
i) Flammability (solid, gas)
   No data available
j) Upper/lower flammability or explosive limits
   Upper explosion limit: 5.6 %(V)
   Lower explosion limit: 0.8 %(V)
k) Vapor pressure
   11 hPa at 20 °C (68 °F)
l) Vapor density
   No data available
m) Density
   0.867 g/cm3 at 25 °C (77 °F) - lit.
   Relative density
   No data available
n) Water solubility
   1 g/l - OECD Test Guideline 105 - insoluble
o) Partition coefficient
   No data available
n-octanol/water

d) Autoignition temperature
   > 450 °C (> 842 °F) at 1,010 hPa

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   none

9.2 Other safety information
   No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
   Vapor/air-mixtures are explosive at intense warming.

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

10.4 Conditions to avoid
   Heating.

10.5 Incompatible materials
   various plastics

10.6 Hazardous decomposition products
   In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
   LD50 Oral - Rat - 3,045 mg/kg
   Remarks: (RTECS)
   Inhalation: No data available
   Dermal: No data available

Skin corrosion/irritation
   Skin - Human
   Result: Skin irritation
   (OECD Test Guideline 439)
   Remarks: (ECHA)

Serious eye damage/eye irritation
   Eyes - Humans
   Result: No eye irritation
Remarks: (ECHA)

Respiratory or skin sensitization
KeratinoSens assay
Result: negative
(OECD Test Guideline 442D)
Remarks: (ECHA)

Germ cell mutagenicity
No data available

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
No data available

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

11.2 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.
Toxicity to daphnia and other aquatic invertebrates

- static test EC50 - Daphnia magna (Water flea) - > 100 mg/l - 48 h (OECD Test Guideline 202)
- Remarks: (ECHA)

Toxicity to algae

- static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 290.44 mg/l - 72 h (OECD Test Guideline 201)
- Remarks: (ECHA)

12.2 Persistence and degradability

Biodegradability

- aerobic - Exposure time 28 d
- Result: 11 % - Not readily biodegradable. (OECD Test Guideline 301B)
- Remarks: (ECHA)

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

- Formation of health-hazardous mixtures possible with water.
- Discharge into the environment must be avoided.

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. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

**DOT (US)**

- UN number: 2709
- Class: 3
- Packing group: III
- Proper shipping name: Butyl benzenes
- Reportable Quantity (RQ):
  - Marine pollutant: yes
  - 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: yes
Marine pollutant: yes

**IATA**
UN number: 2709  Class: 3  Packing group: III
Proper shipping name: Butylbenzene

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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**
Fire Hazard, Acute 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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