

Chemical Safety Data Sheet MSDS / SDS

tert-Butylbenzene

Revision Date:2025-01-11 Revision Number:1

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

Product name : tert-Butylbenzene
CBnumber : CB6161293
CAS : 98-06-6
EINECS Number : 202-632-4
Synonyms : tert-butylbenzene,t-butylbenzene

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Warning

Precautionary statements

P501 Dispose of contents/container to.....

P405 Store locked up.

P403+P235 Store in a well-ventilated place. Keep cool.

P370+P378 In case of fire: Use ... for extinction.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

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

P271 Use only outdoors or in a well-ventilated area.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P240 Ground/bond container and receiving equipment.
P233 Keep container tightly closed.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H335 May cause respiratory irritation
H332 Harmful if inhaled
H319 Causes serious eye irritation
H315 Causes skin irritation
H226 Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: tert-Butylbenzene
Synonyms	: tert-butylbenzene,t-butylbenzene
CAS	: 98-06-6
EC number	: 202-632-4
MF	: C ₁₀ H ₁₄
MW	: 134.22

SECTION 4: First aid measures

Description of first aid measures

General advice

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

If inhaled

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

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: caution if victim vomits. Risk of aspiration! Keep airways free. Pulmonary failure possible after aspiration of vomit. Call a physician immediately.

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

Indication of any immediate medical attention and special treatment needed

SECTION 5: Firefighting measures

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.

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.

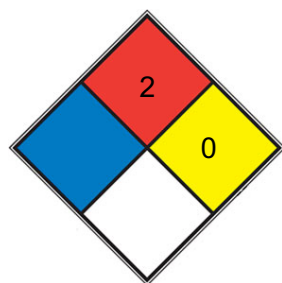
Advice for firefighters

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

Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

NFPA 704



■ HEALTH

Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely

■ FIRE 2 divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

□ SPEC.

□ HAZ.

SECTION 6: Accidental release measures

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.

Environmental precautions

Do not let product enter drains. Risk of explosion.

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 with liquid-absorbent material (e.g.

Chemisorb?). Dispose of properly. Clean up affected area.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols. Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

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

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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
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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.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: -58 °C - lit.
Initial boiling point and boiling range	169 °C - lit.
Flash point	44 °C
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 5,6 %(V) Lower explosion limit: 0,8 %(V)
Vapour pressure	4.79 mm Hg (37.7 °C)
Vapour density	3.16 (169 °C, vs air)
Relative density	0,867 g/cm ³ at 25 °C
Water solubility	29.5mg/l
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available

Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	(x 10 ⁻² atm·m ³ /mol): 1.17 at 25 °C (Hine and Mookerjee, 1975)

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

Vapor/air-mixtures are explosive at intense warming.

Chemical stability

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

Possibility of hazardous reactions

No data available

Conditions to avoid

Heating.

Incompatible materials

Strong oxidizing agents

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

SECTION 11: Toxicological information

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 sensitization

Remarks: (External MSDS)

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.

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

Aspiration hazard, Aspiration may cause pulmonary edema 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.

SECTION 12: Ecological information

Toxicity

Toxicity to fish

LC50 - Leuciscus idus (Golden orfe) - 65 mg/l

Remarks: (Lit.)

Toxicity to daphnia and other aquatic invertebrates

EC50 - Daphnia magna (Water flea) - 41 mg/l Remarks: (Lit.)

Persistence and degradability

No data available

Bioaccumulative potential

No data available

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Toxics Screening Level

The initial threshold screening level (ITSL) for t-Butyl benzene is 10 µg/m³ based on an annual averaging time.

Other adverse effects

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

SECTION 13: Disposal considerations

Waste treatment methods

Product

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

UN number

ADR/RID: 2709 IMDG: 2709 IATA: 2709

UN proper shipping name

ADR/RID: BUTYLBENZENES IMDG: BUTYLBENZENES IATA: Butylbenzenes

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

Packaging group

ADR/RID: III IMDG: III IATA: III

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015: Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Korea Existing Chemicals List (KECL): Not Listed. website: <http://ncis.nier.go.kr>

Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory: Listed. website: <https://www.epa.gov/>
Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>
New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>
European Inventory of Existing Commercial Chemical Substances (EINECS): Listed. website: <https://echa.europa.eu/>
EC Inventory: Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Listed. website: <https://www.mee.gov.cn/>

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
CAS: Chemical Abstracts Service
EC50: Effective Concentration 50%
IATA: International Air Transportation Association
IMDG: International Maritime Dangerous Goods
LC50: Lethal Concentration 50%
LD50: Lethal Dose 50%
RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
STEL: Short term exposure limit
TWA: Time Weighted Average

References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.