

Creation Date 22-Sep-2009

Revision Date 24-Jan-2024

Revision Number 3

## SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

### 1.1. Product identifier

Product Description:	<u>tert-Butylbenzene</u>
Cat No. :	<b>A12378</b>
Synonyms	(1,1-Dimethylethyl)benzene; 2-Methyl-2-phenylpropane
CAS No	98-06-6
EC No	202-632-4
Molecular Formula	C10 H14
REACH registration number	-

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

Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

### 1.3. Details of the supplier of the safety data sheet

Company	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
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E-mail address	begel.sdsdesk@thermofisher.com
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### 1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

**CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567**

#### Physical hazards

Flammable liquids

Category 3 (H226)

#### Health hazards

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Based on available data, the classification criteria are not met

## **Environmental hazards**

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



**Signal Word**

**Warning**

## **Hazard Statements**

H226 - Flammable liquid and vapor

## **Precautionary Statements**

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

## **2.3. Other hazards**

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### **3.1. Substances**

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
tert-Butylbenzene	98-06-6	EEC No. 202-632-4	99	Flam Liq. 3 (H226)

**REACH registration number**

-

Full text of Hazard Statements: see section 16

## **SECTION 4: FIRST AID MEASURES**

### **4.1. Description of first aid measures**

#### **Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

#### **Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Get medical attention.

#### **Ingestion**

Do NOT induce vomiting. Get medical attention.

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**Inhalation** Remove to fresh air. Get medical attention. If not breathing, give artificial respiration.

**Self-Protection of the First Aider** Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

#### **4.2. Most important symptoms and effects, both acute and delayed**

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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

**Notes to Physician** Treat symptomatically. Symptoms may be delayed.

## **SECTION 5: FIREFIGHTING MEASURES**

#### **5.1. Extinguishing media**

##### **Suitable Extinguishing Media**

Carbon dioxide (CO<sub>2</sub>). Dry chemical. Water mist may be used to cool closed containers. Chemical foam. Water mist may be used to cool closed containers.

##### **Extinguishing media which must not be used for safety reasons**

Water may be ineffective. Do not use a solid water stream as it may scatter and spread fire.

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

Flammable. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated. Vapors may form explosive mixtures with air.

##### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

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

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

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

Remove all sources of ignition. Take precautionary measures against static discharges.

#### **6.2. Environmental precautions**

See Section 12 for additional Ecological Information.

#### **6.3. Methods and material for containment and cleaning up**

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges.

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

Refer to protective measures listed in Sections 8 and 13.

## **SECTION 7: HANDLING AND STORAGE**

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## 7.1. Precautions for safe handling

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Take precautionary measures against static discharges. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Wear personal protective equipment/face protection. Keep away from open flames, hot surfaces and sources of ignition.

## Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

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

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Flammables area.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3  
Storage Class (LGK) (Germany)

## 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### Exposure limits

List source(s):

#### Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

See table for values

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
tert-Butylbenzene 98-06-6 ( 99 )				DNEL = 2.17mg/kg bw/day

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
tert-Butylbenzene 98-06-6 ( 99 )				DNEL = 7.64mg/m <sup>3</sup>

#### Predicted No Effect Concentration (PNEC)

See values below.

Component	Fresh water	Fresh water sediment	Water Intermittent	Microorganisms in sewage treatment	Soil (Agriculture)
tert-Butylbenzene 98-06-6 ( 99 )	PNEC = 0.1mg/L	PNEC = 1.727mg/kg sediment dw	PNEC = 1mg/L	PNEC = 2mg/L	PNEC = 2.614mg/kg soil dw

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Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
tert-Butylbenzene 98-06-6 ( 99 )	PNEC = 0.01mg/L	PNEC = 0.1727mg/kg sediment dw	PNEC = 0.1mg/L		

## 8.2. Exposure controls

### Engineering Measures

Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

### Personal protective equipment

#### Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Viton (R)	See manufacturers recommendations	-	EN 374	(minimum requirement)

#### Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

#### Respiratory Protection

No protective equipment is needed under normal use conditions.

#### Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

#### Small scale/Laboratory use

Maintain adequate ventilation

#### Environmental exposure controls

No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

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

Physical State	Liquid	
Appearance	Clear	
Odor	aromatic	
Odor Threshold	No data available	
Melting Point/Range	-58 °C / -72.4 °F	
Softening Point	No data available	
Boiling Point/Range	169 °C / 336.2 °F	@ 760 mmHg
Flammability (liquid)	Flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	44 °C / 111.2 °F	Method - No information available

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<b>Autoignition Temperature</b>	512 °C / 953.6 °F	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	1.15 mPa s at 20 °C	
<b>Water Solubility</b>	0.03 G/L WATER (20°C)	practically insoluble
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Component</b>	<b>log Pow</b>	
tert-Butylbenzene	4.11	
<b>Vapor Pressure</b>	1.33 hPa @ 13 °C	
<b>Density / Specific Gravity</b>	0.860	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Vapor Density</b>	4.6	(Air = 1.0)
<b>Particle characteristics</b>	Not applicable (liquid)	

## 9.2. Other information

<b>Molecular Formula</b>	C10 H14
<b>Molecular Weight</b>	134.22
<b>Explosive Properties</b>	explosive air/vapour mixtures possible

## SECTION 10: STABILITY AND REACTIVITY

### 10.1. Reactivity

None known, based on information available

### 10.2. Chemical stability

Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

<b>Hazardous Polymerization</b>	Hazardous polymerization does not occur.
<b>Hazardous Reactions</b>	No information available.

### 10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.

### 10.5. Incompatible materials

None known.

### 10.6. Hazardous decomposition products

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

### 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

#### Product Information

#### (a) acute toxicity;

<b>Oral</b>	Based on available data, the classification criteria are not met
<b>Dermal</b>	No data available
<b>Inhalation</b>	No data available

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
tert-Butylbenzene	LD50 = 3503 mg/kg ( Rat )	-	-

(b) skin corrosion/irritation; No data available

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(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available  
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

**Other Adverse Effects** The toxicological properties have not been fully investigated.

**Symptoms / effects, both acute and delayed** Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

## 11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

Ecotoxicity effects .

### 12.2. Persistence and degradability

**Persistence** Insoluble in water, May persist, based on information available.

12.3. Bioaccumulative potential May have some potential to bioaccumulate

Component	log Pow	Bioconcentration factor (BCF)
tert-Butylbenzene	4.11	No data available

### 12.4. Mobility in soil

The product is insoluble and floats on water. The product evaporates slowly. Is not likely mobile in the environment due its low water solubility and propensity to bind to soil particles: Spillage unlikely to penetrate soil

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**12.5. Results of PBT and vPvB assessment** No data available for assessment.

**12.6. Endocrine disrupting properties**

**Endocrine Disruptor Information** This product does not contain any known or suspected endocrine disruptors

**12.7. Other adverse effects**  
**Persistent Organic Pollutant**  
**Ozone Depletion Potential**

This product does not contain any known or suspected substance  
This product does not contain any known or suspected substance

## SECTION 13: DISPOSAL CONSIDERATIONS

**13.1. Waste treatment methods**

**Waste from Residues/Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

**European Waste Catalogue (EWC)**

According to the European Waste Catalog, Waste Codes are not product specific, but application specific.

**Other Information**

Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

## SECTION 14: TRANSPORT INFORMATION

**IMDG/IMO**

**14.1. UN number** UN2709  
**14.2. UN proper shipping name** BUTYLBENZENES  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** III

**ADR**

**14.1. UN number** UN2709  
**14.2. UN proper shipping name** BUTYLBENZENES  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** III

**IATA**

**14.1. UN number** UN2709  
**14.2. UN proper shipping name** BUTYLBENZENES  
**14.3. Transport hazard class(es)** 3  
**14.4. Packing group** III

**14.5. Environmental hazards** No hazards identified

**14.6. Special precautions for user** No special precautions required.



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**14.7. Maritime transport in bulk according to IMO instruments** Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

**International Inventories**

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
tert-Butylbenzene	98-06-6	202-632-4	-	-	X	X	-	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
tert-Butylbenzene	98-06-6	X	ACTIVE	X	-	X	X	X

**Legend:** X - Listed '-' - Not Listed      **KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**Authorisation/Restrictions according to EU REACH** Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
tert-Butylbenzene	98-06-6	-	-	-

**Seveso III Directive (2012/18/EC)**

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
tert-Butylbenzene	98-06-6	Not applicable	Not applicable

**Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals**  
Not applicable

**Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?**  
Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

**National Regulations**

**UK** - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
tert-Butylbenzene	WGK1	

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Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
tert-Butylbenzene 98-06-6 ( 99 )	Prohibited and Restricted Substances		

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

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

H226 - Flammable liquid and vapor

### Legend

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

### Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Chemical incident response training.

Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.

### Prepared By

Health, Safety and Environmental Department

### Creation Date

22-Sep-2009

### Revision Date

24-Jan-2024

### Revision Summary

New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

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## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**