

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

1.1. Product identifier

Product Description:	4-tert-Butyltoluene
Cat No. :	A18214
Synonyms	1-Methyl-4-tert-butylbenzene
CAS No	98-51-1
Molecular Formula	C11 H16
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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Acute oral toxicity
Acute Inhalation Toxicity - Vapors
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Specific target organ toxicity - (single exposure)

Category 4 (H302)
Category 2 (H330)
Category 2 (H315)
Category 2 (H319)
Category 3 (H335)

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
H319 - Causes serious eye irritation
H330 - Fatal if inhaled
H302 - Harmful if swallowed
H335 - May cause respiratory irritation
H315 - Causes skin irritation

Precautionary Statements

P310 - Immediately call a POISON CENTER or doctor/physician
P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

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
p-tert-Butyltoluene	98-51-1	EEC No. 202-675-9	96	Flam. Liq. 3 (H226) Acute Tox. 4 (H302) Acute Tox. 2 (H330) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319)

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				STOT SE 3 (H335)
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REACH registration number	-
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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 soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention.
Ingestion	Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Drink plenty of water. Clean mouth with water. Get medical attention. If possible drink milk afterwards.
Inhalation	Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Immediate medical attention is required.
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.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray. Carbon dioxide (CO₂). 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

No information available.

5.2. Special hazards arising from the substance or mixture

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

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂).

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.

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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

Do not flush into surface water or sanitary sewer system.

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. Do not flush into surface water or sanitary sewer system.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

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. Use only in well-ventilated areas. 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. Protect from direct sunlight. Keep container tightly closed in a dry and well-ventilated place.

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): IRE - 2021 Code of Practice for the Chemical Agents Regulations, Schedule 1. Published by the Health and Safety Authority

Component	The United Kingdom	European Union	Ireland
p-tert-Butyltoluene			TWA: 1 ppm 8 hr. TWA: 6.1 mg/m ³ 8 hr.

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			STEL: 3 ppm 15 min STEL: 18.3 mg/m ³ 15 min
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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)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

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

Goggles (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	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

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

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

Recommended Filter type: Particulates filter conforming to EN 143

Small scale/Laboratory use

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Particle filtering: EN149:2001

When RPE is used a face piece Fit Test should be conducted

Environmental exposure controls

Prevent product from entering drains. Do not allow material to contaminate ground water system.

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SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Light yellow	
Odor	Petroleum distillates	
Odor Threshold	No data available	
Melting Point/Range	-54 °C / -65.2 °F	
Softening Point	No data available	
Boiling Point/Range	189 - 192 °C / 372.2 - 377.6 °F	@ 760 mmHg
Flammability (liquid)	Flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	54 °C / 129.2 °F	Method - No information available
Autoignition Temperature	510 °C / 950 °F	
Decomposition Temperature	No data available	
pH	Not applicable	
Viscosity	1.25 mPa s at 25 °C	
Water Solubility	0.06 wt% (20°C)	practically insoluble
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Component	log Pow	
p-tert-Butyltoluene	4.4	
Vapor Pressure	0.65 mmHg @ 25 °C	
Density / Specific Gravity	0.861	
Bulk Density	Not applicable	Liquid
Vapor Density	4.62 (Air = 1.0)	(Air = 1.0)
Particle characteristics	Not applicable (liquid)	

9.2. Other information

Molecular Formula	C11 H16
Molecular Weight	148.25
Explosive Properties	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

Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	No information available.

10.4. Conditions to avoid

Keep away from open flames, hot surfaces and sources of ignition. Excess heat. Exposure to light. Incompatible products.

10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

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Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

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

Product Information

(a) acute toxicity;

Oral

Category 4

Dermal

Based on available data, the classification criteria are not met

Inhalation

Category 2

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
p-tert-Butyltoluene	LD50 = 1550 mg/kg (Rat)	LD50 = 16880 mg/kg (Rabbit)	LC50 = 1.5 mg/L (Rat) 4 h

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(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; Category 3

Results / Target organs

Respiratory system.

(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

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12.1. Toxicity

Ecotoxicity effects

The product contains following substances which are hazardous for the environment. Contains a substance which is: Toxic to aquatic organisms.

Component	Freshwater Fish	Water Flea	Freshwater Algae
p-tert-Butyltoluene	LC50: = 2 mg/L, 96h semi-static (Cyprinus carpio)	EC50: = 3.2 mg/L, 48h (Daphnia magna)	EC50: > 5.6 mg/L, 72h (Desmodesmus subspicatus)

Component	Microtox	M-Factor
p-tert-Butyltoluene	EC50 > 1000 mg/L 5 h	

12.2. Persistence and degradability

Persistence

May persist.

Degradation in sewage treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

12.3. Bioaccumulative potential

Product has a high potential to bioconcentrate

Component	log Pow	Bioconcentration factor (BCF)
p-tert-Butyltoluene	4.4	No data available

12.4. Mobility in soil

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

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

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

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SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number UN2929
14.2. UN proper shipping name Toxic liquid, flammable, organic, n.o.s.
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group II

ADR

14.1. UN number UN2929
14.2. UN proper shipping name Toxic liquid, flammable, organic, n.o.s.
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group II

IATA

14.1. UN number UN2929
14.2. UN proper shipping name TOXIC LIQUID, FLAMMABLE, ORGANIC, N.O.S.*
14.3. Transport hazard class(es) 6.1
Subsidiary Hazard Class 3
14.4. Packing group II

14.5. Environmental hazards No hazards identified
14.6. Special precautions for user No special precautions required.
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
p-tert-Butyltoluene	98-51-1	202-675-9	-	-	X	X	KE-11393	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
p-tert-Butyltoluene	98-51-1	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)
p-tert-Butyltoluene	98-51-1	-	-	-

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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
p-tert-Butyltoluene	98-51-1	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
p-tert-Butyltoluene	WGK3	Class I : 20 mg/m ³ (Massenkonzentration)

Component	France - INRS (Tables of occupational diseases)
p-tert-Butyltoluene	Tableaux des maladies professionnelles (TMP) - RG 84

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
H302 - Harmful if swallowed
H315 - Causes skin irritation
H319 - Causes serious eye irritation
H330 - Fatal if inhaled
H335 - May cause respiratory irritation

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/NDL - 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

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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/MDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

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)

Key literature references and sources for data

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

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

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.

Prepared By

Health, Safety and Environmental Department

Revision Date

12-Feb-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.

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