

According to Regulation (EC) No 1907/2006

4-tert-Butylphenol

Version number: 1
Issued: 2023-08-29



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

1.1. Product identifier

Trade name

4-tert-Butylphenol

CAS number

98-54-4

EC number

202-679-0

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

Relevant identified uses

Research and development.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Street address

Molekula Ltd, Lingfield Way, Darlington,

DL1 4XX Darlington

United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

Email address

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Hazardous to the aquatic environment — Chronic hazard category 1
Skin irritation, hazard category 2
Reproductive toxicity, hazard category 2
Eye irritation, hazard category 2
Specific Target Organ Toxicity — Single exposure, hazard category 3

Hazard statements

H315, H319, H335, H361, H410

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Danger

Hazard statements

H315 Causes skin irritation.
H319 Causes serious eye irritation.
H335 May cause respiratory irritation.
H361 Suspected of damaging fertility or the unborn child.
H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P261 Avoid breathing dust/fumes/gas/mist/vapours/spray.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P273 Avoid release to the environment.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P302 + P352 IF ON SKIN: Wash with plenty of water/.
P304 + P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313 IF exposed or concerned: Get medical advice/attention.
P332 + P313 If skin irritation occurs: Get medical advice/attention.
P337 + P313 If eye irritation persists: Get medical advice/attention.
P362 + P364 Take off contaminated clothing and wash it before reuse.
P403 + P235 Store in a well-ventilated place. Keep cool.

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2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrases M factor acute M factor chronic	Note
4-tert-Butylphenol	98-54-4 202-679-0 - -	100%	Skin Irrit. 2, Repr. 2, Aquatic Chronic 1, Eye Irrit. 2, STOT SE 3	H315, H318, H335, H361f, H410 - -	-

Molecular weight

150.22

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel.

Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. In case of persistent throat irritation or coughing: Seek medical attention and bring these instructions.

Skin contact

IF ON SKIN: Wash with plenty of water. Continue to rinse for at least 15 minutes and seek medical attention. Get medical advice/attention if you feel unwell.

Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

Ingestion

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. Get medical advice/attention if you feel unwell.

Information for doctors

First aiders/ medical personnel need to protect themselves.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure.

Inhalation

Single exposure may cause the following adverse effects: Upper respiratory irritation. Difficulty in breathing.

Skin contact

Single exposure may cause the following adverse effects: Severe skin irritation.

Eye contact

Single exposure may cause the following adverse effects: Severe irritation.

Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. Nausea, vomiting.

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

Treat symptomatically. No special treatment requirement.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

Unsuitable extinguishing media

No specific fire fighting procedure given.

5.2. Special hazards arising from the substance or mixture

Specific hazards: Corrosive.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

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

Vapours are heavier than air and may travel along the floor and in the bottom of containers.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Avoid breathing dust/fume/gas/mist/vapours/spray. Provide adequate ventilation. Avoid contact with skin and eyes. For personal protection, see section 8.

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6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

6.3. Methods and material for containment and cleaning up

Collect spillage with shovel, broom or the like and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2.

7.2. Conditions for safe storage, including any incompatibilities

Store at ambient temperature. Store in a dry place. Store in a closed container.

7.3. Specific end use(s)

No specific usage precautions noted.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No data available

8.2. Exposure controls

Eye / face protection

Wear eye protection.

Hand protection

Wear protective gloves. Recommended gloves: Nitrile.

Glove Thickness: 0.1mm

Breakthrough time: 8 hours

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

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Environmental exposure controls

Avoid discharge into drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Solid

Colour

White.

Odour

No data available

Melting point / freezing point

96 - 101 °C

Boiling point or initial boiling point and boiling range

236 - 238 °C

Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

113 °C

Auto-ignition temperature

501 °C

Decomposition temperature

No data available

pH

No data available

Kinematic viscosity

No data available

Solubility

0.6072 g/l

Partition coefficient n-octanol/water

3

Vapour pressure

1 hPa

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Density and/or relative density

0.908

Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

Forms explosive mixtures with air on intense heating.

15 (approx) Kelvin below the flash point is to be rated as critical.

10.2. Chemical stability

Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Exothermic reaction with:

alkaline substances

oxidising agents

Acid anhydrides.

Acid chlorides Acids.

10.4. Conditions to avoid

Heating.

10.5. Incompatible materials

Strong oxidising agents. Bronze. Copper. Copper alloys Brass. Mild steel

10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

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

Acute toxicity

Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Test animals
4-tert-Butylphenol 98-54-4 / 202-679-0	LD50	>2000 mg/kg	Oral	Rat
4-tert-Butylphenol	LD50	2950 mg/kg	Dermal	Rabbit

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Product / Substance name CAS / EC no.	Dose descriptor	Value / Dose	Exposure route	Test animals
98-54-4 / 202-679-0				

Skin corrosion/irritation

Product / Substance name CAS / EC no.	Result	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	Skin irritation.	Rabbit

Serious eye damage/irritation

Product / Substance name CAS / EC no.	Result	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	Irreversible effects on the eye	Rabbit

Respiratory or skin sensitisation

Product / Substance name CAS / EC no.	Result	Species	Method / Guideline
4-tert-Butylphenol 98-54-4 / 202-679-0	Negative.	Guinea Pig	Maximization Test

Germ cell mutagenicity

Product / Substance name CAS / EC no.	Result	Exposure route	Metabolic activation / Exposure	Species	Method / Guideline
4-tert-Butylphenol 98-54-4 / 202-679-0	Negative.	-	with and without metabolic activation	Escherichia coli/Salmonella typhimurium	Ames test
4-tert-Butylphenol 98-54-4 / 202-679-0	Negative.	-	with and without metabolic activation	lymphocytes	Chromosome aberration: In Vitro Test
4-tert-Butylphenol 98-54-4 / 202-679-0	Negative.	-	with and without metabolic activation	Mouse lymphoma cells	In vitro mammalian cell gene mutation test.
4-tert-Butylphenol 98-54-4 / 202-679-0	Negative.	Oral	-	Mouse bone marrow	in vivo Micronucleus test

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Reproductive toxicity

Product / Substance name CAS / EC no.	Result
4-tert-Butylphenol 98-54-4 / 202-679-0	Suspected of damaging fertility.

Aspiration hazard

Based on available data, the classification criteria are not met.

11.2. Information on other hazards

No data available

SECTION 12: Ecological information

12.1. Toxicity

Acute fish toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	LC50	>1 mg/l	96 hours	Onchorhynchus mykiss (Rainbow trout)

Acute algae toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	NOEC	0.32 mg/l	72 hours	Pseudokirchneriella subcapitata
4-tert-Butylphenol 98-54-4 / 202-679-0	ErC50	14 mg/l	72 hours	Pseudokirchneriella subcapitata

Acute crustacean toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	NOEC	3.2 mg/l	48 hours	Daphnia magna
4-tert-Butylphenol 98-54-4 / 202-679-0	EC50	4.8 mg/l	48 hours	Daphnia magna

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**Micro-/macro organism toxicity**

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	EC50	>10 mg/l	3 hours	Activated sludge.

Chronical toxicity

Product / Substance name CAS / EC no.	Measurement type	Value / Result	Duration of exposure	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	NOEC	0.73 mg/l	21 days	Daphnia magna
4-tert-Butylphenol 98-54-4 / 202-679-0	NOEC	0.01 mg/l	128 days	Pimephales promelas (Fat-head Minnow)

12.2. Persistence and degradability**Persistence and degradability**

Product / Substance name CAS / EC no.	Type of test	Duration	Result	Degradation
4-tert-Butylphenol 98-54-4 / 202-679-0	aerobic	28 days	60%	Not rapidly biodegradable

12.3. Bioaccumulative potential**Bioaccumulative potential**

Product / Substance name CAS / EC no.	Bioconcentration factor (BCF)	Duration	Result	Species
4-tert-Butylphenol 98-54-4 / 202-679-0	20-43	56 days	40 µg/l	Cyprinus carpio (Common carp)

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

No data available

12.6. Endocrine disrupting properties

No data available

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12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

SECTION 14: Transport information

14.1. UN number

3077

14.2. UN proper shipping name

ADR / RID / ADN proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4-tert-Butylphenol)

IMDG proper shipping name

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (4-tert-Butylphenol)

IATA proper shipping name

Environmentally hazardous substance, solid, n.o.s. (4-tert-Butylphenol)

14.3. Transport hazard class(es)

Label

ADR/RID/ADN



9

Environmental hazard

IMDG



9

IATA



9

Environmental hazard

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ADR / RID Class

9

ADR / RID Classification code

M7

ADR / RID hazard identification number

90

IMDG Class

9

IATA Class

9

ADN Class

9

ADN Class Code

M7

14.4. Packing group

ADR / RID / ADN: III

IMDG: III

IATA: III

14.5. Environmental hazards

ADR/RID/ADN: Hazardous for the environment

IMDG EmS

F-A, S-F

14.6. Special precautions for user

Tunnel restriction code: -

Transport category: 3

14.7. Maritime transport in bulk according to IMO instruments

IBC Instruction: IBC08

SECTION 15: Regulatory information

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

EU regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National regulations

Directive: ENVIRONMENTAL HAZARDS

REACH 4-tert-Butylphenol

15.2. Chemical safety assessment

No data available

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SECTION 16: Other information

Phrase meaning

Aquatic Chronic 1 - Hazardous to the aquatic environment — Chronic hazard category 1

Skin Irrit. 2 - Skin irritation, hazard category 2

Repr. 2 - Reproductive toxicity, hazard category 2

Eye Irrit. 2 - Eye irritation, hazard category 2

STOT SE 3 - Specific Target Organ Toxicity — Single exposure, hazard category 3

H315 Causes skin irritation.

H318 Causes serious eye damage.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

H361 Suspected of damaging fertility or the unborn child.

H361f Suspected of damaging fertility

H410 Very toxic to aquatic life with long lasting effects.