

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 20.03.2019

Version 10.4

SECTION 1. Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Catalogue No.	801987
Product name	4-tert-Butylpyrocatechol for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	98-29-3

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal (www.merckgroup.com).
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1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0
Responsible Department	LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number Please contact the regional company representation in your country.**SECTION 2. Hazards identification****2.1 Classification of the substance or mixture**
Classification (REGULATION (EC) No 1272/2008)

Acute toxicity, Category 4, Oral, H302
Acute toxicity, Category 4, Dermal, H312
Skin corrosion, Category 1B, H314
Skin sensitisation, Category 1, H317
Short-term (acute) aquatic hazard, Category 1, H400
Long-term (chronic) aquatic hazard, Category 2, H411
For the full text of the H-Statements mentioned in this Section, see Section 16.

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Catalogue No.
Product name

801987
4-tert-Butylpyrocatechol for synthesis

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H302 + H312 Harmful if swallowed or in contact with skin.

H314 Causes severe skin burns and eye damage.

H317 May cause an allergic skin reaction.

H410 Very toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

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

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Reduced labelling (≤ 125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H314 Causes severe skin burns and eye damage.

H317 May cause an allergic skin reaction.

Precautionary statements

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

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

Contains: 4-tert-butylpyrocatechol

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2.3 Other hazards

None known.

SECTION 3. Composition/information on ingredients

3.1 Substance

Formula 4-[(CH₃)₃C]C₆H₃-1,2-(OH)₂ C₁₀H₁₄O₂ (Hill)
EC-No. 202-653-9
Molar mass 166,22 g/mol

Hazardous components (REGULATION (EC) No 1272/2008)

Chemical name (Concentration)

CAS-No.	Registration number	Classification
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4-tert-butylpyrocatechol (<= 100 %)

98-29-3 *)

Acute toxicity, Category 4, H302
Acute toxicity, Category 4, H312
Skin corrosion, Category 1B, H314
Skin sensitisation, Category 1, H317
Short-term (acute) aquatic hazard, Category 1, H400
Long-term (chronic) aquatic hazard, Category 2, H411

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

3.2 Mixture

Not applicable

SECTION 4. First aid measures

4.1 Description of first aid measures

General advice

First aider needs to protect himself.

After inhalation: fresh air. Call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

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4.2 Most important symptoms and effects, both acute and delayed

cardiovascular disorders, CNS disorders

Risk of blindness!

Irritation and corrosion, Allergic reactions, Cough, Shortness of breath

Risk of blindness!

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water, 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

Combustible.

Vapours are heavier than air and may spread along floors.

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 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

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: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders:

Protective equipment see section 8.

6.2 Environmental precautions

Do not let product enter drains.

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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 Reference to other sections

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Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Protected from light.

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.

Recommended storage temperature see product label.

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

8.2 Exposure controls

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Tightly fitting safety goggles

Hand protection

full contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,11 mm

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Break through time: > 480 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 741 Dermatril® L (full contact), KCL 741 Dermatril® L (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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).

Other protective equipment
protective clothing

Respiratory protection

required when dusts are generated.

Recommended Filter type: Filter P 2 (acc. to DIN 3181) for solid and liquid particles of harmful substances

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Environmental exposure controls

Do not let product enter drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	scales
Colour	beige
Odour	phenol-like
Odour Threshold	No information available.
pH	No information available.
Melting point	52 - 55 °C
Boiling point/boiling range	284 - 286 °C at 1.013 hPa
Flash point	130 °C Method: c.c.
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.

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Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	13,3 hPa at 107 °C < 1 hPa at 25 °C
Relative vapour density	No information available.
Density	1,05 g/cm ³ at 60 °C
Relative density	No information available.
Water solubility	2 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 2,94 (calculated) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Ignition temperature	160 °C
Bulk density	650 - 700 kg/m ³
Viscosity, kinematic	100 mm ² /s at 57 °C

SECTION 10. Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

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10.2 Chemical stability

sensitive to moisture
Sensitivity to light

10.3 Possibility of hazardous reactions

Violent reactions possible with:
Strong oxidizing agents, bases, Strong acids

10.4 Conditions to avoid

Exposure to moisture
Strong heating.

10.5 Incompatible materials

no information available

10.6 Hazardous decomposition products

no information available

SECTION 11. Toxicological information

11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 815 mg/kg
OECD Test Guideline 401

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

Acute inhalation toxicity

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Acute dermal toxicity

LD50 Rat: 1.331 mg/kg
OECD Test Guideline 402

Skin irritation

Rabbit
Result: Causes burns.
OECD Test Guideline 404
Causes burns.

Eye irritation

Causes serious eye damage.
Risk of blindness!
Rabbit
Result: Irreversible effects on the eye
OECD Test Guideline 405

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Product name 4-tert-Butylpyrocatechol for synthesis

Sensitisation

Maximisation Test Guinea pig

Result: positive

Method: OECD Test Guideline 406

May cause an allergic skin reaction.

Germ cell mutagenicity

Genotoxicity in vivo

In vivo micronucleus test

Rat

male and female

Oral

Bone marrow

Exposure time: 90-day

Result: negative

Method: OECD Test Guideline 474

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Repeated dose toxicity

Rat

male and female

Oral

90 d

daily

NOAEL: 70 mg/kg

OECD Test Guideline 408

Subchronic toxicity

Aspiration hazard

This information is not available.

11.2 Further information

Systemic effects:

After absorption of large quantities:

Methaemoglobinemia, CNS disorders, cardiovascular disorders

Other dangerous properties can not be excluded.

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Handle in accordance with good industrial hygiene and safety practice.

SECTION 12. Ecological information

12.1 Toxicity

Toxicity to fish

semi-static test LC50 Danio rerio (zebra fish): 0,12 mg/l; 96 h

Analytical monitoring: yes

OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 Daphnia magna (Water flea): 0,48 mg/l; 48 h

Analytical monitoring: yes

OECD Test Guideline 202

Toxicity to algae

static test EC50 Pseudokirchneriella subcapitata (algae): 10,17 mg/l; 72 h

Analytical monitoring: yes

OECD Test Guideline 201

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)

flow-through test NOEC Daphnia magna (Water flea): 0,135 mg/l; 21 d

Analytical monitoring: yes

OECD Test Guideline 211

12.2 Persistence and degradability

Biodegradability

24,7 %; 28 d

OECD Test Guideline 301B

Not readily biodegradable.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 2,94

(calculated)

(Lit.) Bioaccumulation is not expected.

12.4 Mobility in soil

No information available.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.6 Other adverse effects

Additional ecological information

Discharge into the environment must be avoided.

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SECTION 13. Disposal considerations

Waste treatment methods

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

Land transport (ADR/RID)

14.1 UN number UN 2923
14.2 Proper shipping name CORROSIVE SOLID, TOXIC, N.O.S. (4-TERT-BUTYLPYROCATECHOL)
14.3 Class 8 (6.1)
14.4 Packing group III
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
Tunnel restriction code E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number UN 2923
14.2 Proper shipping name CORROSIVE SOLID, TOXIC, N.O.S. (4-TERT-BUTYLPYROCATECHOL)
14.3 Class 8 (6.1)
14.4 Packing group III
14.5 Environmentally hazardous yes
14.6 Special precautions for user no

Sea transport (IMDG)

14.1 UN number UN 2923
14.2 Proper shipping name CORROSIVE SOLID, TOXIC, N.O.S. (4-TERT-BUTYLPYROCATECHOL)
14.3 Class 8 (6.1)
14.4 Packing group III
14.5 Environmentally hazardous yes
14.6 Special precautions for user yes
EmS F-A S-B

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14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not relevant

SECTION 15. Regulatory information

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

EU regulations

Major Accident Hazard SEVESO III
Legislation ENVIRONMENTAL HAZARDS
E1
Quantity 1: 100 t
Quantity 2: 200 t

Occupational restrictions Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer not regulated

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC not regulated

Substances of very high concern (SVHC) This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1\%$ (w/w).

National legislation

Storage class 6.1C

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out.

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SECTION 16. Other information

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

H302	Harmful if swallowed.
H312	Harmful in contact with skin.
H314	Causes severe skin burns and eye damage.
H317	May cause an allergic skin reaction.
H400	Very toxic to aquatic life.
H411	Toxic to aquatic life with long lasting effects.

Training advice

Provide adequate information, instruction and training for operators.

Labelling

Hazard pictograms



Signal word

Danger

Hazard statements

H302 + H312 Harmful if swallowed or in contact with skin.
H314 Causes severe skin burns and eye damage.
H317 May cause an allergic skin reaction.
H400 Very toxic to aquatic life.
H411 Toxic to aquatic life with long lasting effects.

Precautionary statements

Prevention

P273 Avoid release to the environment.

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

Response

P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/physician.

Contains: 4-tert-butylpyrocatechol

Key or legend to abbreviations and acronyms used in the safety data sheet

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Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.