SAFETY DATA SHEET

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

1.1 Product identifiers

Product name: 4-tert-Butylcatechol
Product Number: 19670
Brand: Aldrich
CAS-No.: 98-29-3

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO  63103
UNITED STATES
Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 4), H302
Acute toxicity, Dermal (Category 4), H312
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Skin sensitization (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.

2.2 GHS Label elements, including precautionary statements
2.3 **Hazards not otherwise classified (HNOC) or not covered by GHS** - none

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-tert-butylpyrocatechol</td>
<td>Acute Tox. 4; Skin Corr. 1B; Eye Dam. 1; Skin</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

Formula: $C_{10}H_{14}O_2$

Molecular weight: 166.22 g/mol

CAS-No.: 98-29-3

EC-No.: 202-653-9

The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada
SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Call in physician.

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

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

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

4.2 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

4.3 Indication of any immediate medical attention and special treatment needed
No data 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
Carbon oxides
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.

For the full text of the H-Statements mentioned in this Section, see Section 16.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 **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.

5.4 **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. For personal protection 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**
For disposal see section 13.

### SECTION 7: Handling and storage

7.1 **Precautions for safe handling**

**Advice on safe handling**
Work under hood. Do not inhale substance/mixture.

**Hygiene measures**
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**

**Storage conditions**
Tightly closed. Dry. hygroscopic

**Storage class**
Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

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

<table>
<thead>
<tr>
<th>Ingredients with workplace control parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component</td>
</tr>
<tr>
<td>4-tert- butylpyrocatechol</td>
</tr>
</tbody>
</table>

Remarks: Skin Dermal Sensitization Notation

8.2 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). Tightly fitting safety goggles.

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 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: Nitrile rubber
Minimum layer thickness: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

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: 0.11 mm
Break through time: 480 min
Material tested: KCL 741 Dermatril® L

Body Protection
protective clothing

Respiratory protection
required when dusts 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.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: flakes
   Color: white

b) Odor
   phenol-like

c) Odor Threshold
   No data available

d) pH
   No data available

e) Melting point/freezing point
   Melting point/range: 53 - 58 °C (127 - 136 °F)

f) Initial boiling point and boiling range
   285 °C 545 °F - lit.

g) Flash point
   113 °C (235 °F) - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   No data available

k) Vapor pressure
   0.001 - 0.011 hPa at 30.35 - 50.15 °C (86.63 - 122.27 °F)

l) Vapor density
   No data available

m) Density
   1.08 kg/m3 at 20 °C (68 °F) - OECD Test Guideline 109
   Relative density
   No data available

n) Water solubility
   4.2 g/l at 20 °C (68 °F) - OECD Test Guideline 105 - soluble

o) Partition coefficient:
   n-octanol/water
   log Pow: 1.98 at 25 °C (77 °F) - Bioaccumulation is not expected.

p) Autoignition temperature
   435 °C (815 °F) at 996 - 1,000 hPa

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   Not explosive

t) Oxidizing properties
   none

9.2 Other safety information

No data available
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.

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

10.3 Possibility of hazardous reactions
Violent reactions possible with:
Strong oxidizing agents
bases
Strong acids

10.4 Conditions to avoid
Avoid moisture.
Strong heating.

10.5 Incompatible materials
Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - male and female - 815 mg/kg
(OECD Test Guideline 401)
Inhalation: No data available
LD50 Dermal - Rat - male and female - 1,331 mg/kg
(OECD Test Guideline 402)
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Causes burns. - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Irreversible effects on the eye
(OECD Test Guideline 405)

Respiratory or skin sensitization
Maximization Test - Guinea pig
Result: positive
(OECD Test Guideline 406)

**Germ cell mutagenicity**
Test Type: Ames test
Test system: Salmonella typhimurium
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative

Test Type: In vivo micronucleus test
Species: Rat
Cell type: Bone marrow
Application Route: Oral
Method: OECD Test Guideline 474
Result: negative

**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.
NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**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**
No data available

11.2 Additional Information
RTECS: UX1400000
Cough, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

**SECTION 12: Ecological information**

12.1 Toxicity
Toxicity to fish
semi-static test LC50 - Danio rerio (zebra fish) - 0.12 mg/l - 96 h (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 (OECD Test Guideline 202)

Toxicity to algae
static test ErC50 - Pseudokirchneriella subcapitata (algae) - 10.17
mg/l - 72 h  
(OECD Test Guideline 201)

static test NOEC - Pseudokirchneriella subcapitata - 0.2 mg/l - 72 h  
(OECD Test Guideline 201)

Toxicity to bacteria  
static test EC50 - activated sludge - 16 mg/l - 3 h  
(OECD Test Guideline 209)

static test NOEC - activated sludge - 0.6 mg/l - 3 h  
(OECD Test Guideline 209)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)  
flow-through test NOEC - Daphnia magna (Water flea) - 0.135 mg/l - 21 d  
(OECD Test Guideline 211)

Toxicity to bacteria

**12.2 Persistence and degradability**

Biodegradability

aerobic - Exposure time 28 d  
Result: 24.7 % - Not readily biodegradable.  
(OECD Test Guideline 310)

**12.3 Bioaccumulative potential**

No data available

**12.4 Mobility in soil**

No data available

**12.5 Results of PBT and vPvB assessment**

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

**12.6 Endocrine disrupting properties**

No data available

**12.7 Other adverse effects**

Discharge into the environment must be avoided.

**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**

**Product**

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

**SECTION 14: Transport information**

**DOT (US)**

UN number: 3261   Class: 8   Packing group: II  
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-tert-butylpyrocatechol)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

Aldrich - 19670  
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IMDG
UN number: 3261  Class: 8  Packing group: II EMS-No: F-A, S-B
Proper shipping name: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (4-tert-butylpyrocatechol)
Marine pollutant: yes

IATA
UN number: 3261  Class: 8  Packing group: II
Proper shipping name: Corrosive solid, acidic, organic, n.o.s. (4-tert-butylpyrocatechol)

SECTION 15: Regulatory information

SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components

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Pennsylvania Right To Know Components

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SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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