

## SAFETY DATA SHEET

Version 8.4  
Revision Date 11/19/2021  
Print Date 05/28/2022

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2,4,6-Trimethylphenol

Product Number : T79006  
Brand : Aldrich  
CAS-No. : 527-60-6

**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)**

Skin irritation (Category 2), H315  
Serious eye damage (Category 1), H318  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335  
Specific target organ toxicity - repeated exposure, Oral (Category 2), Stomach, H373  
Short-term (acute) aquatic hazard (Category 2), H401  
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**

Pictogram



Signal word

Danger

Aldrich - T79006

Page 1 of 10

|                            |                                                                                                                                                                            |
|----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Hazard statement(s)        |                                                                                                                                                                            |
| H315                       | Causes skin irritation.                                                                                                                                                    |
| H318                       | Causes serious eye damage.                                                                                                                                                 |
| H335                       | May cause respiratory irritation.                                                                                                                                          |
| H373                       | May cause damage to organs (Stomach) through prolonged or repeated exposure if swallowed.                                                                                  |
| H411                       | Toxic to aquatic life with long lasting effects.                                                                                                                           |
| Precautionary statement(s) |                                                                                                                                                                            |
| P260                       | Do not breathe dust/ fume/ gas/ mist/ vapors/ 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/ eye protection/ face protection.                                                                                                                   |
| P302 + P352                | IF ON SKIN: Wash with plenty of soap and water.                                                                                                                            |
| P304 + P340 + P312         | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.                                                |
| P305 + P351 + P338 + P310  | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor. |
| P314                       | Get medical advice/ attention if you feel unwell.                                                                                                                          |
| P332 + P313                | If skin irritation occurs: Get medical advice/ attention.                                                                                                                  |
| P362                       | Take off contaminated clothing and wash before reuse.                                                                                                                      |
| P391                       | Collect spillage.                                                                                                                                                          |
| P403 + P233                | Store in a well-ventilated place. Keep container tightly closed.                                                                                                           |
| P405                       | Store locked up.                                                                                                                                                           |
| P501                       | Dispose of contents/ container to an approved waste disposal plant.                                                                                                        |

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                    |
|------------------|------------------------------------|
| Synonyms         | : Mesityl                          |
| Formula          | : C <sub>9</sub> H <sub>12</sub> O |
| Molecular weight | : 136.19 g/mol                     |
| CAS-No.          | : 527-60-6                         |
| EC-No.           | : 208-419-2                        |

| Component                    | Classification                                                                                                          | Concentration |
|------------------------------|-------------------------------------------------------------------------------------------------------------------------|---------------|
| <b>2,4,6-Trimethylphenol</b> |                                                                                                                         |               |
|                              | Skin Irrit. 2; Eye Dam. 1; STOT SE 3; STOT RE 2; Aquatic Acute 2; Aquatic Chronic 2; H315, H318, H335, H373, H401, H411 | <= 100 %      |

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

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.

#### 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: immediately make victim drink water (two glasses at most). Consult a physician.

### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) 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.

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.

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## **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.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

For precautions see section 2.2.

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

#### **Storage conditions**

Tightly closed. Dry.

#### **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

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **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**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact

with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### **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.

### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

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

- |                                            |                                                       |
|--------------------------------------------|-------------------------------------------------------|
| a) Appearance                              | Form: powder<br>Color: light brown                    |
| b) Odor                                    | No data available                                     |
| c) Odor Threshold                          | No data available                                     |
| d) pH                                      | No data available                                     |
| e) Melting point/freezing point            | Melting point/range: 71 - 74 °C (160 - 165 °F) - lit. |
| f) Initial boiling point and boiling range | 220 °C 428 °F - lit.                                  |
| g) Flash point                             | No data available                                     |
| 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                               | No data available |
| l) | Vapor density                                | No data available |
| m) | Density                                      | No data available |
|    | Relative density                             | No data available |
| n) | Water solubility                             | No data available |
| o) | Partition coefficient: n-octanol/water       | No data available |
| p) | Autoignition temperature                     | No data available |
| q) | Decomposition temperature                    | No data available |
| r) | Viscosity                                    | No data available |
| s) | Explosive properties                         | No data available |
| t) | Oxidizing properties                         | No data available |

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

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

No data available

### 10.4 Conditions to avoid

no information available

### 10.5 Incompatible materials

Strong oxidizing agents Bases, Acid chlorides, Acid anhydrides, Oxidizing agents, Brass, Copper

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - > 2,000 mg/kg  
(OECD Test Guideline 423)

Inhalation: No data available

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg  
(OECD Test Guideline 402)

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: slight irritation - 4 h  
(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive to eyes  
(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: Not a skin sensitizer.  
(OECD Test Guideline 406)

#### Germ cell mutagenicity

In vivo tests did not show mutagenic effects

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 476

Result: Equivocal evidence.

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Bone marrow

Application Route: Intraperitoneal

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**

Inhalation - May cause respiratory irritation. - Upper respiratory tract

**Specific target organ toxicity - repeated exposure**

Oral - May cause damage to organs through prolonged or repeated exposure. - Stomach

**Aspiration hazard**

No data available

**11.2 Additional Information**

Repeated dose toxicity - Rat - male and female - Oral - 42 d - NOAEL (No observed adverse effect level) - 10 mg/kg

RTECS: OX6590000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**SECTION 12: Ecological information**

**12.1 Toxicity**

|                                                     |                                                                                                                                                                                                                               |
|-----------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Toxicity to fish                                    | static test LC50 - Oncorhynchus mykiss (rainbow trout) - 9.7 mg/l - 96 h<br>(OECD Test Guideline 203)                                                                                                                         |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna Straus (Water flea) - 3.403 mg/l - 48 h<br>(OECD Test Guideline 202)                                                                                                                         |
| Toxicity to algae                                   | static test ErC50 - Pseudokirchneriella subcapitata (algae) - 5.59 mg/l - 72 h<br>(OECD Test Guideline 201)<br><br>static test NOEC - Pseudokirchneriella subcapitata (algae) - 1.61 mg/l - 72 h<br>(OECD Test Guideline 201) |
| Toxicity to bacteria                                | static test EC50 - activated sludge - > 100 mg/l - 3 h<br>(OECD Test Guideline 209)                                                                                                                                           |

**12.2 Persistence and degradability**

Biodegradability      aerobic - Exposure time 28 d  
Result: 11.3 % - Not readily biodegradable.  
(OECD Test Guideline 301D)

**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

No data available

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## 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. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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## SECTION 14: Transport information

### DOT (US)

UN number: 2430    Class: 8    Packing group: III  
Proper shipping name: Alkylphenols, solid, n.o.s.  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

UN number: 2430    Class: 8    Packing group: III    EMS-No: F-A, S-B  
Proper shipping name: ALKYLPHENOLS, SOLID, N.O.S. (2,4,6-Trimethylphenol)  
Marine pollutant : yes

### IATA

UN number: 2430    Class: 8    Packing group: III  
Proper shipping name: Alkylphenols, solid, n.o.s.

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## 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

No components are subject to the Massachusetts Right to Know Act.

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

2,4,6-Trimethylphenol

CAS-No.  
527-60-6

Revision Date

**New Jersey Right To Know Components**

2,4,6-Trimethylphenol

CAS-No.  
527-60-6

Revision Date

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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](http://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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