

• SAFETY DATA SHEET

Version 6.7
Revision Date 11/06/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : 3,5-Dimethylphenol

Product Number : 144134

Brand : Aldrich

Index-No. : 604-037-00-9

CAS-No. : 108-68-9

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Acute toxicity (Oral) : Category 3

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Acute toxicity (Dermal) : Category 3
Skin corrosion : Category 1B
Serious eye damage : Category 1
Short-term (acute) aquatic hazard : Category 2

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements : H301 + H311 Toxic if swallowed or in contact with skin.
H314 Causes severe skin burns and eye damage.
H401 Toxic to aquatic life.

Precautionary statements :

Prevention:

P260 Do not breathe dust.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response:

P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
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.
P362 Take off contaminated clothing and wash before reuse.

Storage:

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 108-68-9

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
3,5-Xylenol	108-68-9*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

- General advice : First aiders need to protect themselves.
Show this 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 : If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.
Do not attempt to neutralise.
- Most important symptoms and effects, : The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in

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both acute and delayed	section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO ₂) Dry powder
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Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
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Specific hazards during fire fighting	: Combustible.
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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.

Hazardous combustion products	: Carbon oxides
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Specific extinguishing methods	: No data available
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Further information	: Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.
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Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.
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SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	: Do not let product enter drains.
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 carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion	: Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Further information on storage conditions	: Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.
Storage class	: 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials
Recommended storage temperature	: Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible	Basis
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			concentration	
3,5-Xylenol	108-68-9	TWA (Inhalable fraction and vapor)	1 ppm	ACGIH

Engineering measures : No data available

Personal protective equipment

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.

Recommended Filter type: : Filter type P3

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.

Hand protection

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Full contact
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber
Break through time : 480 min
Glove thickness : 0.11 mm
Protective index : Splash contact
Manufacturer : KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.
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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Eye 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 and body protection	: Flame retardant antistatic protective clothing.
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: crystalline
Color	: beige
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: 149 - 151 °F / 65 - 66 °C 142 - 147 °F / 61 - 64 °C Method: lit.
Boiling point/boiling range	: 432 °F / 222 °C Method: lit.
Flash point	: 180 °F / 82 °C
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: 1.4 %(V)
Vapor pressure	: 0.05 hPa (77 °F / 25 °C)

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Relative vapour density	: No data available
Relative density	: No data available
Density	: No data available
Water solubility	: No data available
Partition coefficient: n-octanol/water	: log Pow: 2.35 (77 °F / 25 °C)
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 122.16 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

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.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Violent reactions possible with: Bases Acid chlorides

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Acid anhydrides
Oxidizing agents
Copper

Conditions to avoid : Strong heating.

Incompatible materials : No data available

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

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - 100.1 mg/kg
(Expert judgement)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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

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

Inhalation: Corrosive to respiratory system.

Acute toxicity estimate Dermal - 300.1 mg/kg
(Expert judgement)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Skin corrosion/irritation

Remarks: Causes skin burns.

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

Maximisation Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative

Carcinogenicity

- IARC: No component 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 component 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: ZE6475000

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Systemic effects:

After absorption:

Headache
Dizziness
inebriation
Nausea
Vomiting
Convulsions
Drowsiness
Unconsciousness
Circulatory collapse
respiratory arrest
death

Damage to:

Kidney

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

3,5-Xylenol:

Toxicity to fish	: LC50 (Carassius auratus (goldfish)): 22 mg/l Exposure time: 96 h Remarks: (ECOTOX Database) LC50 (Oncorhynchus mykiss (rainbow trout)): 13 mg/l Exposure time: 96 h Remarks: (IUCLID)
Toxicity to daphnia and other aquatic invertebrates	: EC50 (Daphnia magna (Water flea)): 7.7 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes
Toxicity to algae/aquatic plants	: ErC50 (Pseudokirchneriella subcapitata): > 22 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes

Ecotoxicology Assessment

Chronic aquatic toxicity : This product has no known ecotoxicological effects.

Persistence and degradability

Components:

3,5-Xylenol:

Biodegradability	: aerobic Inoculum: activated sludge Chemical oxygen demand Result: Readily biodegradable. Biodegradation: ca. 89.3 % Exposure time: 2 d Remarks: (ECHA)
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Bioaccumulative potential

Components:

3,5-Xylenol:

Partition coefficient: n-octanol/water : log Pow: 2.35 (77 °F / 25 °C)

Mobility in soil

No data available

Other adverse effects

Components:

3,5-Xylenol:

Additional ecological information : Discharge into the environment must be avoided.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : 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

International Regulations

IATA-DGR

UN/ID No. : UN 2261
Proper shipping name : Xylenols, solid
Class : 6.1
Packing group : II
Labels : Division 6.1 - Toxic substances
Packing instruction (cargo aircraft) : 676
Packing instruction (passenger aircraft) : 669

IMDG-Code

UN number : UN 2261
Proper shipping name : XYLENOLS, SOLID

Class : 6.1
Packing group : II
Labels : 6.1
EmS Code : F-A, S-A
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number : UN 2261
Proper shipping name : Xylenols, solid

Class : 6.1
Packing group : II
Labels : Division 6.1 - Toxic substances
ERG Code : 153
Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

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

SARA 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

SARA 313 : 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.

US State Regulations

Massachusetts Right To Know

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

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH : USA. ACGIH Threshold Limit Values (TLV)
ACGIH / TWA : 8-hour, time-weighted average

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United

States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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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