

MATERIAL SAFETY DATA SHEET

VANILLIN

(For Synthesis) (4-hydroxy-3-methoxybenzaldehyde)

MSDS CAS: - 121-33-5

Section 1: Chemical Product and Company Identification

Section 1: Chemical Product

Product Name: VANILLIN (For Synthesis) (4-Hydroxy-3-methoxybenzaldehyde)

CAS#: 121-33-5

Synonym: 4-Hydroxy-3-methoxybenzaldehyde; Vanillaldehyde; Vanilla; Lioxin; Methylprotocatechuic Aldehyde

Chemical Name: Vanillin

Chemical Formula: (CH₃O) (OH) C₆H₃CHO or C₈-H₈-O₃

Brand: OXFORD

Details Of The Supplier Of The Safety Data Sheet:

Company identification: **OXFORD LAB FINE CHEM LLP**
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Section 2: Composition and Information on Ingredients

Composition:

Name	CAS #	% by Weight
Vanillin	121-33-5	100

Toxicological Data on Ingredients: Vanillin: ORAL (LD₅₀): Acute: 1580 mg/kg [Rat]. 3925 mg/kg [Mouse]. 1400 mg/kg [Guinea pig]. DERMAL (LD₅₀): Acute: & gt; 5010 mg/kg [Rabbit].

Section 3: Hazards Identification

Potential Acute Health Effects:

Hazardous in case of eye contact (irritant), of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Potential Chronic Health Effects:

Slightly hazardous in case of skin contact (sensitizer). CARCINOGENIC EFFECTS: Not available. MUTAGENIC EFFECTS: Not available. TERATOGENIC EFFECTS: Not available. DEVELOPMENTAL TOXICITY: Not available.

Section 4: First Aid Measures

Eye Contact: Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Cold water may be used. Get medical attention.

Skin Contact: Wash with soap and water. Cover the irritated skin with an emollient. Get medical attention if irritation develops. Cold water may be used.

Serious Skin Contact: Not available.

Inhalation: If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.

Serious Inhalation: Not available.

Ingestion: Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Serious Ingestion: Not available.

Section 5: Fire and Explosion Data

Flammability of the Product: May be combustible at high temperature.

Auto-Ignition Temperature: Not available.

Flash Points: Not available.

Flammable Limits: Not available.

Section 5: Fire and Explosion Data (Continued)

Products of Combustion: These products are carbon oxides (CO, CO₂).

Fire Hazards in Presence of Various Substances:

Slightly flammable to flammable in presence of heat. Non-flammable in presence of shocks.

Explosion Hazards in Presence of Various Substances:

Risks of explosion of the product in presence of mechanical impact: Not available. Risks of explosion of the product in presence of static discharge: Not available.

Fire Fighting Media and Instructions:

SMALL FIRE: Use DRY chemical powder. LARGE FIRE: Use water spray, fog or foam. Do not use water jet.

Special Remarks on Fire Hazards:

When heated to decomposition it emits acrid smoke and irritating fumes.

Special Remarks on Explosion Hazards: Not applicable.

Section 6: Accidental Release Measures

Small Spill:

Use appropriate tools to put the spilled solid in a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and dispose of according to local and regional authority requirements.

Large Spill:

Use a shovel to put the material into a convenient waste disposal container. Finish cleaning by spreading water on the contaminated surface and allow to evacuate through the sanitary system.

Section 7: Handling and Storage

Precautions:

Keep away from heat. Keep away from sources of ignition. Empty containers pose a fire risk, evaporate the residue under a fume hood. Ground all equipment containing material. Do not ingest. Do not breathe dust. Avoid contact with eyes. Wear suitable protective clothing. If ingested, seek medical advice immediately and show the container or the label.

Section 7: Handling and Storage (Continued)

Storage:

Keep container tightly closed. Keep container in a cool, well-ventilated area. Moisture sensitive. Sensitive to light. Store in light-resistant containers.

Section 8: Exposure Controls/Personal Protection

Engineering Controls:

Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protection:

Splash goggles. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Gloves.

Personal Protection in Case of a Large Spill:

Splash goggles. Full suit. Dust respirator. Boots. Gloves. A self-contained breathing apparatus should be used to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

Exposure Limits: Not available.

Section 9: Physical and Chemical Properties

Physical state and appearance: Solid.

Odor: pleasant aromatic vanilla odor

Taste: pleasant vanilla taste

Molecular Weight: 152.15 g/mole

Color: White to yellowish.

pH (1% soln/water): Not available.

Boiling Point: 285°C (545°F)

Melting Point: 80°C (176°F)

Critical Temperature: Not available.

Specific Gravity: 1.056 (Water = 1)

Vapor Pressure: Not applicable.

Section 9: Physical and Chemical Properties (Continued)

Vapor Density: 5.2 (Air = 1)

Volatility: Not available.

Odor Threshold: Not available.

Water/Oil Dist. Coeff.: The product is more soluble in oil; $\log(\text{oil/water}) = 1.4$

Ionicity (in Water): Not available.

Dispersion Properties: See solubility in water, diethyl ether, acetone.

Solubility: Soluble in cold water, diethyl ether, acetone. Very soluble in hot benzene, and petroleum ether. Freely soluble in chloroform, carbon disulfide, glacial acetic acid, pyridine. Soluble in oils, and in aqueous solutions of alkali hydroxides.

Solubility in water: 1gram dissolves in 100 ml of water and 16 ml of water @ 80 C.; 11 grams dissolves in 1 liter of water @ 25 C.

Section 10: Stability and Reactivity Data

Stability: The product is stable.

Instability Temperature: Not available.

Conditions of Instability: Excessive heat, incompatible materials, light, moisture

Incompatibility with various substances: Reactive with oxidizing agents, reducing agents, alkalis.

Corrosivity: Non-corrosive in presence of glass.

Special Remarks on Reactivity: Can react violently with Br₂; HClO₄; potassium-tert-butoxide; tert-chlorobenzene + NaOH; formic acid + thallium nitrate. Also incompatible with perchloric acid Moisture sensitive. Sensitive to light.

Special Remarks on Corrosivity: Not available.

Polymerization: Will not occur.

Section 11: Toxicological Information

Routes of Entry: Inhalation. Ingestion.

Toxicity to Animals: Acute oral toxicity (LD₅₀): 1400 mg/kg [Guinea pig]. Acute dermal toxicity (LD₅₀): >5010 mg/kg [Rabbit].

Chronic Effects on Humans: Not available.

Other Toxic Effects on Humans: Hazardous in case of ingestion, of inhalation. Slightly hazardous in case of skin contact (irritant, permeator).

Special Remarks on Toxicity to Animals: Not available.

Special Remarks on Chronic Effects on Humans: May affect genetic material (mutagenic). May cause adverse reproductive effects based on animal test data.

Section 11: Toxicological Information (Continued)

Special Remarks on other Toxic Effects on Humans:

Acute Potential Health Effects: It may cause eye, skin, respiratory tract, and mucous membrane irritation. It may be absorbed by the skin. Ingestion may cause gastrointestinal tract irritation and affect the cardiovascular system, respiration, liver (jaundice), urinary system, behavior/nervous system (muscle weakness, somnolence, coma). **Chronic Potential Health Effects:** Inhalation: Prolonged or repeated inhalation may affect the brain and blood (changes in white and red blood cell count). Ingestion: Prolonged or repeated ingestion may affect the urinary system, liver, heart, and metabolism (weight loss).

Section 12: Ecological Information

Ecotoxicity: Not available.

BOD5 and COD: Not available.

Products of Biodegradation: Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

Toxicity of the Products of Biodegradation: The products of degradation are more toxic.

Special Remarks on the Products of Biodegradation: Not available.

Section 13: Disposal Considerations

Waste Disposal:

Waste must be disposed of in accordance with federal, state and local environmental control regulations.

Section 14: Transport Information

Land transport (ADR-RID)

General information: Not regulated.

Sea transport (IMDG) [English only]

General information: Not regulated.

Air transport (ICAO-IATA) [English only]

General information: Not regulated.

Section 15: Other Regulatory Information

Federal and State Regulations:

TSCA 8(b) inventory: Vanillin TSCA 8(a) PAIR: Vanillin TSCA 8(d) H and S data reporting: Vanillin:
effective date: 9/30/91; sunset date: 6/30/98

Other Regulations:

Canadian DSL: This product on the Canadian Domestic Substances List. EINECS: This product is on the European Inventory of Existing Commercial Chemical Substances.

Other Classifications:

WHMIS (Canada): Not controlled under WHMIS (Canada).

DSCL (EEC): R22- Harmful if swallowed. R36- Irritating to eyes. S2- Keep out of the reach of children. S24/25- Avoid contact with skin and eyes. S46- If swallowed, seek medical advice immediately and show this container or label.

HMIS (U.S.A.):

Health Hazard: 2

Fire Hazard: 1

Reactivity: 0

Personal Protection: E

National Fire Protection Association (U.S.A.):

Health: 2

Flammability: 1

Reactivity: 0

Specific hazard:

Protective Equipment:

Gloves. Lab coat. Dust respirator. Be sure to use an approved/certified respirator or equivalent. Splash goggles.

Section 16 - Additional Information

References: Not available.

Other Special Considerations: Not available.

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