



## Expert Synthesis Solutions

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## SAFETY DATA SHEET

Version: 2

Revision Date: 01/19/18

### SECTION 1: PRODUCT IDENTIFICATION

**Product Name:** 4-Isothiocyanato-3,5-dimethylphenol  
**Catalog No.:** ESS0028  
**Product Use:** For laboratory research purposes

### SECTION 2: HAZARDS IDENTIFICATION

**WHMIS Classification:** CLASS D1B: Toxic material causing immediate and serious toxic effects. Toxic by ingestion.

**GHS Classification:** Acute toxicity, oral (Category 3)

**GHS Label elements:**

**Pictogram:**



**Signal word:** Danger

**Hazard statement:**

H301: Toxic if swallowed.  
H315: Causes skin irritation.  
H319: Causes serious eye irritation.  
H335: May cause respiratory irritation.

**Precautionary statement:**

P261: Avoid breathing dust/fume/gas/mist/vapours/spray.  
P264: Wash skin thoroughly after handling.  
P270: Do not eat, drink or smoke when using this product.  
P271: Use only outdoors or in a well-ventilated area.  
P280: Wear protective gloves/eye protection/face protection.

**Response statements:**

P301+P310+P330: IF SWALLOWED: Immediately call POISON CENTER/doctor. Rinse mouth.  
P302+P352: IF ON SKIN: Wash with plenty of 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: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

**Potential Health Effects**

**Inhalation:**

Harmful in case of inhalation. Causes respiratory tract irritation.

**Skin:**

May be harmful if absorbed through skin. Cause skin irritation.

**Eyes:**

Causes eye irritation.

**Ingestion:**

Harmful if swallowed.

**Other hazards:**

No data available.

### SECTION 3: COMPOSITION / INFORMATION ON INGREDIENTS

**Synonyms:** 4-Isothiocyanato-3,5-dimethylphenol, 4-Hydroxy-2,6-dimethylphenylisothiocyanate, 4-Hydroxy Xylazine metabolite.

**Formula:** C<sub>9</sub>H<sub>9</sub>NOS

**Molecular Weight:** 179.24

**CAS No.:** 1246818-00-7

### SECTION 4: FIRST AID MEASURES

**General Advice:** Consult a physician. Show this SDS. Move out of dangerous area.

**If Inhaled:** Allow the victim to rest in a well-ventilated area. Seek immediate medical attention.

**In case of skin contact:** After contact with skin, wash immediately with plenty of water. Gently and thoroughly wash the contaminated skin with running water and non-abrasive soap. Be particularly careful to clean folds, crevices, creases and groin. Cold water may be used. Cover the irritated skin with an emollient. If irritation persists, seek medical attention. Wash contaminated clothing before reusing.

**In case of eye contact:** Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Do not use an eye ointment. Seek medical attention.

**If swallowed:** Do not induce vomiting. Rinse mouth with water. Examine the lips and mouth to ascertain whether the tissues are damaged, a possible indication that the toxic material was ingested; the absence of such signs, however, is not conclusive. Loosen tight clothing such as a collar, tie, belt or waistband. If the victim is not breathing, perform mouth-to-mouth resuscitation. Seek immediate medical attention.

### SECTION 5: FIRE FIGHTING MEASURES

**Conditions of flammability:** Not flammable or combustible.

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

**Special protective equipment for firefighters:** Wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. During a fire, toxic gases may be generated by thermal decomposition or combustion.

**Hazardous combustion products:** Hazardous decomposition products formed under fire conditions: carbon oxides (CO, CO<sub>2</sub>), Sulphur oxides, Nitrogen oxides.

**Explosion data:** No data available.



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### SECTION 6: ACCIDENTAL RELEASE MEASURES

<b>Personal precautions:</b>	Use proper personal protective equipment as indicated in section 8.
<b>Environmental precautions:</b>	Clean up spills immediately, observing precautions in the Protective Equipment section. Do not let product enter drains.
<b>Methods and materials for containment and cleaning up:</b>	Sweep up, and then place into a suitable container for disposal.

### SECTION 7: HANDLING AND STORAGE

<b>Precautions for safe handling:</b>	Keep away from heat. Keep away from sources of ignition. Avoid formation of dust and aerosols. Provide appropriate exhaust ventilation where dust is formed. Ground all equipment containing material. Do not ingest. Do not breathe dust. Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and show the container or the label. Avoid contact with skin and eyes.
<b>Conditions for safe storage:</b>	Keep container tightly closed in a dry and well ventilated place. Ground all equipment containing material. Recommended long term storage temperature 2-8°C.

### SECTION 8: EXPOSURE CONTROL / PERSONAL PROTECTION

<b>Engineering Controls:</b>	Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits.
<b>Personal protective equipment</b>	
<b>Respiratory protection:</b>	Wear a NIOSH/MSHA or European Standard EN 149 approved full-facepiece airline respirator in the positive pressure mode with emergency escape provisions.
<b>Hand protection:</b>	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.
<b>Eye protection:</b>	Wear safety glasses with side-shields conforming to EN166 Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN166 (EU).
<b>Skin and body protection:</b>	Wear appropriate gloves and clothing to prevent skin exposure.
<b>Hygiene measures:</b>	Handle in accordance with good industrial hygiene and safety practice. Wash hands before break and after the end of work day.

### SECTION 9: PHYSICAL & CHEMICAL PROPERTIES

<b>Appearance:</b>	Pale yellow solid.
<b>Odour:</b>	No data available.
<b>Odour threshold:</b>	No data available.
<b>pH:</b>	No data available.
<b>Melting point/Freezing point:</b>	No data available.
<b>Initial boiling point/boiling range:</b>	No data available.
<b>Flash point:</b>	No data available.
<b>Evaporation rate:</b>	No data available.
<b>Flammability (solid; gas):</b>	No data available.
<b>Lower flammable/explosive limit:</b>	No data available.
<b>Upper flammable/explosive limit:</b>	No data available.
<b>Vapour pressure:</b>	No data available.
<b>Vapour density:</b>	No data available.
<b>Solubility:</b>	Chloroform, DMSO, Methanol
<b>Partition coefficient – n-octanol/water:</b>	No data available.
<b>Autoignition temperature:</b>	No data available.
<b>Decomposition temperature:</b>	No data available.
<b>Viscosity:</b>	No data available.

### SECTION 10: STABILITY & REACTIVITY

<b>Chemical stability:</b>	Stable under recommended storage conditions.
<b>Conditions to avoid:</b>	Not available.
<b>Possibility of hazardous reactions:</b>	No data available.
<b>Incompatibilities:</b>	Strong oxidizing agents.
<b>Hazardous decompositions products:</b>	Hazardous decomposition products formed under fire conditions: carbon oxides (CO, CO <sub>2</sub> ), Sulphur oxides, nitrogen oxides.

### SECTION 11: TOXICOLOGICAL INFORMATION

<b>Acute Toxicity:</b>	No data available.
<b>Potential health effects:</b>	
<b>Inhalation:</b>	Harmful in case of inhalation. Causes respiratory tract irritation.
<b>Skin:</b>	May be harmful if absorbed through skin. Cause skin irritation.
<b>Eyes:</b>	Causes eye irritation.
<b>Ingestion:</b>	Harmful if swallowed.
<b>Signs and symptoms of exposure:</b>	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**

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<b>Ecotoxicity:</b>	No data available.
<b>Persistence and degradability:</b>	No data available.
<b>Bioaccumulative potential:</b>	No data available.
<b>Mobility in soil:</b>	No data available.
<b>Other adverse effects:</b>	An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

**SECTION 13: DISPOSAL CONSIDERATION**

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<b>Product:</b>	Dispose in a manner consistent with federal, state, and local regulations.
<b>Contaminated packaging:</b>	Dispose of as unused product.

**SECTION 14: TRANSPORT INFORMATION**

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<b>TDG (Canada):</b>	UN2811
<b>DOT (US):</b>	UN2811
<b>IMDG:</b>	UN2811
<b>IATA:</b>	UN2811
<b>UN number:</b>	UN2811
<b>UN proper shipping name:</b>	4-Isothiocyano-3,5-dimethylphenol, organic compound, toxic solid.
<b>Transport hazard class:</b>	6.1
<b>Packing group:</b>	III
<b>Special precautions:</b>	Ship at room temperature.

**SECTION 15: REGULATORY INFORMATION**

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<b>General:</b>	WHMIS CLASS D1B: Toxic material causing immediate and serious toxic effects. Toxic by ingestion.
<b>DSL/NDSL (Canada):</b>	This product is not listed on the Canadian DSL/NDSL.
<b>TSCA (US):</b>	This product is not listed on the US EPA TSCA.
<b>ECHA (EU):</b>	A component of this product is listed on the EU ECHA.

**SECTION 16: OTHER INFORMATION**

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**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 regards to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Expert Synthesis Solutions shall not be held liable for any damage resulting from handling or from contact with the above product.