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## Safety Data Sheet

### 1. Identification of the substance/mixture and of the company/undertaking

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#### 1.1. Product identifier

Product name: ROX NHS ester, 6-isomer  
Catalog number(s): 12220, 22220, 42220, 52220, 62220  
Substance name: ROX NHS ester, 6-isomer  
Molecular formula: C<sub>37</sub>H<sub>33</sub>N<sub>3</sub>O<sub>7</sub>  
Molecular weight: 631.67  
CAS number: 117491-83-5; 1890922-83-4; 216699-36-4  
EC number: N/A  
REACH registration number: N/A

**1.2. Relevant identified uses of the substance or mixture and uses advised against**  
Analytical reagent. Reagent for research and development.

#### 1.3. Details of the supplier of the Safety Data Sheet

Supplier: **Lumiprobe Corporation**  
115 Airport Dr Suite 160  
Westminster, Maryland 21157  
USA  
Phone: +1 888 973 6353  
Fax: +1 888 973 6354  
Email: [order@lumiprobe.com](mailto:order@lumiprobe.com)

#### 1.4. Emergency telephone number

+1 888 973 6353 ext 2; +49 (0)511 16596812

### 2. Hazards identification

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#### 2.1. Classification of the substance or mixture

The substance is not hazardous according to EU regulation (EC) No 1272/2008 or GHS regulations., and it does not contain any hazardous substance at more than 1% by weight. US Export Control Classification Number (ECCN) - EAR99 - The substance does not require a license.

#### 2.2. Label elements

Not applicable

#### 2.3. Other hazards

No other hazards identified

### 3. Composition/information on ingredients

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#### 3.1. Substances

Product name: ROX NHS ester, 6-isomer  
CAS number: 117491-83-5; 1890922-83-4; 216699-36-4  
Weight %: >95 %

#### 3.2. Mixtures

Not applicable.

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## 4. First aid measures

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### 4.1. Description of first aid measures

General notes	Wash thoroughly after use.
Inhalation	Move individual to fresh air and seek medical advice.
Skin contact	Wash affected area with water for 15 minutes and seek medical advice if irritation occurs.
Eye contact	Flush eye with water for 15 minutes and seek medical advice if irritation occurs.
Ingestion	Seek medical advice.
Self-protection of first aider	Wear protective gloves.

### 4.2. Most important symptoms and effects, both acute and delayed

We are not aware of any reported health hazards for this product.

### 4.3. Indication of any immediate medical attention and special treatment needed

No immediate medical attention or special treatment indicated.

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## 5. Firefighting measure

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### 5.1. Extinguishing media

Suitable extinguishing media Depending on the surrounding fire. The substance is not flammable.  
Unsuitable extinguishing media Not known.

### 5.2. Special hazards arising from the substance or mixture

No special fire hazards.

### 5.3. Advice for firefighters

No specific precautions arising from the substance.

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## 6. Accidental release measures

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### 6.1. Personal precautions, protective equipment and emergency procedures

For non-emergency personnel avoid breathing in dust. Wear gloves and safety glasses.  
For emergency responders avoid breathing in dust. Wear gloves and safety glasses.

### 6.2. Environmental precautions

Avoid release into environment and sewage water system.

### 6.3. Methods and material for containment and cleaning up

Small spill	Sweep up spilled substance promptly and dispose according to local regulations.
Large spill	Avoid dispersal. Sweep up spilled substance promptly and dispose according to local regulations.

### 6.4. Reference to other sections

See Section 8 for information on appropriate personal protective equipment.  
See Section 13 for additional waste treatment information.

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## 7. Handling and storage

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### 7.1. Precautions for safe handling

Wear protective equipment as specified in section 8.

Do not eat, drink and smoke in work areas. Thoroughly wash hands after use. Remove contaminated clothing and protective equipment before entering eating areas.

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

Storage: 12 months after receipt at -20°C in the dark. Transportation: at room temperature for up to 3 weeks. Avoid prolonged exposure to light. Desiccate.

### 7.3. Specific end use(s)

Analytical reagent. Reagent for research and development.

## 8. Exposure controls/personal protection

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### 8.1. Control parameters

No occupational exposure limits known.

### 8.2. Exposure controls

Appropriate engineering controls:	Work in a fume hood.
Personal protection:	Work in a fume hood with usual precautions.
Eye/face protection:	Wear safety glasses.
Skin protection:	Wear chemical-resistant gloves. Wear a lab coat and appropriate shoes.
Respiratory protection:	Work in a fume hood
Environmental exposure controls:	Do not drain into sewage system

## 9. Physical and chemical properties

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

Appearance	
Odour	Odourless
Odour threshold	Not available
pH	Not available
Melting point / freezing point	Not available
Initial boiling point and boiling range	Not available
Flash point	Substance does not sustain combustion.
Evaporation rate	Not available
Flammability (solid, gas)	Non-flammable
Upper/lower flammability or explosive limits	Not available

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Vapour pressure	Not available
Vapour density	Not available
Relative density	Not available
Solubility(ies)	good in polar organic solvents (DMF, DMSO), low in water
Partition coefficient: n-octanol/water	Not available
Auto-ignition temperature	Not available
Decomposition temperature	Not available
Viscosity	Not available
Explosive properties	Not available
Oxidising properties	Not available

## 9.2. Other information

Not applicable

## 10. Stability and Reactivity

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### 10.1. Reactivity

No specific test data available for this substance.

### 10.2. Chemical stability

The product is stable under normal conditions of storage and use.

### 10.3. Possibility of hazardous reactions

No hazardous reactions will occur under normal conditions of storage and use.

### 10.4. Conditions to avoid

No specific data.

### 10.5. Incompatible materials

No specific data.

### 10.6. Hazardous decomposition products

No dangerous decomposition products should be produced under normal conditions of storage and use.

## 11. Toxicological information

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The toxicological properties of this substance have not been thoroughly investigated.

## 12. Ecological information

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### 12.1. Toxicity

No test data available.

### 12.2. Persistence and degradability

No test data available.

### 12.3. Bioaccumulative potential

No test data available.

**12.4. Mobility in soil**

No test data available.

**12.5. Results of PBT and vPvB assessment**

No test data available.

**12.6. Other adverse effects**

No test data available.

**12.7. Additional information**

We are not aware of any ecological hazards arising from this substance.

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**13. Disposal considerations**

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**13.1. Waste treatment methods**

Waste should not be disposed of by release to sewers. Consult local, state or national regulations for applicable requirements.

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**14. Transport Information**

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**14.1. UN number**

Not regulated.

**14.2. UN proper shipping name**

Not applicable.

**14.3. Transport hazard class(es)**

Not applicable.

**14.4. Packing group**

Not applicable.

**14.5. Environmental hazards**

No.

**14.6. Special precautions for user**

Not available.

**14.7 IATA/ICAO**

Not regulated.

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**15. Regulatory information**

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**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture**

The substance is not listed under relevant regulations.

**15.2. Chemical Safety Assessment**

No Chemical Safety Assessment has been carried out for this substance by the supplier.

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**16. Other information**

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