

Safety Data Sheet

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

1.1. Product identifier

Product name: ROX alkyne, 6-isomer
Catalog number(s): A22B0, B22B0, C22B0, D22B0, E22B0, F22B0
Substance name: ROX alkyne, 6-isomer
Molecular formula: C₃₆H₃₃N₃O₄
Molecular weight: 571.68
CAS number: 2097422-22-3
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 201 International Circle, Suite 135, Hunt Valley, Maryland 21030, USA +1 888 9736353 order@lumiprobe.com | Lumiprobe GmbH Feodor-Lynen-Str. 23 30625 Hannover Germany +49 511 16596811 de@lumiprobe.com |
|-----------|--|---|

1.4. Emergency telephone number

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

2. Hazards identification

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

3.1. Substances

Product name: ROX alkyne, 6-isomer
CAS number: 2097422-22-3
Weight %: >95 %

3.2. Mixtures

Not applicable.

4. First aid measures

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.

5. Firefighting measure

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.

6. Accidental release measures

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.

7. Handling and storage

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

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

7.3. Specific end use(s)

Analytical reagent. Reagent for research and development.

8. Exposure controls/personal protection

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

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

Vapour pressure Not available

Vapour density Not available

| | |
|--|--------------------------------------|
| Relative density | Not available |
| Solubility(ies) | good in DMSO, DMF, methanol, ethanol |
| 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

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

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

12. Ecological information

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.

13. Disposal considerations

13.1. Waste treatment methods

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

14. Transport Information

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.

15. Regulatory information

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.

16. Other information

Date of issue/revision 22.02.2025

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