Material Safety Data Sheet

MRS 2279

Cat. No: 2158

Batch No: 1

(1R,2S,4S)-4-[2-Chloro-6-(methylamino)-9H-purin-9-yl]-2-(phosphonoxy)bicyclo[3.1.0]hexane-1-methanol dihydrogen phosphate ester diammonium salt

1. COMPOSITION/INFORMATION ON INGREDIENTS
For batch specific information, please see Product Information sheet.

2. PHYSICAL AND CHEMICAL PROPERTIES
For batch specific information, please see Product Information sheet.

3. HANDLING AND STORAGE
Use in a chemical fume hood, with air supplied by an independent system. Avoid inhalation, contact with eyes, skin and clothing. Avoid prolonged or repeated exposure. Material should be stored in a tightly sealed container under the storage condition stated on the Product Information sheet and on the vial label.

4. STABILITY AND REACTIVITY
Stability: Stable under normal handling conditions.

5. HAZARDS IDENTIFICATION
Exposure may cause irritation to eyes, mucous membranes, upper respiratory tract and skin.

6. TOXICOLOGICAL INFORMATION
To the best of our knowledge, the chemical, physical and toxicological properties have not been fully investigated.

RTECS No: Not assigned
Target Organs: Eyes; Respiratory system; Skin
Toxicity Data: No data available

7. REGULATORY INFORMATION
Classification: Caution: Substance not yet fully tested.
Safety Phrases: S22 - Do not breathe dust
S24/25 - Avoid contact with skin and eyes
S36/37/39 - Wear suitable protective clothing, gloves and eye/face protection
Risk Phrases:

8. EXPOSURE CONTROLS/PERSONAL PROTECTION
Wear appropriate chemical resistant gloves, safety goggles and other protective clothing to prevent contact with eyes and skin. Laboratory should be equipped with a safety shower and eye wash station. Avoid prolonged or repeated exposure. Do not breathe dust. Do not get in eyes, on skin or on clothing. Wash thoroughly after handling.

9. FIRST-AID MEASURES
In cases of SKIN CONTACT: Wash with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes and wash before wearing. In case of eye contact, flush with copious amounts of water for at least 15 minutes.

In cases of INHALATION: Remove to fresh air and monitor breathing. If breathing becomes difficult, give oxygen. If breathing stops, give artificial respiration.

In cases of INGESTION: If swallowed, rinse mouth out with water, contact local poison centre and call a physician.

10. FIRE-FIGHTING MEASURES
Extinguishing Media: Material is non-combustible. Use extinguishing media appropriate to surrounding fire conditions.

Unusual Fire and Explosive Hazards: May emit toxic gases upon thermal decomposition.

Special Fire-Fighting Procedures: Wear protective clothing to prevent contact with skin and eyes.

11. ACCIDENTAL RELEASE MEASURES
Wear appropriate protective clothing. Cover spillage with suitable absorbent material. Using non-spark tools, sweep up material and place in an appropriate container. Decontaminate spill site with 10% caustic solution and ventilate area until after disposal is complete. Hold all material for appropriate disposal as described under DISPOSAL CONDITIONS.

12. ECOLOGICAL INFORMATION
Data not yet available - treat as potentially toxic if released into the environment.

13. DISPOSAL CONDITIONS
As specific country, federal, state and local environmental regulations are varied and change frequently, we recommend that you contact your local department for Health Services for information on the correct disposal of this product.

14. TRANSPORT INFORMATION
U.N.Number: Proper Shipping Name: IATA Class: IATA Packing Group:

15. OTHER INFORMATION
Due to the nature of this material. It must only be handled by suitably qualified experienced scientists in appropriately equipped and authorised facilities. The above information is believed to be correct but does not purport to be all inclusive and should be used as a guide only for experienced personnel. Always consult your safety advisor and follow appropriate local and national safety legislation. The absence of warning must not, under any circumstance, be taken to mean that no hazard exists.

CAUTION — Not fully tested. For research use only. Not for human use.

customerservice@tocrisusa.com  www.tocris.com  customerservice@tocris.co.uk
technicalsupport@tocrisusa.com  technicalsupport@tocris.co.uk
Product Information

**MRS 2279**

(1R,2S,4S,5S)-4-[2-Chloro-6-(methylamino)-9H-purin-9-yl]-2-(phosphonooxy)bicyclo[3.1.0]hexane-1-methanol dihydrogen phosphate ester diammonium salt

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**Description:** Selective, high affinity competitive antagonist of the P2Y<sub>1</sub> receptor (K<sub>I</sub> = 2.5 nM; IC<sub>50</sub> = 51.6 nM). Fails to block nucleotide signaling at most other P2Y receptors (P2Y<sub>2</sub>, P2Y<sub>4</sub>, P2Y<sub>6</sub>, P2Y<sub>11</sub> and P2Y<sub>12</sub>) and potently inhibits ADP-induced aggregation of human blood platelets in vitro (pKB = 8.05).

**Physical and Chemical Properties:**

Batch Molecular Formula: \(\text{C}_{13}\text{H}_{18}\text{ClN}_{5}\text{O}_{8}\text{P}_{2}\cdot 2\text{NH}_{3}\cdot 2\text{H}_{2}\text{O}\)

Batch Molecular Weight: 539.81

CAS Number: [367909-40-8]

Physical Appearance: Beige solid

Batch Molecular Structure:

![Molecular Structure](image1)

**Storage:** Desiccate at -20°C

**Solubility & Usage Info:**

- **Water to 100 mM**

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**Other Information:**

**References:**


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