

Cayman Chemical Company
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108



1. Identification of the Substance/Mixture and of the Company/Undertaking

Product Code: 11102

Product Name: 3-Deazaneplanocin A (hydrochloride)

Synonyms: 5R-(4-amino-1H-imidazo[4,5-c]pyridin-1-yl)-3-(hydroxymethyl)-3-cyclopentene-1S,2R-diol, monohydrochloride; 2,3-DMMC;

Intended Use: For research use only, not for human or veterinary use.

Manufacturer Information

Company Name: Cayman Chemical Company

Emergency Contact: CHEMTREC Within USA and Canada: +1 (800)424-9300

Alternate Emergency Contact: CHEMTREC Outside USA and Canada: +1 (703)527-3887

Information: Cayman Chemical Company +1 (734)971-3335

Web site address: www.caymanchem.com

2. Hazards Identification

GHS Classification	Placard	Key word	GHS Hazard
Acute Toxicity: Oral, Category 4	Exclamation point	Warning	Harmful if swallowed

GHS Hazard Phrases: H302: Harmful if swallowed.

GHS Precaution Phrases: P264: Wash hands thoroughly after handling.

GHS Response Phrases: P301+312: IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
P330: Rinse mouth.

GHS Storage and Disposal Phrases: Please refer to Section 7 for Storage and Section 13 for Disposal information.

Route(s) of Entry: Inhalation? Yes Skin? Yes Eyes? Yes Ingestion? Yes Other: Injection

Potential Health Effects (Acute and Chronic): Harmful if swallowed.
Material may be irritating to the mucous membranes and upper respiratory tract.
May be harmful by inhalation or skin absorption.
May cause eye, skin, or respiratory system irritation.

Target Organs: No data available.

Signs and Symptoms Of Exposure: To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

Medical Conditions Generally Aggravated By Exposure: No data available.

3. Composition/Information on Ingredients

Hazardous Components (Chemical Name)	CAS #	Concentration	EC#	Risk Phrases
1. 3-Deazaneplanocin A (hydrochloride)	120964-45-6	100.0 %	NA	R22

4. First Aid Measures

Emergency and First Aid Procedures:

In Case of Inhalation: Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.

In Case of Skin Contact: Immediately wash skin with soap and plenty of water for at least 20 minutes. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

In Case of Eye Contact:	Hold eyelids apart and flush eyes with plenty of water for at least 20 minutes. Have eyes examined and tested by medical personnel.
In Case of Ingestion:	Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.
Indication of any immediate medical attention and special treatment needed:	No data available.

5. Fire Fighting Measures

Suitable Extinguishing Media:	Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray. Use water spray to cool fire-exposed containers.
Unsuitable Extinguishing Media:	A solid water stream may be inefficient.
Flammable Properties and Hazards:	No data available.
Flash Pt:	No data.
Autoignition Pt:	No data available.
Explosive Limits:	LEL: No data. UEL: No data.
Hazardous Combustion Products:	No data available.
Fire Fighting Instructions:	As in any fire, wear self-contained breathing apparatus pressure-demand (NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.

6. Accidental Release Measures

Protective Precautions, Protective Equipment and Emergency Procedures:	Avoid raising and breathing dust, and provide adequate ventilation. As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator, and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
Environmental Precautions:	Take steps to avoid release into the environment, if safe to do so.
Steps To Be Taken In Case Material Is Released Or Spilled:	Contain spill and collect, as appropriate. Transfer to a chemical waste container for disposal in accordance with local regulations.

7. Handling and Storage

Precautions To Be Taken in Handling:	Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid prolonged or repeated exposure.
Precautions To Be Taken in Storing:	Keep container tightly closed. Store in accordance with information listed on the product insert.
Hazard Label Information:	Avoid contact with skin and eyes. Do not reuse this container. Use with adequate ventilation. Wash thoroughly after handling.

8. Exposure Controls/Personal Protection

Hazardous Components (Chemical Name)	CAS #	OSHA PEL	ACGIH TLV	Other Limits
1. 3-Deazaneplanocin A (hydrochloride)	120964-45-6	No data.	No data.	No data.
Hazardous Components (Chemical Name)	CAS #	Britain EH40	France VL	Europe
1. 3-Deazaneplanocin A (hydrochloride)	120964-45-6	No data.	No data.	No data.

Protective Equipment Summary - Hazard Label Information:	Compatible chemical-resistant gloves Eye wash station in work area Lab coat Safety glasses Safety shower in work area Vent Hood
Engineering Controls (Ventilation etc.):	Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.
Eye Protection:	Safety glasses
Protective Gloves:	Compatible chemical-resistant gloves
Other Protective Clothing:	Lab coat



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Respiratory Equipment (Specify Type):	NIOSH approved respirator, as conditions warrant.
Work/Hygienic/Maintenance Practices:	Do not take internally. Facilities storing or utilizing this material should be equipped with an eyewash and a safety shower. Wash thoroughly after handling.
Environmental Exposure Controls:	No data available.

9. Physical and Chemical Properties

Information on Basic Physical and Chemical Properties

Physical States:	☐ Gas ☐ Liquid ☒ Solid
Appearance and Odor:	A crystalline solid
Melting Point:	No data.
Boiling Point:	No data.
Flash Pt:	No data.
Evaporation Rate:	No data.
Vapor Pressure (vs. Air or mm Hg):	No data.
Vapor Density (vs. Air = 1):	No data.
Specific Gravity (Water = 1):	No data.
Solubility in Water:	No data.
Solubility Notes:	~5 mg/ml in PBS (pH 7.2); ~3 mg/ml in DMSO;
Autoignition Pt:	No data.
Explosive Properties:	No data available.
Oxidizing Properties:	No data available.
Other Information	
Percent Volatile:	No data.
Formula:	C ₃₁ H ₄₃ N ₃ O ₈
Molecular Weight:	585.70

10. Stability and Reactivity

Reactivity:	No data available.
Stability:	Unstable ☐ Stable ☒
Stability Note(s):	Stable if stored in accordance with information listed on the product insert.
Conditions To Avoid:	No data available.
Polymerization:	Will occur ☐ Will not occur ☒
Incompatibility - Materials To Avoid:	strong oxidizing agents
Hazardous Decomposition Or Byproducts:	carbon dioxide carbon monoxide hydrogen chloride gas nitrogen oxides

11. Toxicological Information

Toxicological Information:	The toxicological effects of this product have not been thoroughly studied.
Chronic Toxicological Effects:	No data available.

Hazardous Components (Chemical Name)	CAS #	NTP	IARC	ACGIH	OSHA
1. 3-Deazaneplanocin A (hydrochloride)	120964-45-6	n.a.	n.a.	n.a.	n.a.



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12. Ecological Information

General Ecological Information: Avoid release into the environment.
Runoff from fire control or dilution water may cause pollution.

13. Disposal Considerations

Waste Disposal Method: Dispose in accordance with local, state, and federal regulations.

14. Transport Information

Globally Harmonized System of Classification and Labelling

Acute Toxicity: Oral, Category 4 - Warning! Harmful if swallowed

LAND TRANSPORT (US DOT)

DOT Proper Shipping Name Not dangerous goods.

LAND TRANSPORT (European ADR/RID)

ADR/RID Shipping Name Not dangerous goods.

AIR TRANSPORT (ICAO/IATA)

ICAO/IATA Shipping Name Not dangerous goods.

Additional Transport Information: Transport in accordance with local, state, and federal regulations.

15. Regulatory Information

European Community Hazard Symbol codes Xn: Harmful

European Community Risk and Safety Phrases

R22 - Harmful if swallowed.

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.

US EPA SARA Title III

Hazardous Components (Chemical Name)	CAS #	Sec.302 (EHS)	Sec.304 RQ	Sec.313 (TRI)	Sec.110
1. 3-Deazaneplanocin A (hydrochloride)	120964-45-6	No	No	No	No

Other US EPA or State Lists

Hazardous Components (Chemical Name)	CAS #	CAA HAP,ODC	CWA NPDES	TSCA	CA PROP.65
1. 3-Deazaneplanocin A (hydrochloride)	120964-45-6	No	No	No	No

Regulatory Information Statement: This SDS was prepared in accordance with 29 CFR 1910.1200, Regulation (EC) No.1272/2008, and European Directive 67/548/EEC as amended.

16. Other Information

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Company Policy or Disclaimer

For research use only, not for human or veterinary use.

DISCLAIMER: This information is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.

N.A.=Not available, N.P.=Not applicable, N.D.=Not determined, N.E.=Not established, N.R.=Not required