

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



Section 1. Identification of the Substance/Mixture and of the

1.1	Product Code:	11214
	Product Name:	NKH477 (hydrochloride)
	Synonyms:	(3R,4aR,5S,6S,6aS,10S,10aR,10bS)-5-(acetyloxy)-3-ethenyldodecahydro-10,10b-dihydroxy-3,4a,7,7,10a-pentamethyl-1-β-alanine, N,N-dimethyl-oxo-1H-naphtho[2,1-b]pyran-6-yl ester, monohydrochloride; Adehl; Colforsin Dapropate;
1.2	Relevant identified uses of the substance or mixture and uses advised against	
	Relevant identified uses:	For research use only, not for human or veterinary use.
1.3	Details of the Supplier of the Safety Data Sheet	
	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

Section 2. Hazards Identification

GHS Classification	Placard	Key word	GHS hazard phrase
Acute Toxicity: Oral, Category 2	Skull and crossbones	Danger	Fatal if swallowed
Toxic To Reproduction, Category 2	Health hazard	Warning	Suspected of damaging fertility or the unborn child

GHS Hazard Phrases:	H300: Fatal if swallowed. H361: Suspected of damaging fertility or the unborn child.
GHS Precaution Phrases:	P264: Wash {hands} thoroughly after handling. P201: Obtain special instructions before use. P202: Do not handle until all safety precautions have been read and understood. P281: Use personal protective equipment as required.
GHS Response Phrases:	P301+310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. P330: Rinse mouth. P308+313: IF exposed or concerned: Get medical attention/advice.
GHS Storage and Disposal Phrases:	Please refer to Section 7 for Storage and Section 13 for Disposal information.
2.3 Adverse Human Health Effects and Symptoms:	Fatal 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. May cause gastrointestinal disturbances. May stimulate contraction of intestinal and reproductive smooth muscle. Suspected of damaging fertility or the unborn child. This chemical has the potential to induce premature labor or abortion. Vasodilator. To the best of our knowledge, the toxicological properties have not been thoroughly investigated.
Target Organs:	Heart, Smooth muscles.
LD 50 / LC 50:	Please refer to Section 11.

Medical Conditions Generally Aggravated By No data available.

Exposure:

Section 3. Composition/Information on Ingredients

Hazardous Components (Chemical Name)	CAS #	Concentration	EC#	Risk Phrases	RTECS #
1. NKH477 (hydrochloride)	138605-00-2	100.0 %	NA	R28-62	AY5992600

Section 4. First Aid Measures

4.1 Description of First Aid Measures:

- 4.1.1 In Case of Inhalation:** Remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.
- 4.1.2 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.
- 4.1.3 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.
- 4.1.4 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.
- 4.2 Important Symptoms and Effects, Both Acute and Delayed:** No data available.
- 4.3 Indication of any immediate medical attention and special treatment needed:** No data available.

Section 5. Fire Fighting Measures

- 5.1 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.
- 5.2 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.
- 5.3 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.

Section 6. Accidental Release Measures

- 6.1 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).
- 6.2 Environmental Precautions:** Take steps to avoid release into the environment, if safe to do so.
- 6.3 Methods and Material For Containment and Cleaning Up:** Contain spill and collect, as appropriate. Transfer to a chemical waste container for disposal in accordance with local regulations.

Section 7. Handling and Storage

- 7.1 Precautions To Be Taken in Handling:** Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid prolonged or repeated exposure.
- 7.2 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.

Section 8. Exposure Controls/Personal Protection

Hazardous Components (Chemical Name)	CAS #	OSHA PEL	ACGIH TLV	Other Limits
1. NKH477 (hydrochloride)	138605-00-2	No data.	No data.	No data.
Hazardous Components (Chemical Name)	CAS #	Britain EH40	France VL	Europe
1. NKH477 (hydrochloride)	138605-00-2	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

8.2.1 Engineering Controls (Ventilation etc.): Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.

8.2.2.1 Eye Protection: Safety glasses

8.2.2.2 Protective Gloves: Compatible chemical-resistant gloves

Other Protective Clothing: Lab coat

8.2.2.3 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.

8.2.3 Environmental Exposure Controls: No data available.

Section 9. Physical and Chemical Properties

9.1 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: ~0.5 1:1 mg/ml in DMSO:PBS (pH 7.2); ~2.5 mg/ml in DMSO; ~20 mg/ml in DMF;

Autoignition Pt: No data.

Explosive Properties: No data available.

Oxidizing Properties: No data available.

9.2 Other Information

Percent Volatile: No data.

Formula: C₂₇H₄₃NO₈ • HCl

Molecular Weight: 546.10

Section 10. Stability and Reactivity

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

Section 11. Toxicological Information

11.1 Information on Toxicological Effects:	The toxicological effects of this product have not been thoroughly studied.
	NKH477 (hydrochloride) - Toxicity Data: Oral LD50 (rat): 12.9 mg/kg; Intravenous LD50 (rat): 6.1 mg/kg;
Chronic Toxicological Effects:	NKH477 (hydrochloride) - Investigated as a reproductive effector. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information. NKH477 (hydrochloride) RTECS Number: AY5992600

Hazardous Components (Chemical Name)	CAS #	NTP	IARC	ACGIH	OSHA
1. NKH477 (hydrochloride)	138605-00-2	n.a.	n.a.	n.a.	n.a.

Section 12. Ecological Information

12.1 Toxicity:	Avoid release into the environment. Runoff from fire control or dilution water may cause pollution.
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Section 13. Disposal Considerations

13.1 Waste Disposal Method:	Dispose in accordance with local, state, and federal regulations.
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Section 14. Transport Information

14.1 LAND TRANSPORT (US DOT)	
DOT Proper Shipping Name	Toxic solids, organic, n.o.s. ((3R,4aR,5S,6S,6aS,10S,10aR,10bS)-5-(acetyloxy)-3-ethenyldodecahydro-10,10b-dihydroxy-3,4a,7,7,10a-pentamethyl-1-β-alanine, N,N-dimethyl-oxo-1H-naphtho[2,1-b]pyran-6-yl ester, monohydrochloride)
DOT Hazard Class:	6.1
DOT Hazard Label:	POISON
UN/NA Number:	2811
Packing Group:	II
14.1 LAND TRANSPORT (European ADR/RID)	
ADR/RID Shipping Name	Toxic solids, organic, n.o.s. ((3R,4aR,5S,6S,6aS,10S,10aR,10bS)-5-(acetyloxy)-3-ethenyldodecahydro-10,10b-dihydroxy-3,4a,7,7,10a-pentamethyl-1-β-alanine, N,N-dimethyl-oxo-1H-naphtho[2,1-b]pyran-6-yl ester, monohydrochloride)
UN Number:	2811



SAFETY DATA SHEET

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Hazard Class: 6.1 - POISON**Packing Group:** II**14.3 AIR TRANSPORT (ICAO/IATA)****ICAO/IATA Shipping Name** Toxic solids, organic, n.o.s.
((3R,4aR,5S,6S,6aS,10S,10aR,10bS)-5-(acetyloxy)-3-ethenyldodecahydro-10,10b-dihydroxy-3,4a,7,7,10a-pentamethyl-1- β -alanine, N,N-dimethyl-oxo-1H-naphtho[2,1-b]pyran-6-yl ester, monohydrochloride)**UN Number:** 2811**Hazard Class:** 6.1 - POISON**Packing Group:** II**IATA Classification:** 6.1**Additional Transport Information:** Transport in accordance with local, state, and federal regulations.

When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.

Section 15. Regulatory Information

European Community Hazard Symbol codes T+: Very Toxic**European Community Risk and Safety Phrases**

- R28 - Very toxic if swallowed.
S22 - Do not breathe dust.
S24/25 - Avoid contact with skin and eyes.
S28 - After contact with skin, wash immediately with plenty of soap-suds.
S36/37/39 - Wear suitable protective clothing, gloves and eye/face protection.
S45 - In case of accident or if you feel unwell, seek medical advice immediately (show the label whenever possible.)

US EPA SARA Title III

Hazardous Components (Chemical Name)	CAS #	Sec.302 (EHS)	Sec.304 RQ	Sec.313 (TRI)	Sec.110
1. NKH477 (hydrochloride)	138605-00-2	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. NKH477 (hydrochloride)	138605-00-2	No	No	No	No

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

Section 16. Other Information

Revision Date: 08/28/2013**Company Policy or Disclaimer**

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