1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1 Product identifiers
Product Name: NKH 477
Catalog Number: 1603
CAS Number: 138605-00-2
IUPAC Name: \(N,N\text{-Dimethyl-}(3R,4aR,5S,6aS,10S,10aR,10bS)-5\text{-}(acetyloxy)-3\text{-ethenyldodecahydro-10,10b-dihydroxy-3,4a,7,10a-pentamethyl-1-oxo-1H-naphtho[2,1-b]pyran-6-yl ester}\) \(\beta\text{-alanine hydrochloride}\)

1.2 Relevant identified uses of the substance or mixture and uses advised against
Identified Uses: Laboratory chemicals, Manufacture of substances

1.3 Details of the supplier of the safety data sheet
Company: Tocris Bioscience
Telephone: +44 (0)117 916-3333
The Watkins Building, Atlantic Road, Bristol, BS11 9QD, UK
Fax: +44 (0)117 916-3344
Internet: www.tocris.com
E-mail address: customerservice@tocris.co.uk

1.4 Emergency Telephone number
For chemical emergency spill, leak, fire, exposure, or accident call CHEMTREC day or night:
Within USA and Canada: 1-800-424-9300. Outside USA and Canada: +1 703-527-3887 (collect calls accepted).

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture
Classification according to Regulation (EC) No 1272/2008 [GHS/CLP]
Acute Toxicity, oral - Category 2

Classification according to EU Directives DSD 67/548/EEC or DPD 1999/45/EC
Very toxic if swallowed

2.2 Labeling elements
Labeling according to Regulation (EC) No 1272/2008 [CLP]

Pictogram(s):

Signal word: Danger
Hazard statement(s):
H300 Fatal if swallowed
Precautionary statement(s):
P264 Wash hands thoroughly after handling
P301+310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician

According to European Directive 67/548/EEC as amended
Hazard symbol(s):

R-phrase(s):
R28 Very toxic if swallowed
S-phrase(s):
S46 If swallowed, seek medical advice immediately and show this container or label

2.3 Other hazards - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances
Product Name: NKH 477
Synonyms: Colforsin dapropate hydrochloride, 6-(3-dimethylaminopropionyl)forskolin hydrochloride
Formula: \(C_{27}H_{43}NO_8\text{HCl}\) Molecular Weight: 546.1
CAS Number: 138605-00-2

4. FIRST AID MEASURES

4.1 Description of first aid measures
General advice
Consult a doctor and show this safety data sheet.

If inhaled
Remove to fresh air and monitor breathing. If breathing becomes difficult, give oxygen. If breathing stops, give artificial ventilation.

respiration. Consult a doctor.

In case of skin contact
Immediately wash skin with copious amounts of soap and water for at least 15 minutes. Remove contaminated clothing and shoes and wash before reuse. Consult a doctor.

In case of eye contact
Flush with copious amounts of water for at least 15 minutes. Consult a doctor.

If swallowed
Rinse mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Consult a doctor.

4.2 Most important symptoms and effects, both acute and delayed
To the best of our knowledge, the chemical, physical and toxicological properties have not been thoroughly investigated.

4.3 Indication of immediate medical attention and special treatment needed
Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

5. FIRE-FIGHTING MEASURES

5.1 Extinguishing media
Suitable extinguishing media
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture
In combustion, may emit toxic fumes.

5.3 Precautions for fire-fighters
Wear suitable protective clothing to prevent contact with skin and eyes and self-contained breathing apparatus.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures
Do not take action without suitable protective clothing - see section 8 of SDS. Evacuate personnel to safe areas. Ensure adequate ventilation. Avoid breathing vapors, mist, dust or gas.

6.2 Environmental precautions
Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up
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 section 13 of SDS.

6.4 Reference to other sections
For required PPE see section 8. For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling
Use in a chemical fume hood, with air supplied by an independent system. Avoid inhalation, contact with eyes, skin and clothing. Avoid the formation of dust and aerosols. Use in a well-ventilated area. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

7.2 Conditions for safe storage, including any incompatibilities.
Store in cool, well-ventilated area. Keep away from direct sunlight. Keep container tightly sealed until ready for use. Recommended storage temperature: Desiccate at +4°C

7.3 Specific end uses
Use in a laboratory fume hood where possible. Refer to employer's COSHH risk assessment.

8. EXPOSURE CONTROLS/PERSoNAL PROTECTION

8.1 Control parameters
Components with workplace control parameters
Contains no substances with occupational exposure limit values.

8.2 Exposure controls
Appropriate engineering controls
Use in a fume hood where applicable. Ensure all engineering measures described under section 7 of SDS are in place. Ensure laboratory is equipped with a safety shower and eye wash station.

Personal protective equipment

Eye/face protection
Use appropriate safety glasses.

Skin protection
Use appropriate chemical resistant gloves (minimum requirement use standard BS EN 374:2003). Gloves should be inspected before use. Wash and dry hands thoroughly after handling.

Body protection
Wear appropriate protective clothing.
Respiratory protection
If risk assessment indicates necessary, use a suitable respirator.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Appearance</td>
<td>White solid</td>
</tr>
<tr>
<td>Odor</td>
<td>No data available</td>
</tr>
<tr>
<td>Odor threshold</td>
<td>No data available</td>
</tr>
<tr>
<td>pH</td>
<td>No data available</td>
</tr>
<tr>
<td>Melting / freezing point</td>
<td>No data available</td>
</tr>
<tr>
<td>Boiling point / range</td>
<td>No data available</td>
</tr>
<tr>
<td>Flash point</td>
<td>No data available</td>
</tr>
<tr>
<td>Evaporation rate</td>
<td>No data available</td>
</tr>
<tr>
<td>Flammability (solid, gas)</td>
<td>No data available</td>
</tr>
<tr>
<td>Upper / lower flammability or explosive limits</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>No data available</td>
</tr>
<tr>
<td>Vapor density</td>
<td>No data available</td>
</tr>
<tr>
<td>Relative density</td>
<td>No data available</td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>No data available</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Decomposition temperature</td>
<td>No data available</td>
</tr>
<tr>
<td>Viscosity</td>
<td>No data available</td>
</tr>
<tr>
<td>Explosive properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Oxidising properties</td>
<td>No data available</td>
</tr>
<tr>
<td>Soluble to 40 mM in water</td>
<td></td>
</tr>
<tr>
<td>Partition coefficient</td>
<td>No data available</td>
</tr>
<tr>
<td>Auto-ignition temperature</td>
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<tr>
<td>Oxidising properties</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2 Other safety information

No data available

10. STABILITY AND REACTIVITY

10.1 Reactivity
Stable under recommended transport or storage conditions.

10.2 Chemical stability
Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions
Hazardous reactions will not occur under normal transport or storage conditions. Decomposition may occur on exposure to conditions or materials listed below.

10.4 Conditions to avoid
Heat, moisture.

10.5 Incompatible materials
Strong acids/alkalis, strong oxidising/reducing agents.

10.6 Hazardous decomposition products
In combustion may emit toxic fumes. No known decomposition information.

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute Toxicity
ORL-RAT LD50: 12900µg/kg; IVN-RAT LD50: 6100µg/kg; IVN-DOG LD50: 1600µg/kg; IVN-RAT TDLo: 27300µg/kg; IVN-DOG TDLo: 27300µg/kg; IVN-RAT TDLo: 11mg/kg

Skin corrosion/irritation
Classified based on available data

Serious eye damage/irritation
Classified based on available data

Respiratory or skin sensitization
Classified based on available data

Germ cell mutagenicity
Classified based on available data

Carcinogenicity
Classified based on available data

Reproductive toxicity
Classified based on available data

Specific target organ toxicity - single exposure
Classified based on available data

Specific target organ toxicity - repeated exposure
Classified based on available data

Aspiration hazard
Classified based on available data

Symptoms / Routes of exposure
Inhalation: There may be shortness of breath with a burning sensation in the throat. Exposure may cause coughing or wheezing. Absorption through the lungs can occur causing symptoms similar to those of ingestion. Severe poisoning causes severe shortness of breath and shock, with blueness of the lips, tongue, ears, face, hands and feet.
Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. Blood may be vomited. There may be vomiting and diarrhea. There may be loss of consciousness. Severe poisoning can cause unconsciousness and severe and persistent nausea and vomiting. Severe poisoning can cause shock, unconsciousness and convulsions.

Skin: Irritation or pain may occur at the site of contact. There may be redness or whiteness of the skin in the area of exposure. Absorption through the skin may be fatal.

Eyes: There may be pain and redness. The vision may become blurred. The eyes may water profusely. Absorption through the eye may cause effects similar to skin and/or ingestion.

Delayed / Immediate Effects: Immediate effects can be expected after short-term exposure.

Additional Information
RTECS No: AY5992600
Exposure may cause irritation of eyes, mucous membranes, upper respiratory tract and skin.

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

12. ECOLOGICAL INFORMATION

12.1 Toxicity
No data available

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
No data available

12.6 Other adverse effects
No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
Transfer to a suitable container and arrange for collection by specialized disposal company in accordance with National legislation.

Contaminated packaging
Dispose of in a regulated landfill site or other method for hazardous or toxic wastes in accordance with National legislation.

14. TRANSPORT INFORMATION

Classified according to the criteria of the UN Model Regulations as reflected in the IMDG Code, ADR, RID and IATA.

14.1 UN-Number
UN2811

14.2 UN proper shipping name
Toxic solid, organic, n.o.s. (NKH 477)

14.3 Transport hazard class(es)
6.1

14.4 Packaging group
II

14.5 Environmental hazards
This product is not classified as environmentally hazardous according to the UN Model Regulations, nor a marine pollutant according to the IMDG Code.

14.6 Special precautions for users
No data available

15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulation (EC) No. 453/2010.

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture
No data available

15.2 Chemical safety assessment
A Chemical Safety Assessment has not been made for this product.

16. OTHER INFORMATION

SDS Revision Details
V2.1 Reclassified based on data review

Nov 16th 2012
Further Information
Copyright © 2017 Tocris Bioscience. This company shall not be held liable for any damage resulting from handling or from contact with the above product. This material must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized 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 legislature. The absence of warning must not, under any circumstance, be taken to mean that no hazard exists.

End of safety data sheet