

according to Regulation (EC) No. 1907/2006 as amended by (EC) No. 1272/2008

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

- 1.1 Product Code:** 10006794
Product Name: (+)-Xestospongina A
Synonyms: [1R-(1R*,4aR*,11R*,12aS*,13R*,16aR*,23R*,24aS*)]-eicosahydro-5H,17H-1,23:11,13-diethano-2H,14H-[1,11]dioxacyclo-eicosino[2,3-b:12,13-b']dipyridine; Araguspogin D; XeA;
- 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
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
Web site address: www.caymanchem.com
Information: Cayman Chemical Company +1 (734)971-3335
- 1.4 Emergency telephone number:**
- Emergency Contact:** CHEMTREC Within USA and Canada: +1 (800)424-9300
CHEMTREC Outside USA and Canada: +1 (703)527-3887

Section 2. Hazards Identification

- 2.1 Classification of the Substance or Mixture:**
2.1.1 Classification according to Regulation (EC) No 1272/2008 [CLP]:
Flammable Liquids, Category 2
Serious Eye Damage/Eye Irritation, Category 2
Target Organ Systemic Toxicity (single exposure), Category 3
- 2.2 Label Elements:**
2.2.1 Labeling according to Regulation (EC) No 1272/2008 [CLP]:



GHS Signal Word: Danger

GHS Hazard Phrases:

H225: Highly flammable liquid and vapor.

H319: Causes serious eye irritation.

H336: May cause drowsiness or dizziness.

GHS Precaution Phrases:

P210: Keep away from heat/sparks/open flames/hot surfaces. - No smoking.

P280: Wear protective gloves/protective clothing/eye protection/face protection.

P264: Wash hands thoroughly after handling.

P261: Avoid breathing dust/fume/gas/mist/vapours/spray.

GHS Response Phrases:

P303+361+353: IF ON SKIN (or hair): Remove/take off immediately all contaminated clothing. Rinse skin with water/shower.

P305+351+338: IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P337+313: If eye irritation persists, get medical advice/attention.

P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.

P312: Call a POISON CENTER/doctor/... if you feel unwell.

GHS Storage and Disposal Phrases:

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

2.3 Adverse Human Health Causes serious eye irritation.

Effects and Symptoms: Material may be irritating to the mucous membranes and upper respiratory tract.
May be harmful by inhalation, ingestion, or skin absorption.
May cause skin or respiratory system irritation.
Vapors may cause drowsiness and dizziness.
To the best of our knowledge, the toxicological properties have not been thoroughly investigated.

Section 3. Composition/Information on Ingredients

CAS # / RTECS #	Hazardous Components (Chemical Name)/ REACH Registration No.	Concentration	EC No./ EC Index No.	GHS Classification
88840-02-2 NA	(+)-Xestospongina A	0.01 %	NA NA	No data available.
67-64-1 AL3150000	Acetone	99.99 %	200-662-2 606-001-00-8	Flam. Liq. 2: H225 Eye Damage 2: H319 TOST (SE) 3: H335 H336

Section 4. First Aid Measures

4.1 Description of First Aid No data available.

Measures:

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 15 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 15 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.

4.2 Important Symptoms and Effects, Both Acute and Delayed: Exposure may cause: dizziness, drowsiness, CNS depression, and narcosis.

Section 5. Fire Fighting Measures

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

Media: Use water spray to cool fire-exposed containers.

Unsuitable Extinguishing A solid water stream may be inefficient.

Media:

5.2 Flammable Properties and Hazards: Can release vapors that form explosive mixtures at temperatures at or above the flashpoint.

Container explosion may occur under fire conditions.
Emits toxic fumes under fire conditions.
Sensitive to static discharge.
Vapors can travel to a source of ignition and flash back.

Flash Pt: -18.00 C Method Used: Closed Cup

Explosive Limits: LEL: 2.5% at 25.0 C UEL: 12.8% at 25.0 C

Autoignition Pt: 465.00 C

- 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.
- Note: Flammable as diluted in acetone.

Section 6. Accidental Release Measures

- 6.1 Protective Precautions,** Avoid breathing vapors and provide adequate ventilation.
- Protective Equipment and Emergency Procedures:** 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.
- Keep away from sources of ignition.
- Take precautionary measures against static discharge.
- 7.2 Precautions To Be Taken in Storing:** Keep away from heat, sparks, and flame.
- Keep container tightly closed.
- Store in accordance with information listed on the product insert.

Section 8. Exposure Controls/Personal Protection

8.1 Exposure Parameters:

CAS #	Partial Chemical Name	Britain EH40	France VL	Europe
88840-02-2	(+)-Xestospongina A	No data.	No data.	No data.
67-64-1	Acetone	TWA: 1210 mg/m3 (500 ppm) STEL: 3620 mg/m3 (1500 ppm)	TWA: 1210 mg/m3 (500 ppm) STEL: 2420 mg/m3 (1000 ppm)	TWA: 1210 mg/m3
CAS #	Partial Chemical Name	OSHA TWA	ACGIH TWA	Other Limits
88840-02-2	(+)-Xestospongina A	No data.	No data.	No data.
67-64-1	Acetone	PEL: 1000 ppm	TLV: 500 ppm STEL: 750 ppm	No data.



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8.2 Exposure Controls:

- 8.2.1 Engineering Controls** Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.
- 8.2.2 Personal protection equipment:**
- Eye Protection:** Safety glasses
- Protective Gloves:** Compatible chemical-resistant gloves
- Other Protective Clothing:** Lab coat
- Respiratory Equipment** NIOSH approved respirator, as conditions warrant.
- (Specify Type):**
- 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.
- No data available.

Section 9. Physical and Chemical Properties

9.1 Information on Basic Physical and Chemical Properties

- Physical States:** [] Gas [X] Liquid [] Solid
- Appearance and Odor:** Solution
- Melting Point:** No data.
- Boiling Point:** No data.
- Flash Pt:** -18.00 C Method Used: Closed Cup
- Evaporation Rate:** No data.
- Explosive Limits:** LEL: 2.5% at 25.0 C UEL: 12.8% at 25.0 C
- Vapor Pressure (vs. Air or mm Hg):** 180 MM_HG at 20.0 C
- Vapor Density (vs. Air = 1):** No data.
- Specific Gravity (Water = 1):** No data.
- Solubility in Water:** No data.
- Autoignition Pt:** 465.00 C

9.2 Other Information

- Percent Volatile:** No data.
- Molecular Formula & Weight:** C₂₈H₅₀N₂O₂ 446.7

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.
- Polymerization:** Will occur [] Will not occur [X]
- 10.4 Conditions To Avoid:** heat, flames and sparks
- 10.5 Incompatibility - Materials** acids
- To Avoid:** bases
- oxidizing agents
- phosphorous oxychloride
- reducing agents
- 10.6 Hazardous** carbon dioxide
- Decomposition Or** carbon monoxide
- Byproducts:**

Section 11. Toxicological Information

11.1 Information on Toxicological Effects:	The toxicological effects of this product have not been thoroughly studied. Acetone - Toxicity Data: Oral LD50 (rat): 5,800 mg/kg; Oral LD50 (rabbit): 5,340 mg/kg; Oral LD50 (mouse): 3,000 mg/kg; Oral TDLO (man): 2,857 mg/kg; Inhalation TCLO (human): 10 mg/m3 (6 hr); Inhalation LC50 (rat): 50,100 mg/m3 (8 hr); Acetone - Irritation Data: Eye (human): 186,300 ppm mild; Eye (rabbit): 20 mg (24h) moderate; Skin (rabbit): 500 mg (24 hr) mild;
Chronic Toxicological Effects:	Acetone - Investigated as a mutagen, reproductive effector, and teratogen. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information. Acetone RTECS Number: AL3150000
Carcinogenicity:	NTP? No IARC Monographs? No OSHA Regulated? No

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
88840-02-2	(+)-Xestospongins A	n.a.	n.a.	n.a.	n.a.
67-64-1	Acetone	n.a.	n.a.	A4	n.a.

Section 12. Ecological Information

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

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:	Acetone Solution		
DOT Hazard Class:	3	FLAMMABLE LIQUID	
UN/NA Number:	1090	Packing Group:	II



14.1 LAND TRANSPORT (European ADR/RID):

ADR/RID Shipping Name:	Acetone Solution		
UN Number:	1090	Packing Group:	II
Hazard Class:	3 - FLAMMABLE LIQUID		



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14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Acetone Solution

UN Number: 1090

Packing Group: II

Hazard Class: 3 - FLAMMABLE LIQUID

IATA Classification: 3

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

EPA SARA (Superfund Amendments and Reauthorization Act of 1986) Lists

CAS #	Hazardous Components (Chemical Name)	S. 302 (EHS)	S. 304 RQ	S. 313 (TRI)
88840-02-2	(+)-Xestospongina A	No	No	No
67-64-1	Acetone	No	Yes 5000 LB	No

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
88840-02-2	(+)-Xestospongina A	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No
67-64-1	Acetone	CAA HAP,ODC: No; CWA NPDES: No; TSCA: Yes - Inventory, 4 Test; CA PROP.65: No

Regulatory Information Statement: This SDS was prepared in accordance with 29 CFR 1910.1200 and Regulation (EC) No.1272/2008.

Section 16. Other Information

Revision Date: 01/20/2015**Additional Information About This Product:** No data available.**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.