

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:** 22151  
**Product Name:** Hepoxilin A3 methyl ester  
**Synonyms:** methyl (5Z,9E)-8-hydroxy-10-((2S,3S)-3-((Z)-oct-2-en-1-yl)oxiran-2-yl)deca-5,9-dienoateHxA3 methyl ester;
- 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:**  
 Flammable Liquids, Category 2  
 Skin Corrosion/Irritation, Category 2  
 Toxic To Reproduction, Category 2  
 Specific Target Organ Toxicity (single exposure), Category 3  
 Specific Target Organ Toxicity (repeated exposure), Category 2  
 Aspiration Toxicity, Category 1  
 Aquatic Toxicity (Chronic), Category 2

**2.2 Label Elements:**



**GHS Signal Word:** **Danger**

**GHS Hazard Phrases:**

- H225: Highly flammable liquid and vapor.  
 H304: May be fatal if swallowed and enters airways.  
 H315: Causes skin irritation.  
 H336: May cause drowsiness or dizziness.  
 H361: Suspected of damaging fertility or the unborn child.  
 H373: May cause damage to {organs} through prolonged or repeated exposure.  
 H411: Toxic to aquatic life with long lasting effects.

**GHS Precaution Phrases:**

P201: Obtain special instructions before use.  
P202: Do not handle until all safety precautions have been read and understood.  
P210: Keep away from {heat/sparks/open flames/hot surfaces}. - No smoking.  
P260: Do not breathe {dust/fume/gas/mist/vapors/spray}.  
P264: Wash {hands} thoroughly after handling.  
P273: Avoid release to the environment.  
P280: Wear {protective gloves/protective clothing/eye protection/face protection}.  
P281: Use personal protective equipment as required.

**GHS Response Phrases:**

P301+310: IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.  
P302+352: IF ON SKIN: Wash with plenty of soap and water.  
P303+361+353: IF ON SKIN (or hair): Remove/take off immediately all contaminated clothing. Rinse skin with water/shower.  
P304+340: IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.  
P308+313: IF exposed or concerned: Get medical attention/advice.  
P312: Call a POISON CENTER or doctor/physician if you feel unwell.  
P314: Get medical attention/advice if you feel unwell.  
P331: Do NOT induce vomiting.  
P332+313: If skin irritation occurs, get medical advice/attention.  
P362: Take off contaminated clothing and wash before re-use.  
P391: Collect spillage.

**GHS Storage and Disposal Phrases:**

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

- 2.3 Adverse Human Health** Aspiration hazard if swallowed-may be fatal if enters lungs, will cause damage.
- Effects and Symptoms:** Causes skin irritation.  
Material may be irritating to the mucous membranes and upper respiratory tract.  
May be fatal if swallowed and enters airways.  
May be harmful by inhalation, ingestion, or skin absorption.  
May cause drowsiness or dizziness.  
May cause damage to organs through prolonged or repeated exposure.  
May cause eye or respiratory system irritation.  
Suspected of damaging fertility or the unborn child.  
Toxic to aquatic life with long lasting effects.  
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   |
|-----------------------|--|---------------|---------------------------|--|
| NA<br>NA              | Hepoxilin A3 methyl ester                                    | 0.1 %         | NA<br>NA                  | No data available.   |
| 121-44-8<br>YE0175000 | Triethylamine  | 1.0 %         | 204-469-4<br>612-004-00-5 | Flam. Liq. 2: H225<br>Acute Tox.(O) 4: H302<br>Acute Tox.(D) 4: H312<br>Skin Corr. 1A: H314<br>Acute Tox.(I) 4: H332 |
| 110-54-3<br>MN9275000 | n-Hexane   | 98.9 %        | 203-777-6<br>601-037-00-0 | Flam. Liq. 2: H225<br>Asp. Toxic. 1: H304<br>Skin Corr. 2: H315<br>STOT (SE) 3: H336                                 |

|   |
|---|
| Toxic Repro. 2: H361f<br>STOT (RE) 2: H373<br>Aquatic (C) 2: H411 |
|---|

### Section 4. First Aid Measures

- 4.1 Description of First Aid 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:** Eye contact may cause: redness, blurred vision, or tearing. Ingestion may cause: chemical pneumonitis, chest pain, CNS depression, dizziness, drowsiness, gastrointestinal discomfort, giddiness, headache, lung irritation, muscle weakness, nausea, numb extremities, pulmonary edema, slowed reaction time, slurred speech, and unconsciousness. Prolonged or repeated skin contact may cause dermatitis, dryness, or cracking. Vapors may cause drowsiness and dizziness.

### 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:** Can release vapors that form explosive mixtures at temperatures at or above the flash point.
- 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.  
No data available.
- Flash Pt:** -21.70 C
- Explosive Limits:** LEL: 1.1% at 25.0 C UEL: 7.5% at 25.0 C
- Autoignition Pt:** 225.00 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 n-hexane.

### 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. 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 #    | Chemical Name | Jurisdiction | Recommended Exposure Limits                            | Notations       |
|----------|---------------|--------------|--|-----------------|
| 121-44-8 | Triethylamine | ACGIH TLV    | TLV: 0.5 ppm<br>STEL: 1 ppm                            |                 |
|          |               | Europe       | TWA: 8.4 mg/m3 (2.0 ppm)<br>STEL: 12.6 mg/m3 (3.0 ppm) | Skin Absorption |
|          |               | France VL    | TWA: 4.2 mg/m3 (1 ppm)<br>STEL: 12.6 mg/m3 (3 ppm)     |                 |
|          |               | OSHA PELs    | PEL: 25 ppm  |                 |
|          |               | Britain EH40 | TWA: 8 mg/m3 (2 ppm)<br>STEL: 17 mg/m3 (4 ppm)         | Skin Absorption |
| 110-54-3 | n-Hexane      | ACGIH TLV    | TLV: 50 ppm  |                 |
|          |               | Europe       | TWA: 72 mg/m3 (20 ppm)                                 |                 |
|          |               | France VL    | TWA: 72 mg/m3 (20 ppm)                                 |                 |
|          |               | OSHA PELs    | PEL: 500 ppm   |                 |
|          |               | Britain EH40 | TWA: 72 mg/m3 (20 ppm)<br>STEL: ()                     |                 |

**8.2 Exposure Controls:**

- 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 Personal protection equipment:**
- Eye Protection:** Safety glasses
- Protective Gloves:** Compatible chemical-resistant gloves
- Other Protective Clothing:** Lab coat
- 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.

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:** A solution in hexane/1% TEA

**pH:** No data.

**Melting Point:** No data.

**Boiling Point:** No data.

**Flash Pt:** -21.70 C

**Evaporation Rate:** No data.

**Flammability (solid, gas):** No data available.

**Explosive Limits:** LEL: 1.1% at 25.0 C UEL: 7.5% at 25.0 C

**Vapor Pressure (vs. Air or mm Hg):** 124 MM\_HG at 20.0 C

**Vapor Density (vs. Air = 1):** No data.

**Specific Gravity (Water = 1):** No data.

**Solubility in Water:** No data.

**Octanol/Water Partition Coefficient:** No data.

**Autoignition Pt:** 225.00 C

**Decomposition Temperature:** No data.

**Viscosity:** No data.

### 9.2 Other Information

**Percent Volatile:** No data.

**Molecular Formula & Weight:** C<sub>21</sub>H<sub>34</sub>O<sub>4</sub> 350.5

## 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 To Avoid:** oxidizing agents

**10.6 Hazardous Decomposition or Byproducts:** carbon dioxide  
carbon monoxide

### Section 11. Toxicological Information

**11.1 Information on Toxicological Effects:** The toxicological effects of this product have not been thoroughly studied.

**Chronic Toxicological Effects:** Hexane - Toxicity Data: Oral LD50 (rat): 15,840 mg/kg; Inhalation TCLO (human): 5,400 mg/m<sup>3</sup> (10m); Inhalation LC50 (rat): 48,000 ppm (4h); Hexane - Irritation Data: Eyes (rabbit): 10 mg mild; Hexane - Investigated as a mutagen and reproductive effector. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information. Hexane RTECS Number: MN9275000

| CAS #    | Hazardous Components (Chemical Name) | NTP  | IARC | ACGIH | OSHA |
|----------|--------------------------------------|------|------|-------|------|
| NA       | Hepoxilin A3 methyl ester            | n.a. | n.a. | n.a.  | n.a. |
| 121-44-8 | Triethylamine                        | n.a. | n.a. | A4    | n.a. |
| 110-54-3 | n-Hexane                             | 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.

**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.

### Section 13. Disposal Considerations

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

### Section 14. Transport Information

**14.1 LAND TRANSPORT (US DOT):**

**DOT Proper Shipping Name:** Hexane Solution  
**DOT Hazard Class:** 3 FLAMMABLE LIQUID  
**UN/NA Number:** UN1208 **Packing Group:** II



**14.1 LAND TRANSPORT (European ADR/RID):**

**ADR/RID Shipping Name:** Hexane Solution  
**UN Number:** 1208 **Packing Group:** II  
**Hazard Class:** 3 - FLAMMABLE LIQUID



# SAFETY DATA SHEET

## Hepoxilin A3 methyl ester

Revision: 06/13/2017  
Supersedes Revision: 04/17/2017

### 14.3 AIR TRANSPORT (ICAO/IATA):

|                                 |                      |                             |    |
|---------------------------------|----------------------|-----------------------------|----|
| <b>ICAO/IATA Shipping Name:</b> | Hexane Solution      | <b>Packing Group:</b>       | II |
| <b>UN Number:</b>               | 1208                 | <b>IATA Classification:</b> | 3  |
| <b>Hazard Class:</b>            | 3 - FLAMMABLE LIQUID |                             |    |

**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) |
|----------|--------------------------------------|--------------|-------------|--------------|
| NA       | Hepoxilin A3 methyl ester            | No           | No          | No           |
| 121-44-8 | Triethylamine                        | No           | Yes 5000 LB | Yes          |
| 110-54-3 | n-Hexane                             | No           | Yes 5000 LB | Yes          |

| CAS #    | Hazardous Components (Chemical Name) | Other US EPA or State Lists   |
|----------|--------------------------------------|---|
| NA       | Hepoxilin A3 methyl ester            | CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; CA PROP.65: No                |
| 121-44-8 | Triethylamine                        | CAA HAP,ODC: HAP; CWA NPDES: Yes; TSCA: Yes - Inventory; CA PROP.65: No |
| 110-54-3 | n-Hexane                             | CAA HAP,ODC: HAP; CWA NPDES: No; TSCA: Yes - Inventory; 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:** 06/13/2017

**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.