

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:** 18656
Product Name: Nitecapone
Synonyms: 3-[(3,4-dihydroxy-5-nitrophenyl)methylene]-2,4-pentanedione; OR-462;
- 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:**
- 2.2 Label Elements:**
- GHS Signal Word:** None
- GHS Hazard Phrases:**
 Based on evaluation of currently available data this substance or mixture is not classifiable according to GHS.
- GHS Precaution Phrases:**
 No phrases apply.
- GHS Response Phrases:**
 No phrases apply.
- GHS Storage and Disposal Phrases:**
 Please refer to Section 7 for Storage and Section 13 for Disposal information.
- 2.3 Adverse Human Health** Material may be irritating to the mucous membranes and upper respiratory tract.
Effects and Symptoms: May be harmful by inhalation, ingestion, or skin absorption.
 May cause eye, skin, or respiratory system irritation.
 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
116313-94-1 SA1942500	2,4-Pentanedione, 3-((3,4-dihydroxy-5-nitrophenyl)methylene)-	100.0 %	NA NA	No data available.

Section 4. First Aid Measures

4.1 Description of First Aid Measures:

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.

Section 5. Fire Fighting Measures

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

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

Unsuitable Extinguishing Media: A solid water stream may be inefficient.

Media:

5.2 Flammable Properties and Hazards: No data available.

Hazards:

No data available.

Flash Pt: No data.

Explosive Limits: LEL: No data. UEL: No data.

Autoignition Pt: No data.

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, Avoid raising and breathing dust, 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.

Precautions:

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.

Section 8. Exposure Controls/Personal Protection

8.1 Exposure Parameters:

CAS #	Partial Chemical Name	Britain EH40	France VL	Europe
116313-94-1	2,4-Pentanedione,	No data.	No data.	No data.

	3-((3,4-dihydroxy-5-nitrophenyl)methylene)-			
CAS #	Partial Chemical Name	OSHA TWA	ACGIH TWA	Other Limits
116313-94-1	2,4-Pentanedione, 3-((3,4-dihydroxy-5-nitrophenyl)methylene)-	No data.	No data.	No data.

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 [] Liquid [X] Solid

Appearance and Odor: A crystalline solid

Melting Point: No data.

Boiling Point: No data.

Flash Pt: No data.

Evaporation Rate: No data.

Flammability (solid, gas): No data available.

Explosive Limits: LEL: No data. UEL: No data.

Vapor Pressure (vs. Air or mm Hg): No data.

Hg):

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

Specific Gravity (Water = 1): No data.

Solubility in Water: No data.

Solubility Notes: ~0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2); ~5 mg/ml in EtOH; ~30 mg/ml in DMSO & DMF;

Autoignition Pt: No data.

9.2 Other Information

Percent Volatile: No data.
Molecular Formula & Weight: C₁₂H₁₁NO₆ 265.2

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: No data available.
10.5 Incompatibility - Materials To Avoid: strong oxidizing agents
10.6 Hazardous Decomposition or Byproducts: No data available.

Section 11. Toxicological Information

11.1 Information on Toxicological Effects: The toxicological effects of this product have not been thoroughly studied.
Nitecapone - Toxicity Data: Oral LD50 (mouse): >2 gm/kg; Intraperitoneal LD50 (mouse): 507 mg/kg;
Chronic Toxicological Effects: Nitecapone - Investigated as a drug.
Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here.
See actual entry in RTECS for complete information.
Nitecapone RTECS Number: SA1942500

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
116313-94-1	2,4-Pentanedione, 3-((3,4-dihydroxy-5-nitrophenyl)methylene)-	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: Not dangerous goods.

DOT Hazard Class:

UN/NA Number:

14.1 LAND TRANSPORT (European ADR/RID):

ADR/RID Shipping Name: Not dangerous goods.

UN Number:

Hazard Class:

14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Not dangerous goods.

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

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)
116313-94-1	2,4-Pentanedione, 3-((3,4-dihydroxy-5-nitrophenyl)methylene)-	No	No	No

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
116313-94-1	2,4-Pentanedione, 3-((3,4-dihydroxy-5-nitrophenyl)methylene)-	CAA HAP,ODC: No; CWA NPDES: No; TSCA: No; 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: 12/16/2015

Additional Information About This Product: No data available.

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