

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:** 15376
Product Name: Roquefortine C
Synonyms: (3E,5aS,10bR)-10b-(1,1-dimethyl-2-propen-1-yl)-6,10b,11,11aS-tetrahydro-3-(1H-imidazol-5-ylmethylene)-2H-pyrazino[1',2':1,5]pyrrolo[2,3-b]indole-1,4(3H,5aH)-dione; NSC 292134;
- 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]:**
Acute Toxicity: Inhalation, Category 3
Acute Toxicity: Oral, Category 3
Acute Toxicity: Skin, 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:

H301: Toxic if swallowed.

H311: Toxic in contact with skin.

H331: Toxic if inhaled.

GHS Precaution Phrases:

P261: Avoid breathing {dust/fume/gas/mist/vapors/spray}.

P264: Wash {hands} thoroughly after handling.

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

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.

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

P311: Call a POISON CENTER or doctor/physician.

P321: Specific treatment {see ... on this label}.

P330: Rinse mouth.

Section 6. Accidental Release Measures

- 6.1 Protective Precautions,** Avoid raising and breathing dust, and provide adequate ventilation.
- Protective Equipment and** As conditions warrant, wear a NIOSH approved self-contained breathing apparatus, or respirator,
- Emergency Procedures:** and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves).
- 6.2 Environmental** Take steps to avoid release into the environment, if safe to do so.
- Precautions:**
- 6.3 Methods and Material For** Contain spill and collect, as appropriate.
- Containment and Cleaning** Transfer to a chemical waste container for disposal in accordance with local regulations.
- Up:**

Section 7. Handling and Storage

- 7.1 Precautions To Be Taken** Avoid breathing dust/fume/gas/mist/vapours/spray.
- in Handling:** Avoid prolonged or repeated exposure.
- 7.2 Precautions To Be Taken** Keep container tightly closed.
- in Storing:** 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
58735-64-1	2H-Pyrazino(1',2':1,5)pyrrolo(2,3-b)indole-1,4-(3H,5a h)-dione, 6,10b,11,11a-tetrahydro-10b-(1,1-dimethyl-2-propenyl)-3-(1H-imidazol-2-yl)-	No data.	No data.	No data.
CAS #	Partial Chemical Name	OSHA TWA	ACGIH TWA	Other Limits
58735-64-1	2H-Pyrazino(1',2':1,5)pyrrolo(2,3-b)indole-1,4-(3H,5a h)-dione, 6,10b,11,11a-tetrahydro-10b-(1,1-dimethyl-2-propenyl)-3-(1H-imidazol-2-yl)-	No data.	No data.	No data.

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.
- (Ventilation etc.):**
- 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 ☐ Liquid ☒ Solid
Appearance and Odor: A white to off-white 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.
Vapor Density (vs. Air = 1): No data.
Specific Gravity (Water = 1): No data.
Solubility in Water: No data.
Solubility Notes: Soluble in: acetone, EtOH, MeOH, chloroform, dichloromethane, DMSO, & DMF;
Autoignition Pt: No data.

9.2 Other Information

Percent Volatile: No data.
Molecular Formula & Weight: C₂₂H₂₃N₅O₂ 389.5

Section 10. Stability and Reactivity

10.1 Reactivity: No data available.
10.2 Stability: Unstable ☐ Stable ☒
10.3 Stability Note(s): Stable if stored in accordance with information listed on the product insert.
Polymerization: Will occur ☐ Will not occur ☒
10.4 Conditions To Avoid: No data available.
10.5 Incompatibility - Materials To Avoid: No data available.
10.6 Hazardous Decomposition or Byproducts: carbon dioxide
carbon monoxide
nitrogen oxides

Section 11. Toxicological Information

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

Chronic Toxicological Effects: Roquefortine C - Toxicity Data: Intraperitoneal LD50 (mouse): 15 mg/kg;

Roquefortine C - Investigated as a drug and natural product.

Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here.

See actual entry in RTECS for complete information.

Roquefortine C RTECS Number: UQ4730500

CAS #	Hazardous Components (Chemical Name)	NTP	IARC	ACGIH	OSHA
58735-64-1	2H-Pyrazino(1',2':1,5)pyrrolo(2,3-b)indole-1,4-(3H,5a h)-dione, 6,10b,11,11a-tetrahydro-10b-(1,1-dimethyl-2-propenyl)-3-(1H-imidazole-2-yl)-	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: Toxins, extracted from living sources, solid, n.o.s. (Roquefortine C)

DOT Hazard Class: 6.1 POISON

UN/NA Number: UN3462 **Packing Group:** III



14.1 LAND TRANSPORT (European ADR/RID):

ADR/RID Shipping Name: Toxins, extracted from living sources, solid, n.o.s. (Roquefortine C)

UN Number: 3462 **Packing Group:** III

Hazard Class: 6.1 - POISON

14.3 AIR TRANSPORT (ICAO/IATA):

ICAO/IATA Shipping Name: Toxins, extracted from living sources, solid, n.o.s. (Roquefortine C)

UN Number: 3462 **Packing Group:** III

Hazard Class: 6.1 - POISON **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.



SAFETY DATA SHEET

Roquefortine C

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)
58735-64-1	2H-Pyrazino(1',2':1,5)pyrrolo(2,3-b)indole-1,4-(3H, 5a h)-dione, 6,10b,11,11a-tetrahydro-10b-(1,1-dimethyl-2-propenyl)-3-(1H-imi	No	No	No

CAS #	Hazardous Components (Chemical Name)	Other US EPA or State Lists
58735-64-1	2H-Pyrazino(1',2':1,5)pyrrolo(2,3-b)indole-1,4-(3H, 5a h)-dione, 6,10b,11,11a-tetrahydro-10b-(1,1-dimethyl-2-propenyl)-3-(1H-imi	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: 05/07/2015

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.