

Safety Data Sheet

according to UK REACH Regulation

Roquefortine C

Revision date: 28.05.2018

Product code: LS-1167

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GB CLP Regulation
Signal word: Danger

Pictograms:

Hazard statements

 H301+H311 Toxic if swallowed or in contact with skin.
 H330 Fatal if inhaled.

Precautionary statements

 P260 Do not breathe dust/fume/gas/mist/vapours/spray.
 P264 Wash hands thoroughly after handling.
 P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection.
 P284 Wear respiratory protection.
 P301+P310 IF SWALLOWED: Immediately call a POISON CENTER/doctor.
 P330 Rinse mouth.
 P302+P352 IF ON SKIN: Wash with plenty of water.
 P312 Call a POISON CENTER/doctor if you feel unwell.
 P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
 P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
 P310 Immediately call a POISON CENTER/doctor.
 P403+P233 Store in a well-ventilated place. Keep container tightly closed.
 P405 Store locked up.
 P501 Dispose of contents/container to an approved disposal site.

Special labelling of certain mixtures

Restricted to professional users.

Additional advice on labelling

Warning - substance not yet tested completely.

2.3. Other hazards

No information available.

SECTION 3: Composition/information on ingredients
3.1. Substances
Chemical characterization

(5aS,10bR,Z)-3-((1H-imidazol-4-yl)methylene)-10b-(2-methylbut-3-en-2-yl)-2,3,6,10b,11,11a-hexahydro-4H-pyrazino[1',2':1,5]pyrrolo[2,3-b]indole-1,4(5aH)-dione

 Sum formula: C₂₂H₂₃N₅O₂

Molecular weight: 389,46 g/mol

Hazardous components

CAS No	Chemical name	Quantity
	EC No	
	Index No	
	REACH No	
	GHS Classification	
58735-64-1	Roquefortine C	<= 100 %
	206-146-3	
	Acute Tox. 2, Acute Tox. 3, Acute Tox. 3; H330 H311 H301	

Full text of H and EUH statements: see section 16.

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Specific Conc. Limits, M-factors and ATE

CAS No	EC No	Chemical name	Quantity
		Specific Conc. Limits, M-factors and ATE	
58735-64-1	206-146-3	Roquefortine C	<= 100 % %
		inhalation: ATE = 0,5 mg/l (vapours); inhalation: ATE = 0,05 mg/l (dusts or mists); dermal: ATE = 300 mg/kg; oral: ATE = 100 mg/kg	

SECTION 4: First aid measures**4.1. Description of first aid measures****General information**

First aider: Pay attention to self-protection! Remove affected person from the danger area and lay down. In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

After inhalation

Provide fresh air. No mouth-to-mouth or mouth-to-nose resuscitation. Use Ambu bag or ventilator. Call a physician immediately. Remove casualty to fresh air and keep warm and at rest. In case of irregular breathing or respiratory arrest provide artificial respiration.

In all cases of doubt, or when symptoms persist, seek medical advice.

After contact with skin

After contact with skin, wash immediately with polyethylene glycol, followed by plenty of water. Take off immediately all contaminated clothing and wash it before reuse. Call a physician immediately. After contact with skin, wash immediately with plenty of water and soap.

In all cases of doubt, or when symptoms persist, seek medical advice.

After contact with eyes

After eye contact: Rinse immediately carefully and thoroughly with eye-bath or water. Consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink plenty of water. Induce vomiting when the affected person is not unconscious. Call a physician immediately. Rinse mouth thoroughly with water. Never give anything by mouth to an unconscious person or a person with cramps.

In all cases of doubt, or when symptoms persist, seek medical advice.

4.2. Most important symptoms and effects, both acute and delayed

No data available

4.3. Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

SECTION 5: Firefighting measures**5.1. Extinguishing media****Suitable extinguishing media**

Co-ordinate fire-fighting measures to the fire surroundings. Water spray. alcohol resistant foam. Dry extinguishing powder. Carbon dioxide (CO₂). Sand.

Unsuitable extinguishing media

High power water jet.

5.2. Special hazards arising from the substance or mixture

Non-flammable. Thermal decomposition can lead to the escape of irritating gases and vapours.

In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).

5.3. Advice for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing. Full protection suit.

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Additional information

Suppress gases/vapours/mists with water spray jet. Collect contaminated fire extinguishing water separately.
Do not allow entering drains or surface water.
Usual measures for fire prevention.

SECTION 6: Accidental release measures**6.1. Personal precautions, protective equipment and emergency procedures****General measures**

Avoid dust formation. Avoid contact with skin, eyes and clothes. Use personal protection equipment. Provide adequate ventilation. Avoid breathing dust/fume/gas/mist/vapours/spray.
In case of fire: Evacuate area.

6.2. Environmental precautions

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

6.3. Methods and material for containment and cleaning up**Other information**

Take up mechanically. Treat the recovered material as prescribed in the section on waste disposal. Take up mechanically, placing in appropriate containers for disposal. Avoid dust formation.
Clear contaminated areas thoroughly.

6.4. Reference to other sections

Safe handling: see section 7
Personal protection equipment: see section 8
Disposal: see section 13 Treat the recovered material as prescribed in the section on waste disposal.

SECTION 7: Handling and storage**7.1. Precautions for safe handling****Advice on safe handling**

If handled uncovered, arrangements with local exhaust ventilation have to be used. Avoid dust formation. Do not breathe dust. Provide adequate ventilation.
Avoid dust formation. Avoid breathing dust/fume/gas/mist/vapours/spray.
Avoid contact with skin, eyes and clothes.

Advice on protection against fire and explosion

Usual measures for fire prevention.

Advice on general occupational hygiene

Remove contaminated, saturated clothing immediately. Draw up and observe skin protection programme.
Wash hands and face before breaks and after work and take a shower if necessary. When using do not eat or drink. Avoid contact with skin, eyes and clothes. Provide adequate ventilation. When using do not eat, drink or smoke. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities**Requirements for storage rooms and vessels**

Keep container tightly closed. Keep locked up. Store in a place accessible by authorized persons only.
Provide adequate ventilation as well as local exhaust at critical locations. Keep container tightly closed in a cool, well-ventilated place.
Handle and store contents under inert gas. Protect from moisture. Protect from light!
storage temperature: -20 °C

Hints on joint storage

No special measures are necessary.

7.3. Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

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SECTION 8: Exposure controls/personal protection
8.1. Control parameters
Additional advice on limit values

To date, no national critical limit values exist.

8.2. Exposure controls

Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation have to be used. Do not breathe dust. The receiver of our product is singularly responsible for adhering to existing laws and regulations.

Individual protection measures, such as personal protective equipment
Eye/face protection

Wear eye/face protection.

Hand protection

When handling with chemical substances, protective gloves must be worn with the CE-label including the four control digits. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves. Wear suitable gloves.

Skin protection

Wear suitable protective clothing. Wear suitable protective clothing.

Respiratory protection

If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

Environmental exposure controls

Discharge into the environment must be avoided. Do not empty into drains.

SECTION 9: Physical and chemical properties
9.1. Information on basic physical and chemical properties

Physical state:	solid
Colour:	whitish/ yellowish
Odour:	No data available

Changes in the physical state

Melting point/freezing point:	303 °C
Boiling point or initial boiling point and boiling range:	768 °C
Sublimation point:	not determined
Softening point:	not determined
Pour point:	not determined
:	No data available
Flash point:	418 °C

Flammability

Solid/liquid:	No data available
Gas:	not applicable

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Explosive properties

No data available

Lower explosion limits:

No data available

Upper explosion limits:

No data available

Auto-ignition temperature:

No data available

Self-ignition temperature

Solid:

No data available

Gas:

not applicable

Decomposition temperature:

No data available

Oxidizing properties

No data available

pH-Value:

not determined

Viscosity / dynamic:

not applicable

Viscosity / kinematic:

not applicable

Flow time:

not applicable

Water solubility:

No data available

Solubility in other solvents

Soluble in: Dimethylsulfoxide (DMSO), Dimethylformamide (DMF), Methanol (MeOH), Ethanol (EtOH)

Partition coefficient n-octanol/water:

1,45

Vapour pressure:

not determined

Vapour pressure:

not determined

Density:

1,37 g/cm³

Bulk density:

not determined

Relative vapour density:

No data available

9.2. Other information**Information with regard to physical hazard classes**

Sustaining combustion:

No data available

Other safety characteristics

Solvent separation test:

No data available

Solvent content:

No data available

Solid content:

No data available

Evaporation rate:

not determined

Further Information**SECTION 10: Stability and reactivity****10.1. Reactivity**

No data available

10.2. Chemical stability

Stable under recommended storage conditions.

10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoid

Protect from moisture.

Keep away from heat.

Protect from light!

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10.5. Incompatible materials

 Oxidizing agents, strong.
 Strong acid

10.6. Hazardous decomposition products

 Thermal decomposition can lead to the escape of irritating gases and vapours.
 In case of fire may be liberated: Carbon dioxide (CO₂). Carbon monoxide (CO). Nitrogen oxides (NO_x).

SECTION 11: Toxicological information
11.1. Information on hazard classes as defined in GB CLP Regulation
Toxicokinetics, metabolism and distribution

No data available

Acute toxicity

 Fatal if inhaled.
 Toxic if swallowed.
 Toxic in contact with skin.
 LD50: Intraperitoneal - Mouse: 15 mg/kg

CAS No	Chemical name				
	Exposure route	Dose	Species	Source	Method
58735-64-1	Roquefortine C				
	oral	ATE 100 mg/kg			
	dermal	ATE 300 mg/kg			
	inhalation vapour	ATE 0,5 mg/l			
	inhalation aerosol	ATE 0,05 mg/l			

Irritation and corrosivity

Based on available data, the classification criteria are not met.

Sensitising effects

Based on available data, the classification criteria are not met.

Carcinogenic/mutagenic/toxic effects for reproduction

 Based on available data, the classification criteria are not met.
 IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

STOT-single exposure

Based on available data, the classification criteria are not met.

STOT-repeated exposure

Based on available data, the classification criteria are not met.

Aspiration hazard

Based on available data, the classification criteria are not met.

Specific effects in experiment on an animal

No data available

Additional information on tests

Special hazards arising from the substance or mixture. Classification according to Regulation (EC) No 1272/2008 [CLP]: health hazard properties.

Practical experience

No data available

11.2. Information on other hazards

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Other information

Potential hazards: Neurotoxins

Other adverse effects: Spasms - central nervous system

Roquefortine C is potentially a neurotoxic compound that activates and inhibits detoxification enzymes P-glycoprotein (P-gp) and cytochrome P450-3A.

Further information

RTECS: UQ4730500

Warning - substance not yet tested completely.

SECTION 12: Ecological information**12.1. Toxicity**

No data available

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No data available

Partition coefficient n-octanol/water

CAS No	Chemical name	Log Pow
58735-64-1	Roquefortine C	1,45

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

12.7. Other adverse effects

Warning - substance not yet tested completely.

Further information

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil.

SECTION 13: Disposal considerations**13.1. Waste treatment methods****Disposal recommendations**

Do not allow to enter into surface water or drains. Do not allow to enter into soil/subsoil. Dispose of waste according to applicable legislation. Dispose of waste according to applicable legislation.

Consult the appropriate local waste disposal expert about waste disposal.

Contaminated packaging

This material and its container must be disposed of as hazardous waste. Handle contaminated packages in the same way as the substance itself. Handle contaminated packages in the same way as the substance itself.

SECTION 14: Transport information**Land transport (ADR/RID)**

14.1. UN number:	UN 2811
14.2. UN proper shipping name:	TOXIC SOLID, ORGANIC, N.O.S. (Roquefortine C)
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	II
Hazard label:	6.1

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Classification code:	T2
Special Provisions:	274 614
Limited quantity:	500 g
Excepted quantity:	E4
Transport category:	2
Hazard No:	60
Tunnel restriction code:	D/E

Inland waterways transport (ADN)

14.1. UN number:	UN 2811
14.2. UN proper shipping name:	TOXIC SOLID, ORGANIC, N.O.S. (Roquefortine C)
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	II
Hazard label:	6.1



Classification code:	T2
Special Provisions:	274 614 802
Limited quantity:	500 g
Excepted quantity:	E4

Marine transport (IMDG)

14.1. UN number:	UN 2811
14.2. UN proper shipping name:	TOXIC SOLID, ORGANIC, N.O.S. (Roquefortine C)
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	II
Hazard label:	6.1



Special Provisions:	274
Limited quantity:	500 g
Excepted quantity:	E4
EmS:	F-A, S-A

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number:	UN 2811
14.2. UN proper shipping name:	TOXIC SOLID, ORGANIC, N.O.S.
14.3. Transport hazard class(es):	6.1
14.4. Packing group:	II
Hazard label:	6.1



Special Provisions:	A3 A5
Limited quantity Passenger:	1 kg
Passenger LQ:	Y644

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Excepted quantity:	E4	
IATA-packing instructions - Passenger:		669
IATA-max. quantity - Passenger:		25 kg
IATA-packing instructions - Cargo:		676
IATA-max. quantity - Cargo:		100 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No data available

14.7. Maritime transport in bulk according to IMO instruments

not applicable

SECTION 15: Regulatory information**15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture****EU regulatory information**

Information according to 2012/18/EU (SEVESO III): H2 ACUTE TOXIC

Additional information

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH)

National regulatory information

Employment restrictions: Observe restrictions to employment for juveniles according to the 'juvenile work protection guideline' (94/33/EC). Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

Water hazard class (D): 3 - highly hazardous to water

Skin resorption/Sensitization: Permeates easily through outer skin and causes poisoning.

15.2. Chemical safety assessment

For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information**Abbreviations and acronyms**

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service

LC50: Lethal concentration, 50%

LD50: Lethal dose, 50%

Relevant H and EUH statements (number and full text)

H301	Toxic if swallowed.
H301+H311	Toxic if swallowed or in contact with skin.
H311	Toxic in contact with skin.
H330	Fatal if inhaled.

Further Information

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights. The receiver of our product is singularly

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responsible for adhering to existing laws and regulations. Warning - substance not yet tested completely.

The product is intended for research, analysis and scientific education.

The receiver of our product is singularly responsible for adhering to existing laws and regulations.

The information is based on the present level of our knowledge. It does not, however, give assurance of product properties and establishes no contract legal rights.

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.