

Safety Data Sheet

according to UK REACH Regulation

(-)-Paraherquamide A

Revision date: 19.03.2026

Product code: BI080

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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

(-)-Paraherquamide A

Further trade names

(1'R ,5'aS ,7'R ,8'aS ,9'aR)-2',3',8'a,9'-tetrahydro-1'-hydroxy-1',4,4,8',8', 11'-hexamethyl-spiro[4H,8H-[1,4]dioxepino[2,3-g]indole-8,7'(8'H)-[5H,6H-5a,9a](iminomethano)[1H]cyclopent[f]indolizine]-9,10'(10H)-dione

Substance name: (-)-Paraherquamide A

CAS No: 77392-58-6

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture

Reference standard for analysis.

1.3. Details of the supplier of the safety data sheet

Company name: WITEGA Laboratorien Berlin-Adlershof GmbH

Street: James-Franck-Strasse 4

Place: D-12489 Berlin

Telephone: +493063922001

Telefax: +493063922007

E-mail: witega@witega.de

Internet: www.witega.de

1.4. Emergency telephone number:

+493063922001

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

GB CLP Regulation

Acute Tox. 1; H300

Full text of hazard statements: see SECTION 16.

2.2. Label elements

GB CLP Regulation

Signal word: Danger

Pictograms:



Hazard statements

H300 Fatal if swallowed.

Precautionary statements

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

P262 Do not get in eyes, on skin, or on clothing.

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

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

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3.1. Substances

Sum formula: C₂₈H₃₅N₃O₅
Molecular weight: 493.59 g/mol g/mol

Relevant ingredients

| CAS No | Chemical name | Quantity |
|------------|------------------------------------|----------|
| | EC No | |
| | Index No | |
| | REACH No | |
| | Classification (GB CLP Regulation) | |
| 77392-58-6 | (-)-Paraherquamide A | 100 % |
| | Acute Tox. 1; H300 | |

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

Specific Conc. Limits, M-factors and ATE

| CAS No | EC No | Chemical name | Quantity |
|------------|-------|--|----------|
| | | Specific Conc. Limits, M-factors and ATE | |
| 77392-58-6 | | (-)-Paraherquamide A | 100 % |
| | | oral: LD50 = 5 mg/kg | |

SECTION 4: First aid measures

4.1. Description of first aid measures

General information

In case of accident or unwellness, seek medical advice immediately (show directions for use or safety data sheet if possible).

After inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

After contact with skin

Remove contaminated, saturated clothing immediately. Subsequently wash off with: Water and soap

After contact with eyes

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

After ingestion

Rinse mouth immediately and drink plenty of water. Get immediate medical advice/attention.
Do NOT induce vomiting. Never give anything by mouth to an unconscious person or a person with cramps.

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

No data available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

Water spray jet. Foam. Dry extinguishing powder. Carbon dioxide (CO₂).

5.2. Special hazards arising from the substance or mixture

In case of fire may be liberated: Pyrolysis products, toxic. In case of fire and/or explosion do not breathe fumes.

5.3. Advice for firefighters

In case of fire: Wear self-contained breathing apparatus.

SECTION 6: Accidental release measures

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6.1. Personal precautions, protective equipment and emergency procedures

General advice

Use personal protection equipment. Do not breathe gas/fumes/vapour/spray.

6.2. Environmental precautions

Do not allow to enter into surface water or drains.

6.3. Methods and material for containment and cleaning up

Other information

Take up dust-free and set down dust-free.

6.4. Reference to other sections

Disposal: see section 13

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

If handled uncovered, arrangements with local exhaust ventilation should be used if possible.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take precautionary measures against static discharges.

Advice on general occupational hygiene

Use personal protection equipment.

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

Keep container tightly closed in a cool, well-ventilated place. Avoid: UV-radiation/sunlight

Further information on storage conditions

storage temperature: 2-8°C

7.3. Specific end use(s)

none

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

8.2. Exposure controls

Appropriate engineering controls

If handled uncovered, arrangements with local exhaust ventilation should be used if possible. If local exhaust ventilation is not possible or not sufficient, the entire working area should be ventilated by technical means.

Individual protection measures, such as personal protective equipment

Eye/face protection

Eye glasses with side protection

Hand protection

Wear suitable gloves. 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.

Skin protection

lab coat

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

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SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| | |
|---|-------------------|
| Physical state: | solid |
| Colour: | white |
| Odour: | odourless |
| Melting point/freezing point: | 264-266 °C |
| Boiling point or initial boiling point and boiling range: | No data available |
| Flammability: | No data available |
| Lower explosion limits: | No data available |
| Upper explosion limits: | No data available |
| Flash point: | No data available |
| Auto-ignition temperature: | No data available |
| Decomposition temperature: | No data available |
| pH-Value: | No data available |
| Water solubility: | No data available |
| Solubility in other solvents | |
| No data available | |
| Partition coefficient n-octanol/water: | No data available |
| Vapour pressure: | No data available |
| Density: | No data available |
| Relative vapour density: | No data available |

9.2. Other information

Information with regard to physical hazard classes

Explosive properties

No data available

Self-ignition temperature

Solid:

No data available

Gas:

No data available

Oxidizing properties

No data available

Other safety characteristics

Evaporation rate:

No data available

Further Information

none

SECTION 10: Stability and reactivity

10.1. Reactivity

Reacts with : Oxidising agent, Alkali (lye), Etchant and acids

10.2. Chemical stability

The product is chemically stable under recommended conditions of storage, use and temperature.

10.3. Possibility of hazardous reactions

No known hazardous reactions.

10.4. Conditions to avoid

Do not expose to temperatures exceeding 50 °C/122 °F.

10.5. Incompatible materials

Oxidising agent, Alkali (lye), Etchant and acids

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10.6. Hazardous decomposition products

In case of fire may be liberated: Pyrolysis products, toxic.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in GB CLP Regulation

Acute toxicity

Fatal if swallowed.

| CAS No | Chemical name | | | | |
|------------|----------------------|--------------|---------|--------|--------|
| | Exposure route | Dose | Species | Source | Method |
| 77392-58-6 | (-)-Paraherquamide A | | | | |
| | oral | LD50 5 mg/kg | Mouse | | |

Irritation and corrosivity

Skin corrosion/irritation: Based on available data, the classification criteria are not met.

Serious eye damage/eye irritation: 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

Germ cell mutagenicity: Based on available data, the classification criteria are not met.

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

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

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

SECTION 12: Ecological information

12.1. Toxicity

No data available

12.2. Persistence and degradability

No data available

12.3. Bioaccumulative potential

No indication of bioaccumulation potential.

12.4. Mobility in soil

No data available

12.5. Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of UK REACH.

This substance does not meet the PBT/vPvB criteria of REACH, Annex XIII.

12.6. Endocrine disrupting properties

This substance does not have endocrine disrupting properties with respect to non-target organisms.

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

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13.1. Waste treatment methods

Disposal recommendations

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

Contaminated packaging

This material and its container must be disposed of as hazardous waste.

SECTION 14: Transport information

Land transport (ADR/RID)

14.1. UN number or ID 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: I
Hazard label: 6.1



Classification code: T2
Special Provisions: 274 614
Limited quantity: 0
Excepted quantity: E5
Transport category: 1
Hazard No: 66
Tunnel restriction code: C/E

Inland waterways transport (ADN)

14.1. UN number or ID 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: I
Hazard label: 6.1



Classification code: T2
Special Provisions: 274 614 802
Limited quantity: 0
Excepted quantity: E5

Marine transport (IMDG)

14.1. UN number or ID 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: I
Hazard label: 6.1



Marine pollutant: no
Special Provisions: 274
Limited quantity: 0
Excepted quantity: E5

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EmS: F-A, S-A

Air transport (ICAO-TI/IATA-DGR)

14.1. UN number or ID 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: I
Hazard label: 6.1



Special Provisions: A3 A5
Limited quantity Passenger: Forbidden
Passenger LQ: Forbidden
Excepted quantity: E5
IATA-packing instructions - Passenger: 666
IATA-max. quantity - Passenger: 5 kg
IATA-packing instructions - Cargo: 673
IATA-max. quantity - Cargo: 50 kg

14.5. Environmental hazards

ENVIRONMENTALLY HAZARDOUS: No

14.6. Special precautions for user

No transport as bulk according to IBC Code.

14.7. Maritime transport in bulk according to IMO instruments

No transport as bulk according to IBC Code.

SECTION 15: Regulatory information

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

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.

15.2. Chemical safety assessment

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

SECTION 16: Other information

Abbreviations and acronyms

Acute Tox: Acute toxicity

Relevant H and EUH statements (number and full text)

H300 Fatal if swallowed.

Further Information

This information is based on our present state of knowledge. However, it should not constitute a guarantee for any specific product properties and shall not establish a legally valid relationship. The substances are only for R&D. Do not use as a drug, in household or other applications.