

Safety Data Sheet

according to UK REACH Regulation

Lubabegron hemifumarate

Revision date:

Product code: OP278

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

1.1. Product identifier

Lubabegron hemifumarate

Further trade names

2-[4-{2-[[[(2S)-2-Hydroxy-3-[2-(2-thienyl)phenoxy]propyl]amino]-2-methylpropyl}phenoxy]-3-pyridinecarbonitrile
(2E)-2-butenedioate (2:1 salt)

Substance name: Lubabegron hemifumarate

CAS No: 391926-19-5

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

Flam. Sol. 1; H228

Repr. 1A; H360

Eye Dam. 1; H318

STOT RE 1; H372

Aquatic Chronic 4; H413

Full text of hazard statements: see SECTION 16.

2.2. Label elements

GB CLP Regulation

Signal word: Danger

Pictograms:



Hazard statements

H228 Flammable solid.

H318 Causes serious eye damage.

H360 May damage fertility or the unborn child.

H372 Causes damage to organs through prolonged or repeated exposure.

H413 May cause long lasting harmful effects to aquatic life.

2.3. Other hazards

No data available

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SECTION 3: Composition/information on ingredients

3.1. Substances

Sum formula: C₂₉H₂₉N₃O₃S ? ½ C₄H₄O₄
Molecular weight: 557.66 g/mol

Hazardous components

CAS No	Chemical name			Quantity
	EC No	Index No	REACH No	
	Classification (GB CLP Regulation)			
391926-19-5	Lubabegron hemifumarate			100 %
	Flam. Sol. 1, Repr. 1A, Eye Dam. 1, STOT RE 1, Aquatic Chronic 4; H228 H360 H318 H372 H413			

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

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

Changes in the physical state

Melting point/freezing point: 150-152 °C
Boiling point or initial boiling point and boiling range: No data available
Flash point: No data available

Flammability

Solid/liquid: No data available
Gas: No data available

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: 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

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.

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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

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

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

Irritation and corrosivity

Causes serious eye damage.

Skin corrosion/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

May damage fertility or the unborn child. (Lubabegron hemifumarate)

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

Carcinogenicity: 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

Causes damage to organs through prolonged or repeated exposure. (Lubabegron hemifumarate)

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

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SECTION 13: Disposal considerations

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)

14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.

Inland waterways transport (ADN)

14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.

Marine transport (IMDG)

14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.

Air transport (ICAO-TI/IATA-DGR)

14.2. UN proper shipping name: No dangerous good in sense of this transport regulation.

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

No dangerous good in sense of this transport regulation.

SECTION 15: Regulatory information

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

EU regulatory information

Restrictions on use (REACH, annex XVII):

Entry 40

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

15.2. Chemical safety assessment

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

SECTION 16: Other information

Relevant H and EUH statements (number and full text)

H228	Flammable solid.
H318	Causes serious eye damage.
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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.