

According to Regulation (EC) No 1907/2006

According to Regulation (EC) No 2020/878

Aprepitant

Version number: 1
Issued: 2024-02-23



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

1.1. Product identifier

Trade name

Aprepitant

CAS number

170729-80-3

EC number

677-636-6

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

Relevant identified uses

Research and development. Laboratory Chemicals. Manufacture of substances.

Not suitable for use in

Not suitable for human consumption or veterinary purposes.

1.3. Details of the supplier of the safety data sheet

Supplier

Molekula Group

Address

Molekula Ltd, Lingfield Way, Darlington,
DL1 4XX Darlington
United Kingdom

Telephone

+44 (0) 3302 000 333

Email

info@molekula.com

Web site

www.molekula.com

Contact person

Kevin Banks

Email

+44 (0) 7769276927

1.4. Emergency telephone number

Poison center/Additional emergency number

0344 892 0111 - National Poisons Information Service (Newcastle Centre)

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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

Classification

Carcinogenicity, hazard category 2

Hazardous to the aquatic environment — Chronic hazard category 3

Specific Target Organ Toxicity — Repeated exposure, hazard category 2

Eye irritation, hazard category 2

Acute toxicity, oral, hazard category 4

Hazard statements

H302, H319, H351, H373, H412

2.2. Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms



Signal word

Warning

Hazard statements

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

H351 Suspected of causing cancer.

H373 May cause damage to organs through prolonged or repeated exposure.

H412 Harmful to aquatic life with long lasting effects.

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Precautionary statements

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P260 Do not breathe dust/fumes/gas/mist/vapours/spray.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P314 Get medical advice/attention if you feel unwell.
P330 Rinse mouth.
P301 + P312 IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313 IF exposed or concerned: Get medical advice/attention.
P337 + P313 If eye irritation persists: Get medical advice/attention.
P405 Store locked up.
P501 Dispose of contents/container to local regulations.

2.3. Other hazards

No data available

SECTION 3: Composition/information on ingredients

3.2. Mixtures

Chemical name	CAS No. EC No. REACH No. Index No.	Concentration	Classification	H-phrase M factor acute M factor chronic	Note
Aprepitant	170729-80-3 677-636-6 - -	100%	Acute Tox. 4 - oral, Eye Irrit. 2, Carc. 2, STOT RE 2, Aquatic Chronic 3	H302, H319, H351, H373, H412 - -	-

Molecular weight

534.43

Substance additional information

For the complete text of H- / EUH-statements mentioned in this section, see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

Get medical attention if any discomfort continues. Show this Safety Data Sheet (SDS) to medical personnel.

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Inhalation

IF INHALED: Remove person to fresh air and keep comfortable for breathing. In case of persistent throat irritation or coughing: Seek medical attention and bring these instructions.

Skin contact

IF ON SKIN: Wash with plenty of water. Continue to rinse for at least 15 minutes and seek medical attention. Get medical advice/attention if you feel unwell.

Eye contact

Remove contact lenses if present. Rinse eyes with water. Continue to rinse for at least 15 minutes and seek medical attention.

Ingestion

IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. Get medical advice/attention if you feel unwell.

Information for doctors

First aiders/ medical personnel need to protect themselves.

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

The severity of the symptoms described will vary dependant of the concentration and the length of exposure.

Inhalation

Single exposure may cause the following adverse effects: Upper respiratory irritation. Difficulty in breathing.

Skin contact

Single exposure may cause the following adverse effects: Severe skin irritation.

Eye contact

Single exposure may cause the following adverse effects: Severe irritation.

Ingestion

Single exposure may cause the following adverse effects: Severe abdominal pain. Nausea, vomiting.

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

Treat symptomatically. No special treatment requirement.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

In case of fire: Use foam, carbon dioxide, dry powder or water fog to extinguish.

Unsuitable extinguishing media

No specific fire fighting procedure given.

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5.2. Special hazards arising from the substance or mixture

Specific hazards: None.

Thermal decomposition or combustion may liberate carbon oxides and other toxic gases or vapours.

Carbon dioxide (CO₂). Carbon monoxide (CO).

Nitrous gases (NO_x).

Hydrogen fluoride (HF).

5.3. Advice for firefighters

Special protective equipment for fire-fighters

Evacuate area. Avoid breathing gas, fume, vapours or spray. Cool containers exposed to heat with water spray and remove container, if no risk is involved.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Avoid breathing dust/fume/gas/mist/vapours/spray. Provide adequate ventilation. Avoid contact with skin and eyes. For personal protection, see section 8.

6.2. Environmental precautions

Avoid discharge into drains, water courses or onto the ground.

6.3. Methods and material for containment and cleaning up

Collect spillage with shovel, broom or the like and reuse, if possible. Dispose of large amounts of spillage/waste according to agreement with local authorities.

6.4. Reference to other sections

For personal protection, see section 8. For waste disposal, see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Preventive handling precautions

For precautions see section 2.2. Wear protective clothing, gloves, eye and face protection. Avoid contact with skin and eyes. Do not breathe dust/fume/gas/mist/vapours/spray. Avoid ingestion and inhalation.

General hygiene

Observe good chemical hygiene practices. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove contaminated clothing and launder thoroughly before re-use. Wash skin thoroughly after handling.

7.2. Conditions for safe storage, including any incompatibilities

Store in a dry place. Store in a closed container.

Recommended storage temperature: -20 to -15°C (-4 to 5°F)

7.3. Specific end use(s)

No specific usage precautions noted.

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SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No data available

8.2. Exposure controls

Personal Protective Equipment Symbols



Eye / face protection

Wear eye protection.

Hand protection

Wear protective gloves. Recommended gloves: Viton rubber (fluor rubber).

Always inspect gloves before use. If signs of wear and tear are noticed then the gloves should be replaced.

No specific hygiene procedures noted, but good personal hygiene practices are always advisable, especially when working with chemicals. Wash contaminated skin thoroughly after handling.

Other skin protection

Wash skin thoroughly after handling.

Respiratory protection

Provide adequate ventilation. If ventilation is insufficient, suitable respiratory protection must be provided.

Environmental exposure controls

Avoid discharge into drains.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state

Solid

Colour

White / off-white.

Odour

No data available

Melting point / freezing point

242 - 246 °C

Boiling point or initial boiling point and boiling range

No data available

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Flammability

No data available

Lower and upper explosion limit

No data available

Flash point

No data available

Auto-ignition temperature

No data available

Decomposition temperature

No data available

pH

7.2

Kinematic viscosity

No data available

Solubility

No data available

Partition coefficient n-octanol/water

No data available

Vapour pressure

No data available

Density and/or relative density

1.51 g/cm³

Relative vapour density

No data available

Particle characteristics

No data available

9.2. Other information

No data available

SECTION 10: Stability and reactivity

10.1. Reactivity

There are no known reactivity hazards associated with this product.

10.2. Chemical stability

Stable under the prescribed storage conditions.

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10.3. Possibility of hazardous reactions

No data available

10.4. Conditions to avoid

No data available

10.5. Incompatible materials

Strong oxidising agents.

10.6. Hazardous decomposition products

See section 5.

SECTION 11: Toxicological information

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Acute toxicity

Product / Substance name CAS / EC no.	Exposure route	Remarks
Aprepitant 170729-80-3 / 677-636-6	Oral	Harmful if swallowed.

Carcinogenicity

Product / Substance name CAS / EC no.	Other
Aprepitant 170729-80-3 / 677-636-6	Carcinogen Category 2.

STOT-repeated exposure

Product / Substance name CAS / EC no.	Result
Aprepitant 170729-80-3 / 677-636-6	May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard

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

11.2. Information on other hazards

No data available

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SECTION 12: Ecological information

12.1. Toxicity

Acute fish toxicity

Product / Substance name CAS / EC no.	Value / Result
Aprepitant 170729-80-3 / 677-636-6	Harmful to aquatic life with long lasting effects.

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. Endocrine disrupting properties

This product does not contain any known or suspected endocrine disruptors.

12.7. Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Disposal considerations

Dispose of contents/container in accordance with local/regional/national/international regulations.

SECTION 14: Transport information

14.1. UN number

Not applicable

14.2. UN proper shipping name

Not applicable

14.3. Transport hazard class(es)

Not applicable

14.4. Packing group

Not applicable

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14.5. Environmental hazards

Not applicable

14.6. Special precautions for user

Not applicable

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 regulations

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

This material safety data sheet complies with the requirements of Regulation (EU) 2020/878.

National regulations

No data available

15.2. Chemical safety assessment

No data available

SECTION 16: Other information

Phrase meaning

Carc. 2 - Carcinogenicity, hazard category 2

Aquatic Chronic 3 - Hazardous to the aquatic environment — Chronic hazard category 3

STOT RE 2 - Specific Target Organ Toxicity — Repeated exposure, hazard category 2

Eye Irrit. 2 - Eye irritation, hazard category 2

Acute Tox. 4 - oral - Acute toxicity, oral, hazard category 4

H302 Harmful if swallowed.

H319 Causes serious eye irritation.

H351 Suspected of causing cancer.

H373 May cause damage to organs through prolonged or repeated exposure.

H412 Harmful to aquatic life with long lasting effects.