

Safety Data Sheet

1. Identification of the substance

- 1.1. *Product identifiers:* *Product Name:* 5-{{(2R,3S)-2-[(1R)-1-[3,5-bis(Trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)morpholin-4-yl]methyl}-2,3-dihydro-1H-1,2,4-triazol-3-one
Synonyms: Aprepitant
Catalog number: QA-9914
CAS Number: 170729-80-3
- 1.2. *Identified use:* Laboratory chemicals, for scientific research and development only.
- 1.3. *Supplier:* Combi-Blocks, Inc., 7949 Silverton Ave # 915, San Diego, CA 92126, USA. Tel: 858-635-8950. Email: sales@combi-blocks.com.
- 1.4. *Emergency Contact:* During normal business hours (Monday-Friday 8am-5pm PST), call 1-858-635-8950. After business hours, call Infotrac at 1-800-535-5053 (USA) or 1-352-323-3500 (international).

2. Hazards identification

- 2.1. *Classification of the substance or mixture:*
 GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
 Acute toxicity, oral (Category 4), H302
 Skin corrosion/irritation (Category 2), H315
 Serious eye damage/eye irritation (Category 2), H319
 Specific target organ toxicity, single exposure; Respiratory tract irritation (Category 3), H335

2.2. GHS Label elements, including precautionary statements:

Pictograms



Signal word

Warning

Hazard statement(s).

H302 Harmful if swallowed
 H315 Causes skin irritation
 H319 Causes serious eye irritation
 H335 May cause respiratory irritation

Precautionary statement(s).

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
 P264 Wash thoroughly after handling.
 P270 Do not eat, drink or smoke when using this product.
 P271 Use only outdoors or in a well-ventilated area.
 P280 Wear protective gloves/protective clothing/eye protection/face protection.
 P301+P312+P330 If swallowed: Call a POISON CENTER or doctor/physician if you feel unwell. Rinse mouth.
 P302+P352 If on skin: Wash with soap and water.
 P304+P340+P312 If inhaled: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician 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.
 P332+P313 If skin irritation occurs: Get medical advice/attention.
 P337+P313 If eye irritation persists: get medical advice/attention.
 P362 Take off contaminated clothing and wash before reuse.
 P403+P233 Store in a well ventilated place. Keep container tightly closed.
 P405 Store locked up.
 P501 Dispose of contents/container to an approved waste disposal plant.

3. Composition/information on ingredients.

3.1. Substances

COMPONENT	CLASSIFICATION	CONCENTRATION
5-{{[(2R,3S)-2-{{[(1R)-1-{{3,5-bis(Trifluoromethyl)phenyl}ethoxy}-3-(4-fluorophenyl)morpholin-4-yl]methyl}}-2,3-dihydro-1H-1,2,4-triazol-3-one	H302, H315, H319, H335	≤ 100

See Section 2 for full text of hazard statements.

4. First aid measures

4.1. Description of first aid measures.

- General advice:* Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
- If inhaled:* Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or doctor/physician if you feel unwell.
- In case of skin contact:* Wash with soap and water.
- In case of eye contact:* Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do – continue rinsing.
- If swallowed:* Call a POISON CENTER or doctor/physician if you feel unwell. Rinse mouth.

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

See Section 2.2 and/or in Section 11.

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

No data.

5. Fire fighting measures

- 5.1. *Extinguishing media:* Use dry sand, dry chemical or alcohol-resistant foam for extinction.
- 5.2. *Special hazards arising from the substance or mixture:* Carbon monoxide, nitrogen oxides, hydrogen fluoride.
- 5.3. *Advice for firefighters:* Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4. *Further information:* No data available.

6. Accidental release measures

- 6.1. *Personal precautions, protective equipment and emergency procedures:*
Ensure adequate ventilation. Use personal protective equipment.
- 6.2. *Environmental precautions:*
Should not be released into the environment. See Section 12 for additional ecological information.
- 6.3. *Methods and materials for containment and cleaning up:*
Sweep up or vacuum up spillage and collect in suitable container for disposal.
- 6.4. *Reference to other sections:*
Refer to protective measures listed in Sections 8 and 13.

7. Handling and storage

- 7.1. *Precautions for safe handling:* Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge. For precautions see section 2.2.
- 7.2. *Conditions for safe storage, including any incompatibilities:* Store refrigerated. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
- 7.3. *Specific end use(s):* Laboratory chemicals, for scientific research and development only.

8. Exposure Controls / Personal protection

- 8.1. *Control parameters:*
Components with workplace control parameters: Contains no substances with occupational exposure limit values.
- 8.2. *Exposure controls:*
Appropriate engineering controls: Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use only under a chemical fume hood.

Personal protective equipment:

- Eye/face protection:* Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.
- Skin protection:* Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands
- Body Protection:* Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.
- Respiratory protection:* No protective equipment is needed under normal use conditions.
- Control of environmental exposure:* Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. Physical and chemical properties*9.1. Information on basic physical and chemical properties*

(a)	Appearance:	Solid
(b)	Odour:	No data
(c)	Odour Threshold:	No data
(d)	pH:	No data
(e)	Melting point/freezing point:	250 - 260°C
(f)	Initial boiling point and boiling range:	No data
(g)	Flash point:	No data
(h)	Evaporatoin rate:	No data
(i)	Flammability (solid, gas):	No data
(j)	Upper/lower flammability or explosive limits:	No data
(k)	Vapour pressure:	No data
(l)	Vapour density:	No data
(m)	Relative density:	No data
(n)	Water solubility:	No data
(o)	Partition coefficient: n-octanol/water:	No data
(p)	Auto-ignition:	No data
(q)	Decomposition temperature:	No data
(r)	Viscosity:	No data
(s)	Explosive properties:	No data
(t)	Oxidizing properties:	No data

9.2. Other safety information:

Formula	C ₂₃ H ₂₁ F ₇ N ₄ O ₃
Molecular weight	534.4
CAS Number	170729-80-3

10. Stability and reactivity

- 10.1. *Reactivity* No data
- 10.2. *Chemical stability* Stable under recommended storage conditions.
- 10.3. *Possibility of hazardous reactions* No data
- 10.4. *Conditions to avoid*
- 10.5. *Incompatible material* No data.
- 10.6. *Hazardous decomposition products:*

Hazardous decomposition products formed under fire conditions: Carbon monoxide, nitrogen oxides, hydrogen fluoride.

Other decomposition products: No data

In the event of fire: See Section 5.

11. Toxicological information

11.1 Information on toxicological effects

<i>Acute toxicity:</i>	Harmful if swallowed. .
<i>Skin irritation/corrosion:</i>	No data available.
<i>Eye damage/irritation:</i>	Causes serious eye irritation.
<i>Respiratory or skin sensitization:</i>	May cause respiratory irritation.
<i>Germ cell mutagenicity:</i>	No data available.
<i>Carcinogenicity:</i>	No data available.
<i>Reproductive toxicity:</i>	No data available.
<i>Specific target organ system toxicity - single exposure:</i>	No data available.
<i>Specific target organ system toxicity - repeated exposure:</i>	No data available.
<i>Aspiration hazard:</i>	No data available.
<i>Additional information:</i>	To the best of our knowledge, the chemical, physical and toxicological properties of this substance have not been thoroughly investigated.

12. Ecological information

12.1. Toxicity	No data available.
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.

13. Disposal Considerations

13.1. Waste treatment methods

<i>Product</i>	Arrange disposal as special waste, by licensed disposal company, in consultation with local waste disposal authority, in accordance with national and regional regulations.
<i>Contaminated packaging</i>	Dispose of as unused product.

14. Transportation information

DOT (US), IMDG and IATA:

No known hazard for air and ground transportation.

15. Regulatory information

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302, or have known CAS numbers that exceed the threshold reporting levels established by SARA Title III, Section 313.

16. Other information

This MSDS is correct to the best of our knowledge at the date of publication but does not purport to be all inclusive and shall be used only as a guide. Combi-Blocks shall not be held liable for any injury or damage resulting from handling or from contact with the above product.