

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)
No data.
- 2.2. *GHS Label elements, including precautionary statements:*
No known hazard.

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		≤ 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. In severe cases or if symptoms persist, seek medical attention.
- In case of skin contact:* Immediately wash skin with copious amounts of water for at least 15 minutes while removing contaminated clothing and shoes. If irritation persists, seek medical attention.
- In case of eye contact:* Immediately flush with plenty of water. After initial flushing, remove any contact lenses and continue flushing for at least 15 minutes. Keep eye wide open while rinsing. Get medical attention.
- If swallowed:* Wash out mouth with copious amounts of water for at least 15 minutes. Seek medical attention.

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 electro-static 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.
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:
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)	Evaporatoion 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	$C_{23}H_{21}F_7N_4O_3$
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:*

<i>Hazardous decomposition products formed under fire conditions:</i>	Carbon monoxide, nitrogen oxides, hydrogen fluoride.
<i>Other decomposition products:</i>	No data
<i>In the event of fire:</i>	See Section 5.

11. Toxicological information

11.1 Information on toxicological effects

<i>Acute toxicity:</i>	.
<i>Skin irritation/corrosion:</i>	No data available.
<i>Eye damage/irritation:</i>	No data available.
<i>Respiratory or skin sensitization:</i>	No data available.
<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.

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| 12.2. <i>Persistence and degradability</i> | No data available. |
| 12.3. <i>Bioaccumulative potential</i> | No data available |
| 12.4. <i>Mobility in soil</i> | No data available |
| 12.5. <i>Results of PBT and vPvB assessment</i> | No data available. |
| 12.6. <i>Other adverse effects</i> | No data available. |

13. Disposal Considerations

13.1. *Waste treatment methods*

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| <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.