

# PHYSICAL AND CHEMICAL PROPERTIES

Product Name:	Aprepitant
Catalog Number:	BCC1101
Cas No.:	170729-80-3
Formula:	C23H21F7N4O3
M.Wt:	534.43
Purity:	>98%
Physical Description:	N/A
Synonyms:	Emend; MK-869; MK-0869; Aprepitantum
Chemical Name:	5-[[(2S,3R)-2-[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophe
	nyl)morpholin-4-yl]methyl]-1,2-dihydro-1,2,4-triazol-3-one
SMILES:	CC(C1=CC(=C1)C(F)(F)F)C(F)(F)F)OC2C(N(CCO2)CC3=NC(=O)N)
	N3)C4=CC=C(C=C4)F
Solubility:	$DMSO :\ge 100 \text{ mg/mL} (187.12 \text{ mM})$
	$*"\geq"$ means soluble, but saturation unknown.

## STORAGE AND SHIPPING

Storage:	Store the product in sealed, cool and dry condition.
General tips:	For obtaining a higher solubility, please warm the tube at $37^{\circ}$ and shake it in
	the ultrasonic bath for a while. Stock solution can be stored below -20 $^{\circ}$ for
	several months.
Shipping Condition:	Ship with RT, or blue ice upon request

## **INTENDED USE**

- 1. Reference standards;
- 2. Pharmacological research;
- 3. Food research;
- 4. Synthetic precursor compounds;
- 5. Intermediates & Fine Chemicals;
- 6. Others.

## **CAUTION!**

## FOR RESEARCH PURPOSES ONLY.

## NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

Specific storage and handling information for each product is indicated on the product datasheet. Most BioCrick products are stable under the recommended conditions. Products are sometimes shipped at a temperature that differs from the recommended storage temperature. Short-term storage of many products are stable in the short-term at temperatures that differ from that required for long-term storage. We ensure that the product is shipped under conditions that will maintain the quality of the reagents. Upon receipt of the product, follow the storage recommendations on the product data sheet.

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