

# **Product Datasheet**

## PHYSICAL AND CHEMICAL PROPERTIES

Product Name: HOE 140
Catalog Number: BCC5964
Cas No.: 130308-48-4

**Formula:** C59H89N19O13S

M.Wt: 1304.52
Purity: >98%
Physical Description: N/A

Synonyms: Icatibant

**Chemical Name:** (2S)-2-[[(3aS,7aS)-1-[2-[(2S)-2-[[(2S)-2-[[(4R)-1-[1-[2-[[(2R)-2-amino-5-

(diaminomethylideneamino)pentanoyl]amino]-5-(diaminomethylideneamino)pentanoyl]pyrrolidine-2-carbonyl]-4-hydroxypyrrolidine-2-carbonyl]amino]acetyl]amino]-3-thiophen-2-ylpropanoyl]amino]-3-hydroxypropanoyl]-3,4-dihydro

-1H-isoquinoline-3-carbonyl]-2,3,3a,4,5,6,7,7a-

octahydroindole-2-carbonyl]amino]-5-(diaminomethylideneamino)pentanoic

acid;acetic acid

**SMILES:** CC(=0)O.C1CCC2C(C1)CC(N2C(=0)C3CC4=CC=C4CN3C(=0)C(C

O)NC(=O)C(CC5=CC=CS5)NC(=O)CNC(=O)C6CC(CN6C(=O)C7CCCN7 C(=O)C(CCCN=C(N)N)NC(=O)C(CCCN=C(N)N)N)O)C(=O)NC(CCCN=C

(N)N)C(=O)O

**Solubility:**  $H2O : \ge 50 \text{ mg/mL } (38.33 \text{ mM})$ 

\*"≥" 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° and shake it in

the ultrasonic bath for a while. Stock solution can be stored below -20° 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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