Product Datasheet

PHYSICAL AND CHEMICAL PROPERTIES

Product Name: Simeprevir

Catalog Number: BCC1949

Cas No.: 923604-59-5

Formula: C38H47N5O7S2

M.Wt: 749.96

Purity: >98%

Physical Description: N/A

Synonyms: TMC435

Chemical Name: (1R,4R,6S,7Z,15R,17R)-N-cyclopropylsulfonyl-17-[7-methoxy-8-methyl-2-(4-propan-2-yl-1,3-thiazol-2-yl)quinolin-4-yl]oxy-13-methyl-2,14-dioxo-3,13-diazatricyclo[13.3.0.04,6]octadec-7-ene-4-carboxamide

SMILES: CC1=C(C=CC2=C1N=C(C=C2OC3CC4C(C3)C(=O)N(CCCCC=CC5CC5(NC4=O)C(=O)NS(=O)(=O)C6CC6)C)C7=NC(=CS7)C(C)C)OC

Solubility: DMSO : 14.29 mg/mL (19.05 mM; Need ultrasonic)

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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