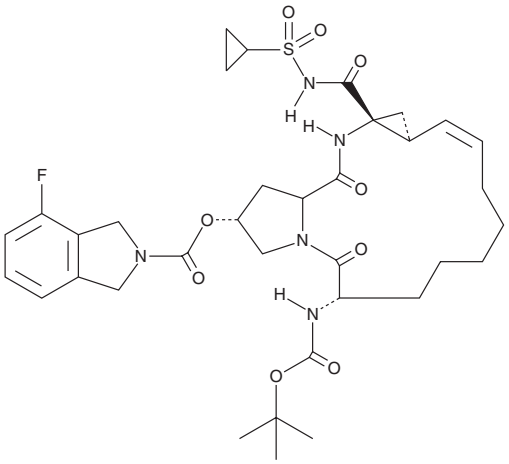
# PRODUCT INFORMATION

## Danoprevir

*Item No. 24185*

**CAS Registry No.:** 850876-88-9
**Formal Name:** 4-fluoro-1,3-dihydro-2H-isoindole-2-carboxylic acid, (2R,6S,13aS,14aR,16aS)-14a-[[(cyclopropylsulfonyl)amino]carbonyl]-6-[[(1,1-dimethylethoxy)carbonyl]amino]-1,2,3,5,6,7,8,9,10,11,13a,14,14a,15,16,16a-hexadecahydro-5,16-dioxocyclopropa[e]pyrrolo[1,2-a][1,4]diazacyclopentadecin-2-yl ester
**Synonyms:** ITMN-191, R-7227
**MF:** $C_{35}H_{46}FN_5O_9S$
**FW:** 731.8
**Purity:** ≥95%
**Supplied as:** A crystalline solid
**Storage:** -20°C
**Stability:** ≥4 years



*Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.*

### Laboratory Procedures

Danoprevir is supplied as a crystalline solid. A stock solution may be made by dissolving the danoprevir in the solvent of choice, which should be purged with an inert gas. Danoprevir is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of danoprevir in these solvents is approximately 15, 25, and 30 mg/ml, respectively.

Danoprevir is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, danoprevir should first be dissolved in DMF and then diluted with the aqueous buffer of choice. Danoprevir has a solubility of approximately 0.20 mg/ml in a 1:4 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

Danoprevir is an orally bioavailable inhibitor of hepatitis C virus (HCV) nonstructural protein 3/4A (NS3/4A; $IC_{50}$ = 1 nM), a serine protease essential for HCV replication.[1] It is selective for NS3/4A over a panel of 53 proteases at a concentration of 10 µM. Danoprevir inhibits replication of the HCV genotypes 1a, 1b, 4, 5, and 6 ($IC_{50}$s = 0.2-0.4 nM) as well as 2b and 3a ($IC_{50}$s = 1.6 and 3.5 nM, respectively) *in vitro*. It also reduces the number of HCV genotype 1b replicons in Huh-7 cells ($EC_{50}$ = 1.8 nM).

### Reference


1. Seiwert, S.D., Andrews, S.W., Jiang, Y., *et al.* Preclinical characteristics of the hepatitis C virus NS3/4A protease inhibitor ITMN-191 (R7227). *Antimicrob. Agents Chemother.* **52(12)**, 4432-4441 (2008).





**CAYMAN CHEMICAL**
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
**PHONE:** [800] 364-9897
[734] 971-3335
**FAX:** [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM