

# PRODUCT INFORMATION



## Boceprevir

Item No. 18379

**CAS Registry No.:** 394730-60-0  
**Formal Name:** (1R,2S,5S)-N-[3-amino-1-(cyclobutylmethyl)-2,3-dioxopropyl]-3-[(2S)-2-[[[(1,1-dimethylethyl)amino]carbonyl]amino]-3,3-azabicyclo[3.1.0]hexane-2-carboxamide

**Synonyms:** SCH 503034

**MF:** C<sub>27</sub>H<sub>45</sub>N<sub>5</sub>O<sub>5</sub>

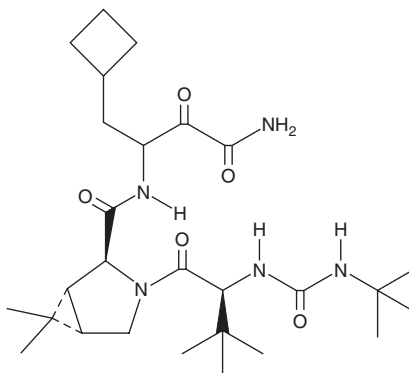
**FW:** 519.7

**Purity:** ≥98%

**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

Boceprevir is supplied as a crystalline solid. A stock solution may be made by dissolving the boceprevir in the solvent of choice, which should be purged with an inert gas. Boceprevir is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of boceprevir in ethanol and DMF is approximately 25 mg/ml and approximately 16 mg/ml in DMSO.

Boceprevir is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, boceprevir should first be dissolved in ethanol and then diluted with the aqueous buffer of choice. Boceprevir has a solubility of approximately 0.14 mg/ml in a 1:6 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

Boceprevir is an inhibitor of hepatitis C virus (HCV) non-structural protease 3/4A (NS3/4A;  $K_i = 14$  nM for the HCV genotype 1b enzyme).<sup>1</sup> Boceprevir inhibits HCV replication in Huh7 cells ( $EC_{50} = 200$  nM).<sup>2</sup> It also inhibits severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) main protease ( $M^{pro}$ ;  $K_i = 1.8$   $\mu$ M) and reduces cytopathic effects of SARS-CoV-2 in Vero cells ( $EC_{50} = 1.31$   $\mu$ M).<sup>3</sup> Formulations containing boceprevir have been used in the treatment of HCV.

### References

1. Malcolm, B.A., Liu, R., Lahser, F., *et al.* SCH 503034, a mechanism-based inhibitor of hepatitis C virus NS3 protease, suppresses polyprotein maturation and enhances the antiviral activity of alpha interferon in replicon cells. *Antimicrob. Agents Chemother.* **50(3)**, 1013-1020 (2006).
2. Trembling, P.M., Tanwar, S., and Dusheiko, G.M. Boceprevir: An oral protease inhibitor for the treatment of chronic HCV infection. *Expert Rev. Anti. Infect. Ther.* **10(3)**, 269-279 (2012).
3. Ma, C., Sacco, M.D., Hurst, B., *et al.* Boceprevir, GC-376, and calpain inhibitors II, XII inhibit SARS-CoV-2 viral replication by targeting the viral main protease. *Cell Res.* **30(8)**, 678-692 (2020).

#### WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 12/22/2022

#### 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