

Product Name: Takinib

Catalog No.: 6430

Batch No.: 1

CAS Number: 1111556-37-6

IUPAC Name: *N*¹-(1-Propyl-1*H*-benzimidazol-2-yl)-1,3-benzenedicarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₈N₄O₂·¼H₂O

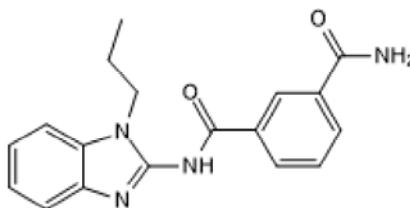
Batch Molecular Weight: 326.87

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.14	5.7	17.14
Found	66.51	5.68	17.22

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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CAS Number: 1111556-37-6

IUPAC Name: *N*¹-(1-Propyl-1*H*-benzimidazol-2-yl)-1,3-benzenedicarboxamide

Description:

Potent and selective TAK1/MAP3K7 kinase inhibitor (IC₅₀ = 8.2-9.5 nM). Selective for TAK1 over IRAK4, IRAK1, GCK, CLK2 and MINK1 (IC₅₀ values = 120, 390, 430, 430 and 1900 nM, respectively). Demonstrates weak inhibition at Src and Yes1. Exhibits no inhibition of MAP2K or other MAP3K family members. Induces apoptosis following TNF-α stimulation in in vitro models of rheumatoid arthritis and metastatic breast cancer.

Physical and Chemical Properties:

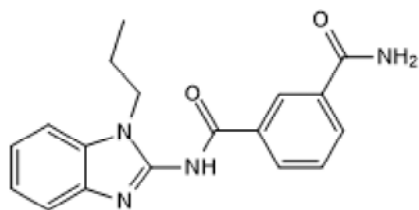
Batch Molecular Formula: C₁₈H₁₈N₄O₂·¼H₂O

Batch Molecular Weight: 326.87

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Totzke *et al* (2017) Takinib, a selective TAK1 inhibitor, broadens the therapeutic efficacy of TNF-α inhibition for cancer and autoimmune disease. *Cell Chem.Biol.* **24** 1029. PMID: 28820959.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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