Ibrutinib deacryloylpiperidine

Cat. No.: HY-78727

CAS No.: 330786-24-8

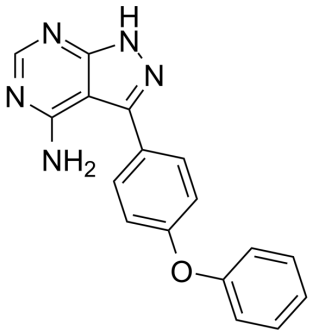
Molecular Formula: $C_{17}H_{13}N_5O$

Molecular Weight: 303.32

Target: Btk

Pathway: Protein Tyrosine Kinase/RTK

Storage: 4°C, protect from light
* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (82.42 mM; Need ultrasonic)
H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	3.2968 mL	16.4842 mL	32.9685 mL
	5 mM	0.6594 mL	3.2968 mL	6.5937 mL
	10 mM	0.3297 mL	1.6484 mL	3.2968 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
Solubility: 2.5 mg/mL (8.24 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Ibrutinib deacryloylpiperidine (IBT4A) is an impurity of Ibrutinib[1]. Ibrutinib is a selective, irreversible Btk inhibitor with an IC_{50} of 0.5 nM[2].

REFERENCES

[1]. Somana Siva Prasad, et al. A QUALITY BY DESIGN APPROACH FOR DEVELOPMENT OF SIMPLE AND ROBUST REVERSED PHASE STABILITY INDICATING HPLC METHOD FOR ESTIMATION OF IBRUTINIB AND ITS IMPURITIES.

[2]. Honigberg LA, et al. The Bruton tyrosine kinase inhibitor PCI-32765 blocks B-cell activation and is efficacious in models of autoimmune disease and B-cell malignancy. Proc Natl Acad Sci U S A. 2010 Jul 20;107(29):13075-80.

Caution: Product has not been fully validated for medical applications. For research use only.

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