

Product Name: VX 745

Catalog No.: 3915

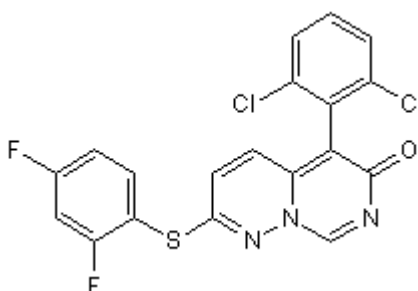
Batch No.: 1

CAS Number: 209410-46-8

IUPAC Name: 5-(2,6-Dichlorophenyl)-2-[2,4-difluorophenyl]thio]-6*H*-pyrimido[1,6-*b*]pyridazin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₉Cl₂F₂N₃OS
Batch Molecular Weight: 436.26
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
 ethanol to 5 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.31	2.08	9.63
Found	52.78	2.01	9.55

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

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Description:

Highly potent and selective p38 α inhibitor (IC₅₀ = 10 nM). Also blocks TNF α production in LPS-stimulated HWB in vitro (IC₅₀ = 177 nM). Displays 1000-fold selectivity over closely related kinases, including ERK1, MK2 and JNK1-3.

Physical and Chemical Properties:

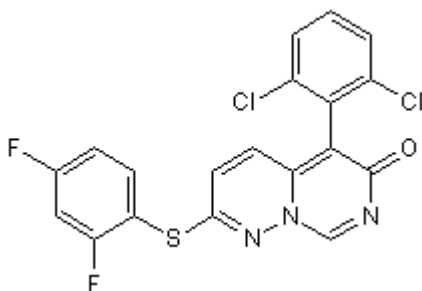
Batch Molecular Formula: C₁₉H₉Cl₂F₂N₃OS

Batch Molecular Weight: 436.26

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 5 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.

References:

Bagley et al (2007) Rapid synthesis of VX-745: p38 MAP kinase inhibition in Werner syndrome cells. *Bioorg.Med.Chem.Lett.* **17** 5107. PMID: 17659871.

Goldstein et al (2010) Selective p38 α inhibitors clinically evaluated for the treatment of chronic inflammatory disorders. *J.Med.Chem.* **53** 2345. PMID: 19950901.

Duffy et al (2011) The discovery of VX-745: a novel and selective p38 α kinase inhibitor. *ACS Med.Chem.Lett.* **2** 758.

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USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

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