

Product Name: CID 2745687

Catalog No.: 4293

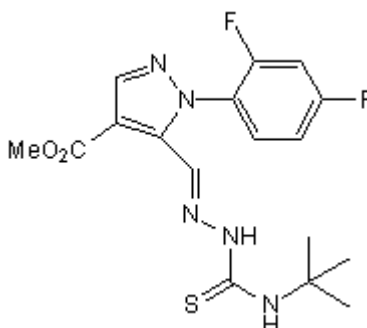
Batch No.: 1

CAS Number: 264233-05-8

IUPAC Name: 1-(2,4-Difluorophenyl)-5-[[2-[[[(1,1-dimethylethyl)amino]thioxomethyl]hydrazinylidene]methyl]-1*H*-pyrazole-4-carboxylic acid methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₉F₂N₅O₂S
Batch Molecular Weight: 395.43
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 10 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 | 51.64 | 4.84 | 17.71 |
| Found | 51.73 | 4.8 | 17.77 |

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Description:

Competitive, reversible antagonist of the orphan receptor GPR35 ($K_i = 12.8$ nM). Blocks the GPR35-mediated increase in ERK1/2 phosphorylation and β -arrestin recruitment induced by pamoic acid (Cat. No. 4298).

Physical and Chemical Properties:

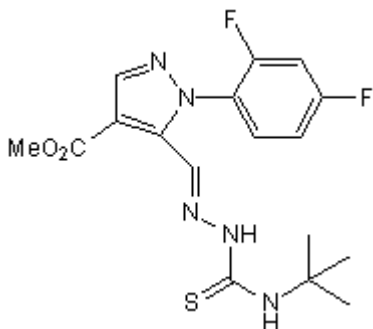
Batch Molecular Formula: $C_{17}H_{19}F_2N_5O_2S$

Batch Molecular Weight: 395.43

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 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:

Zhao *et al* (2010) Targeting of the orphan receptor GPR35 by pamoic acid: a potent activator of extracellular signal-regulated kinase and β -arrestin2 with antinociceptive activity. *Mol.Pharmacol.* **78** 560. PMID: 20826425.

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