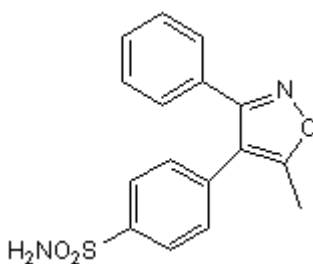


Product Name: Valdecoxib
CAS Number: 181695-72-7
IUPAC Name: 4-(5-Methyl-3-phenylisoxazol-4-yl)benzenesulfonamide

Catalog No.: 4206 **Batch No.:** 1
EC Number: 448-010-8

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₄N₂O₃S
Batch Molecular Weight: 314.36
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 61.13 | 4.49 | 8.91 |
| Found | 60.9 | 4.5 | 8.93 |

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

Product Name: Valdecoxib

Catalog No.: 4206 **Batch No.:** 1

CAS Number: 181695-72-7

EC Number: 448-010-8

IUPAC Name: 4-(5-Methyl-3-phenylisoxazol-4-yl)benzenesulfonamide

Description:

Selective and potent COX-2 inhibitor (in vitro IC₅₀ values are 0.005 and 140 μM for human recombinant COX-2 and COX-1 respectively). Displays potent anti-inflammatory activity in vivo.

Physical and Chemical Properties:

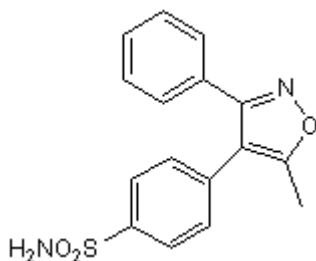
Batch Molecular Formula: C₁₆H₁₄N₂O₃S

Batch Molecular Weight: 314.36

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

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.

References:

Talley et al (2000) 4-[5-methyl-3-phenylisoxazol-4-yl]-benzenesulfonamide, valdecoxib: a potent and selective inhibitor of COX-2. *J.Med.Chem.* **43** 775. PMID: 10715145.

Walker et al (2001) A three-step kinetic mechanism for selective inhibition of cyclo-oxygenase-2 by diarylheterocyclic inhibitors. *Biochem.J.* **357** 709. PMID: 11463341.

Gierse et al (2005) Valdecoxib: assessment of cyclooxygenase-2 potency and selectivity. *J.Pharmacol.Exp.Ther.* **312** 1206. PMID: 15494548.

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