

Product Name: SC 236

Catalog No.: 3919

Batch No.: 1

CAS Number: 170569-86-5

IUPAC Name: 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl] benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₆H₁₁ClF₃N₃O₂S

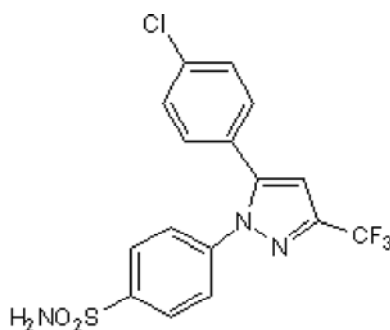
Batch Molecular Weight: 401.79

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	47.83	2.76	10.46
Found	47.53	2.67	10.42

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

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Description:

Selective COX-2 inhibitor (IC₅₀ values are 0.005 and 17.8 μM for COX-2 and COX-1 respectively). Displays anti-inflammatory properties and potent antimetastatic activity against both experimental metastases and spontaneous metastases arising following primary tumor excision.

Physical and Chemical Properties:

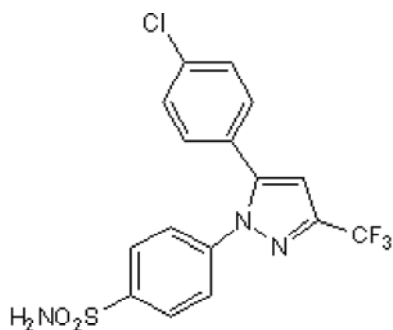
Batch Molecular Formula: C₁₆H₁₁ClF₃N₃O₂S

Batch Molecular Weight: 401.79

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



References:

Roche-Nagle et al (2004) Antimetastatic activity of a cyclooxygenase-2 inhibitor. *Br.J.Cancer* **91** 359. PMID: 15213717.

Penning et al (1997) Synthesis and biological evaluation of the 1,5-diarylpyrazole class of cyclooxygenase-2 inhibitors: identification of 4-[5-(4-Methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (SC-58635, Celecoxib). *J.Med.Chem.* **40** 1347. PMID: 9135032.

Gierse et al (1996) A single amino acid difference between cyclooxygenase-1 (COX-1) and -2 (COX-2) reverses the selectivity of COX-2 specific inhibitors. *J.Biol.Chem.* **271** 15810. PMID: 8663121.

Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

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