

Product Name: SC 560

Catalog No.: 1550

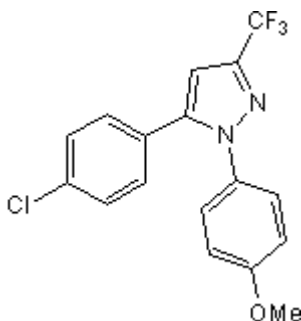
Batch No.: 1

CAS Number: 188817-13-2

IUPAC Name: 5-(4-Chlorophenyl)-1-(4-methoxyphenyl)-3-(trifluoromethyl)-1*H*-pyrazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₂ClF₃N₂O
Batch Molecular Weight: 352.74
Physical Appearance: Light brown solid
Solubility: DMSO to 100 mM
 ethanol to 25 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Ethyl acetate:Petroleum ether [9:1])
Melting Point: Between 62 - 65°C
HPLC: Shows >98.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.89	3.43	7.94
Found	58.15	3.56	7.77

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

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IUPAC Name: 5-(4-Chlorophenyl)-1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole

Description:

Highly selective cyclooxygenase-1 (COX-1) inhibitor (IC₅₀ values are 0.009 and 6.3 μM for COX-1 and COX-2 respectively). Inhibits COX-1-derived platelet thromboxane B₂, gastric PGE₂ and dermal PDE₂ production. Significantly reduces ovarian surface epithelial tumor growth in vivo. Orally active.

Physical and Chemical Properties:

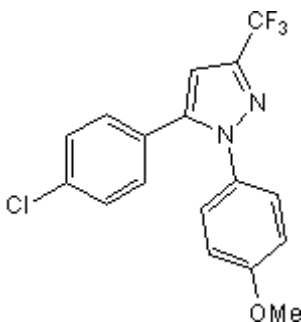
Batch Molecular Formula: C₁₇H₁₂ClF₃N₂O

Batch Molecular Weight: 352.74

Physical Appearance: Light brown solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 25 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:

Smith et al (1998) Pharmacological analysis of cyclooxygenase-1 in inflammation. Proc Natl Acad Sci U S A **95** 13313. PMID: 9789085.

Daikoku et al (2005) Cyclooxygenase-1 is a potential target for prevention and treatment of ovarian epithelial cancer. Cancer Res. **65** 3735. PMID: 15867369.

Takeuchi et al (2005) COX inhibition and NSAID-induced gastric damage - roles in various pathogenic events. Curr.Top.Med.Chem. **5** 475. PMID: 15974942.

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