

Product Name: DuP 697

Catalog No.: 1430

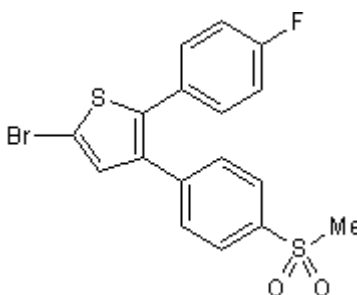
Batch No.: 1

CAS Number: 88149-94-4

IUPAC Name: 5-Bromo-2-(4-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-thiophene

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₇H₁₂BrFO₂S₂
Batch Molecular Weight: 411.3
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.27 (Ethyl acetate:Petroleum ether [1:3])
Melting Point: At 135°C
HPLC: Shows >99.3% purity
¹H NMR: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.64	2.94	
Found	49.48	2.89	

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

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Description:

Potent and selective inhibitor of cyclooxygenase-2 (IC₅₀ values are 10 and 800 nM for COX-2 and COX-1 respectively). Inhibits prostaglandin synthesis and is anti-inflammatory in vivo. Orally active.

Physical and Chemical Properties:

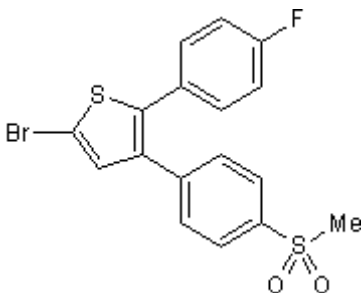
Batch Molecular Formula: C₁₇H₁₂BrFO₂S₂

Batch Molecular Weight: 411.3

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

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:

Gans et al (1990) Anti-inflammatory and safety profile of DuP 697, a novel orally effective prostaglandin synthesis inhibitor. *J.Pharmacol.Exp.Ther.* **254** 180. PMID: 2366180.

Gierse et al (1995) Expression and selective inhibition of the constitutive and inducible forms of human cyclo-oxygenase. *Biochem.J.* **305** 479. PMID: 7832763.

Rossoni et al (2002) Inhibition of cyclo-oxygenase-2 exacerbates ischaemia-induced acute myocardial dysfunction in the rabbit. *Br.J.Pharmacol.* **135** 1540. PMID: 11906968.

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

www.RnDSystems.com