Product Name: SC 58125

CAS Number: 162054-19-5

IUPAC Name: 5-(4-Fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{17}\text{H}_{12}\text{F}_{4}\text{N}_{2}\text{O}_{2}\text{S} \)

Batch Molecular Weight: 384.35

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:

![Molecular Structure Image]

2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

\(^1\text{H} \text{NMR:} \) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>53.12</td>
<td>3.15</td>
<td>7.29</td>
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<tr>
<td>Found</td>
<td>52.86</td>
<td>2.96</td>
<td>7.21</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: SC 58125
Catalog No.: 2895
Batch No.: 2

CAS Number: 162054-19-5
IUPAC Name: 5-(4-Fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazole

Description:
Selective cyclooxygenase 2 (COX-2) inhibitor (IC_{50} values are 0.04 and >100 μM for COX-2 and COX-1 respectively). Anti-inflammatory; blocks edema and hyperalgesia in vivo following an inflammatory insult, without causing gastric mucosal damage. Also displays antitumor activity.

Physical and Chemical Properties:
Batch Molecular Formula: C_{17}H_{12}F_{3}N_{2}O_{2}S
Batch Molecular Weight: 384.35
Physical Appearance: White 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: