1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{12}ClF_{3}N_{2}O$
Batch Molecular Weight: 352.74
Physical Appearance: Light brown solid
Solubility: DMSO to 100 mM, ethanol to 25 mM
Storage: Store at +4°C

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
$^1$H 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>57.89</td>
<td>3.43</td>
<td>7.94</td>
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<tr>
<td>Found</td>
<td>58.15</td>
<td>3.56</td>
<td>7.77</td>
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</table>
Product Name: SC 560
CAS Number: 188817-13-2
IUPAC Name: 5-(4-Chlorophenyl)-1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole

Description:
Highly selective cyclooxygenase-1 (COX-1) inhibitor (IC 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:
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Batch Molecular Weight: 352.74
Physical Appearance: Light brown solid
Minimum Purity: >98%

Batch Molecular Structure:

![Molecular Structure](image)

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: