Product Name: Celecoxib
Catalog No.: 3786
Batch No.: 1
CAS Number: 169590-42-5
IUPAC Name: 4-[5-(4-Methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]-benzenesulfonamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{17}H_{14}F_{3}N_{3}O_{2}S
Batch Molecular Weight: 381.37
Physical Appearance: White solid
Solubility: DMSO to 25 mM
            ethanol to 50 mM
Storage: Store at RT

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity
1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
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<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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<td>53.54</td>
<td>3.7</td>
<td>11.02</td>
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<td>53.72</td>
<td>3.7</td>
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</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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CAS Number: 169590-42-5
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Description:
Selective cyclooxygenase-2 (COX-2) inhibitor (IC50 values are 15 and 0.04 μM for COX-1 and COX-2 respectively). Anti-inflammatory with shorter plasma half-life in vivo than SC 58121 (Cat. No. 2895). Displays chemopreventive activity in in vivo tumor models.

Physical and Chemical Properties:
Batch Molecular Formula: C21H14F3N3O5S
Batch Molecular Weight: 381.37
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
DMSO to 25 mM
ethanol to 50 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: