Product Name: A 425619 Catalog No.: 5781 Batch No.: 1

CAS Number: 581809-67-8
IUPAC Name: N-5-Isoquinolinyl-N'-[4-(trifluoromethyl)phenyl]methyl]urea

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{18}H_{14}F_{3}N_{3}O
Batch Molecular Weight: 345.32
Physical Appearance: Tan solid
Solubility: DMSO to 100 mM ethanol to 100 mM
Storage: Store at RT
Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: R_f = 0.42 (Dichloromethane:Methanol [95:5])
HPLC: Shows 98.9% purity
^1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
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<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
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<tr>
<td>Hydrogen</td>
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<td>4.06</td>
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<tr>
<td>Nitrogen</td>
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</table>
Product Information

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CAS Number: 581809-67-8
IUPAC Name: N-5-Isoquinolinyl-N’-[(4-(trifluoromethyl)phenyl)methyl]urea

Description:
Potent TRPV1 antagonist (IC₅₀ = 3-9 nM). Blocks capsaicin-evoked currents in rat DRG neurons and inhibits TRPV1-activation by anandamide (Cat. No. 1339) and N-arachidonoyl-dopamine. Reduces pain in inflammatory, postoperative and osteoarthritic in vivo pain models.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₈H₁₄F₃N₅O
Batch Molecular Weight: 345.32
Physical Appearance: Tan solid
Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:
DMSO to 100 mM
ethanol 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: