Product Name: Leflunomide
CAS Number: 75706-12-6
IUPAC Name: 5-Methyl-N-[4-(trifluoromethyl)phenyl]-4-isoxazolecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{12}H_{9}F_{3}N_{2}O_{2}
Batch Molecular Weight: 270.21
Physical Appearance: White crystalline solid
Solubility: ethanol to 100 mM
DMSO to 100 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: R_{t} = 0.61 (Ethyl acetate:Petroleum ether [1:2])
Melting Point: Between 166 - 167°C
HPLC: Shows 100% purity
\textsuperscript{1}H NMR: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
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<td>10.37</td>
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<td>Found</td>
<td>53.44</td>
<td>3.31</td>
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</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Description:
Inhibitor of dihydroorotate dehydrogenase (IC$_{50}$ = 2.5 μM). Inhibits de novo pyrimidine synthesis in human T cells in vitro; also inhibits lymphocyte proliferation. Exhibits efficacy in several animal models of autoimmune disease, arthritis and graft rejection. Active metabolite, teriflunomide (A77 1726, Cat. No. 5069), also available.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{12}$H$_9$F$_3$N$_2$O$_2$
Batch Molecular Weight: 270.21
Physical Appearance: White crystalline solid
Minimum Purity: >99%

Storage: Store at +4°C

Solubility & Usage Info:
ethanol to 100 mM
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: