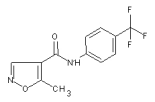

Formula: C12H9F3N2O2

MW: 270.21

CAS: 75706-12-6

MDL NUMBER: MFCD00867593

IUPAC: (5-methylisoxazol-4-yl)-N-[4-(trifluoromethyl)phenyl]carboxamide

Smiles: c1c(c(C)on1)C(Nc1ccc(cc1)C(F)(F)F)=O

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 1

N+O: 4

Chiral Centers: 0

LogP: 1.92

LogS: -3.45

LIPINSKI: 4

Synonyms: LEFLUNOMIDE;HWA 486;ALPHA,ALPHA,ALPHA-TRIFLUORO-5-METHYL-4-ISOXAZOLECARBOXY-P-TOLUIDIDE;5-METHYLISOXAZOLE-4-(4-TRIFLUOROMETHYLCARBOXANILIDE);5-METHYL-N-[4-(TRIFLUOROMETHYL)PHENYL]-4-ISOXAZOLECARBOXAMIDE;N-(4-TRIFLUOROMETHYLPHENYL)-5-METHYLISOXAZOL-4-CARBOXAMIDE;5-methylisoxazole-4-carboxylicacid(4-trifluoromethyl)anilide;5-methyl-n-(4-(trifluoromethyl)phenyl)-4-isoxazolecarboxamid

CAS:75706-12-6

MF:C12H9F3N2O2

MW:270.21

EINECS:

Product Categories:Active Pharmaceutical Ingredients;API;Osteoarthritis and Rheumatoid Arthritis;Inhibitors;Intermediates & Fine Chemicals;Pharmaceuticals;Cytokine signaling Leflunomide

Chemical Properties: mp 163-168C storage temp. 2-8C

CAS DataBase Reference: 75706-12-6(

CAS DataBase Reference: ) Xn,Xi Risk Statements 22-36/37/38 Safety Statements 26-36 RIDADR UN 2811 6.1/PG 3 WGK Germany 3 RTECS NY2354200 Hazardous Substances Data75706-12-6(Hazardous Substances Data) Leflunomide Leflunomide

Usage And Synthesis:

Chemical Properties: Off White Crystalline Solid UsageAn immunosuppressive. Inhibits T and B cell proliferation. Activity is attributed mainly to its metabolite, a malononitrile derivative, which is beleived to inhibit dihydroorotate dehydrogenase as well as several protein tyrosine kinases. Therape Biological ActivityImmunosuppressant agent. In vitro the active metabolite A77 1726 (RS-61980) inhibits dihydroorotate dehydrogenase (K i = 2.7 u M) and de novo pyrimidine synthesis in T-cells; blocks lymphocyte cell cycle progression and proliferation. A77 1726 also inhibits anti-CD3/CD28-induced cytokine production in PBMC cells (IC 50 = 21-27 u g/ml). In vivo reduces inflammation in several animal models of autoimmune disease, arthritis, asthma and graft rejection. Leflunomide