5-methyl-N-(4-(trifluoromethyl)phenyl)-4-isoxazole

Other names: Leflunomide
Inchi: InChI=1S/C12H9F3N2O2/c1-7-10(6-16-19-7)11(18)17-9-4-2-8(3-5-9)12(13,14)15/h2-6H,
InchiKey: VHOGYURTWQBHIL-UHFFFAOYSA-N
Formula: C12H9F3N2O2
SMILES: Cc1oncc1C(=O)Nc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 270.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.53		Crippen Method
logp	3.254		Crippen Method
mcvol	169.430	ml/mol	McGowan Method
tf	442.15	K	Enhancement of dissolution behavior of antiarthritic drug leflunomide using solid dispersion methods

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Enhancement of dissolution behavior of antiarthritic drug leflunomide using solid dispersion methods: https://www.doi.org/10.1016/j.tca.2017.09.003
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point