

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:	<chem>Cc1oncc1C(=O)Nc1ccc(C(F)(F)F)cc1</chem>
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

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