Sulfamoxole

Other names:	2-(p-Aminobenzenesulfonamido)-4,5-dimethyloxazole
	2-(p-Aminobenzolsulfonamido)-4,5-dimethyloxazol
	4,5-Dimethyl-2-sulfanilamidooxazole
	4-Amino-N-(4,5-dimethyl-2-oxazolyl)benzenesulfonamide
	Benzenesulfonamide, 4-amino-N-(4,5-dimethyl-2-oxazolyl)-
	Justamil
	N1-(4,5-Dimethyl-2-oxazolyl)sulfanilamide
	N1-(4,5-Dimethyloxazol-2-yl)-sulfanilamide
	NSC 683535
	Oxasulfa
	Oxazole, 2-(p-aminophenylsulfonylamino)-4,5-dimethyl-
	Sulfabutin
	Sulfadimethyloxazole
	Sulfamoxolum
	Sulfanilamide, N1-(4,5-dimethyl-2-oxazolyl)-
	Sulfano
	Sulfavigor
	Sulfmidil
	Sulfune
	Sulfuno
	Sulphamoxole
	Tardamid
	Tardamide
	p-Aminobenzenesulfonyl-2-amino-4,5-dimethyloxazole
Inchi:	InChI=1S/C11H13N3O3S/c1-7-8(2)17-11(13-7)14-18(15,16)10-5-3-9(12)4-6-10/h3-6H,12
InchiKey:	CYFLXLSBHQBMFT-UHFFFAOYSA-N
Formula:	C11H13N3O3S
SMILES:	Cc1nc(NS(=O)(=O)c2ccc(N)cc2)oc1C
Mol. weight [g/mol]:	267.30
CAS:	729-99-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Aqueous Solubility Prediction Method
logp	1.674		Crippen Method
mcvol	186.530	ml/mol	McGowan Method

tf	481.00 ± 1.00	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C729997&Units=SI

Legend

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