N(1)-(4,5-DIMETHYL-2-OXAZOLYL)SULFANILAMI

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
sulfamoxole

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]: 267.31

Physical Properties

Property code	Value	Unit	Source
hvap	113.65	kJ/mol	Cheméo Relay (1.0)
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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C729997&Units=SI

Legend

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point