Sulfameter

Other names:	5-Methoxysulfadiazine
	Benzenesulfonamide, 4-amino-N-(5-methoxy-2-pyrimidinyl)-
	Sulfanilamide, N
Inchi:	InChI=1S/C11H12N4O3S/c1-18-9-6-13-11(14-7-9)15-19(16,17)10-4-2-8(12)3-5-10/h2-7H
InchiKey:	GPTONYMQFTZPKC-UHFFFAOYSA-N
Formula:	C11H12N4O3S
SMILES:	COc1cnc(NS(=O)(=O)c2ccc(N)cc2)nc1
Mol. weight [g/mol]:	280.30
CAS:	651-06-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.58		Aqueous Solubility Prediction Method
logp	0.868		Crippen Method
mcvol	192.210	ml/mol	McGowan Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tf	486.70 ± 0.50	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C651069&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point