Sulfisomidine

Other names: 4-amino-N-(2,6-dimethylpyrimidin-4-yl)benzenesulfonamide
Benzenesulfonamide, 4-amino-N-(2,6-dimethyl-4-pyrimidinyl)-
Sulfanilamide, N
Inchi: InChI=1S/C12H14N4O2S/c1-8-7-12(15-9(2)14-8)16-19(17,18)11-5-3-10(13)4-6-11/h3-7H
InchiKey: YZMCKZRAOLZXAZ-UHFFFAOYSA-N
Formula: C12H14N4O2S
SMILES: Cc1cc(NS(=O)(=O)c2ccc(N)cc2)nc(C)n1
Mol. weight [g/mol]: 278.33
CAS: 515-64-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Aqueous Solubility Prediction Method
logp	1.476		Crippen Method
mcvol	200.430	ml/mol	McGowan Method
tf	523.60 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	42.70	kJ/mol	523.60	NIST Webbook

Sources

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=C515640&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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