SULPHAMETHOXYDIAZINE

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]: 280.31

Physical Properties

Property code	Value	Unit	Source
hvap	118.95	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	0.868		Crippen Method
mcvol	192.210	ml/mol	McGowan Method
tb	700.46	K	Cheméo Relay (1.0)
tf	492.03	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C651069
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point