Sulfamerazine

Other names:	2-(4-Aminobenzenesulfonamido)-4-methylpyrimidine
	2-(p-Aminobenzosulfonamido)-4-methylpyrimidine
	2-Sulfa-4-methylpyrimidine
	2-Sulfanilamido-4-methylpyrimidine
	2632 R. P.
	2643-RP
	A-310
	Benzenesulfonamide, 4-amino-N-(4-methyl-2-pyrimidinyl)-
	Cremomerazine
	Debenal-M
	Kelamerazine
	Mebacid
	Mesulfa
	Methylpyrimal
	Methylsulfazine
	Metilsulfadiazin
	Metilsulfazin
	N-(4-Methyl-2-pyrimidyl)sulfanilamide
	Percoccide
	Pirimal-M
	Pyralcid
	Pyrimal m
	RP 2632
	Romezin
	Septacil
	Septosyl
	Solumedin
	Solumedine
	Sulfameradine
	Sulfamerazin
	Sulfamethyldiazine
	Sulfanilamide, N
	Sulphamerazine
	Sumedine
	Veta-Merazine
Inchi:	InChI=1S/C11H12N4O2S/c1-8-6-7-13-11(14-8)15-18(16,17)10-4-2-9(12)3-5-10/h2-7H,12
InchiKey:	QPPBRPIAZZHUNT-UHFFFAOYSA-N
Formula:	C11H12N4O2S
SMILES:	Cc1ccnc(NS(=O)(=O)c2ccc(N)cc2)n1
Mol. weight [g/mol]:	264.30

CAS: 127-79-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.24		Aqueous Solubility Prediction Method
log10ws	-3.12		Aqueous Solubility Prediction Method
logp	1.168		Crippen Method
mcvol	186.340	ml/mol	McGowan Method
rinpol	2573.00		NIST Webbook
rinpol	2573.00		NIST Webbook
tf	508.69	K	Aqueous Solubility Prediction Method
tf	508.69	K	Aqueous Solubility Prediction Method
tf	506.40 ± 1.00	K	NIST Webbook
tf	515.20 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	41.30	kJ/mol	508.50	NIST Webbook
hfust	31.60	kJ/mol	515.20	NIST Webbook
hfust	31.60	kJ/mol	515.20	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C127797&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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

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

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point