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
4-amino-N-(4-methyl-2-pyrimidinyl)benzenesulfonamide
A-310
Cremomerazine
Debenal-M
Kelamerazine
Mebacid
Mesulfa
Methylpyrimal
Metilsulfadiazin
Metilsulfazin
N-(4-methyl-2-pyrimidyl)sulfanilamide
N1-(4-methyl-2-pyrimidinyl)sulfanilamide
N1-(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
benzenesulfonamide, 4-amino-N-(4-methyl-2-pyrimidinyl)-
methylsulfazine
sulfanilamide, N1-(4-methyl-2-pyrimidinyl)-

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]: 264.31

Physical Properties

Property code	Value	Unit	Source
hvap	121.81	kJ/mol	Cheméo Relay (1.0)
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

Solubility and solution thermodynamics of sulfamerazine and sulfamethazine in some ethanol + water mixtures: https://www.doi.org/10.1016/j.fluid.2013.09.018
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

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

Legend

hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point