Sulfamethoxazole

Other names:	3-(para-Aminophenylsulphonamido)-5-methylisoxazole
	3-Sulfanilamido-5-methylisoxazole
	4-Amino-N-(5-methyl-3-isoxazolyl)benzenesulfonamide
	5-Methyl-3-sulfanilamidoisoxazole
	5-Methyl-3-sulfonylamidoisoxazole
	A047
	Azo-gantanol
	Bactrim
	Benzenesulfonamide, 4-amino-N-(5-methyl-3-isoxazolyl)-
	Gantanol
	MS 53
	Metoxal
	N
	N'-(5-Methyl-3-isoxazole)sulfanilamide
	N'-(5-Methyl-3-isoxazolyl)sulfanilamide
	N'-(5-Methylisoxazol-3-yl)sulphanilamide
	N1-(5-Methyl-3-isoxazolyl)sulfanilamide
	Radonil
	Ro 4-2130
	Ro 6-2580/11
	Simsinomin
	Sinomin
	Sulfamethalazole
	Sulfamethoxazol
	Sulfamethylisoxazole
	Sulfanilamide, N'-(5-methyl-3-isoxazolyl)-
	Sulfanilamide, N1-(5-methyl-3-isoxazolyl)-
	Sulfisomezole
	Sulphamethoxazole
Inchi:	InChI=1S/C10H11N3O3S/c1-7-6-10(12-16-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6H,11H2,1
InchiKey:	JLKIGFTWXXRPMT-UHFFFAOYSA-N
Formula:	C10H11N3O3S
SMILES:	Cc1cc(NS(=O)(=O)c2ccc(N)cc2)no1
Mol. weight [g/mol]:	253.28
CAS:	723-46-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Aqueous Solubility Prediction Method
logp	1.366		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
rinpol	2387.00		NIST Webbook
tf	439.50 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	33.80	kJ/mol	440.70	NIST Webbook
hfust	35.26	kJ/mol	440.00	NIST Webbook

Sources

Solubilities of Sulfamethazine, Sulfadimethoxine, Sulfamethoxydiazine, Sulfamonomethoxine, Sulfamethoxazole, and Sulfaquinoxaline in 1-Octanol from (298.15 to 333.15) K:	https://www.doi.org/10.1021/je800867a
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=C723466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of Sulfadiazine, Sulfamethazine, Sulfadimethoxine, Sulfamethoxydiazine, Sulfamonomethoxine, Sulfamethoxazole, and Sulfachloropyridazine in Water from (298.15 to 333.15) K:	https://www.doi.org/10.1021/je0603978

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

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