

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,11H2,12H
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

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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/ci9903071>

Solubilities of Sulfadiazine, Sulfamethazine, Sulfadimethoxine, Sulphonethoxazine, Sulfamethoxazole, Sulfadimethoxine, Sulfamethoxazole, and Sulfamethopetazine in Water from 298.15 K to 333.15 K: <https://www.doi.org/10.1021/je0603978>

<https://www.doi.org/10.1021/je800867a>

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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