SULPHASOMIZOLE

Other names:	Benzenesulfonamide, 4-amino-N-(3-methyl-5-isothiazolyl)-
	Amidozol
	Amidozole
	Bidizole
	N1-(3-Methyl-5-isothiazolyl)sulfanilamide
	Sulfamizole
	Sulfanilamide, N1-(3-methyl-5-isothiazolyl)-
	Sulfasomizol
	Sulphasomizole
	2132 TH
	3-Methyl-5-sulfanilamidoisothiazole
	Sulphasomisole
	NSC 139593
Inchi:	InChI=1S/C10H11N3O2S2/c1-7-6-10(16-12-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6,13H,11
InchiKey:	JVYKJZPZFIUYAB-UHFFFAOYSA-N
Formula:	C10H11N3O2S2
SMILES:	Cc1cc(NS(=O)(=O)c2ccc(N)cc2)sn1
Mol. weight [g/mol]:	269.35

Physical Properties

Property code	Value	Unit	Source
hvap	120.65	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.61		Cheméo Relay (1.0)
logp	1.835		Crippen Method
mcvol	182.920	ml/mol	McGowan Method
tf	443.89	K	Cheméo Relay (1.0)

Sources

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point