

Sulfasomizole

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:	<chem>Cc1cc(NS(=O)(=O)c2ccc(N)cc2)sn1</chem>
Mol. weight [g/mol]:	269.34
CAS:	632-00-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.835		Crippen Method
mcpvol	182.920	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C632008&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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