Dimetotiazine

Other names:	10H-Phenothiazine-2-sulfonamide, 10-[2-(dimethylamino)propyl]-N,N-dimethyl- Phenothiazine-2-sulfonamide, 10-(2-(dimethylamino)propyl)-N,N-dimethyl- Banistyl Dimethodin Dimethothiazine 10-(2-(Dimethylamino)propyl)-N,N-dimethylphenothiazine-2-sulfonamide Dimethylsulfamido-3-(dimethylamino-2-propyl)-10-phenothiazine 3-Dimethylsulfonamido 10-(2-dimethylaminopropyl)phenothiazine Dimetiotazine Fonazine 8599 R.P. Dimethiotazine RP-8599
Inchi:	InChI=1S/C19H25N3O2S2/c1-14(20(2)3)13-22-16-8-6-7-9-18(16)25-19-11-10-15(12-17(
InchiKey:	VWNWVCJGUMZDIU-UHFFFAOYSA-N
Formula:	C19H25N3O2S2
SMILES:	CC(CN1c2ccccc2Sc2ccc(S(=O)(=O)N(C)C)cc21)N(C)C
Mol. weight [g/mol]:	391.55
CAS:	7456-24-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	3.490		Crippen Method
mcvol	294.570	ml/mol	McGowan Method
rinpol	3047.00		NIST Webbook
rinpol	3060.00		NIST Webbook
rinpol	3050.00		NIST Webbook
rinpol	3078.00		NIST Webbook
rinpol	3078.00		NIST Webbook
rinpol	3047.00		NIST Webbook
rinpol	3050.00		NIST Webbook
rinpol	3060.00		NIST Webbook
rinpol	3078.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7456248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices