Thioproperazine

Other names:	10H-Phenothiazine-2-sulfonamide, N,N-dimethyl-10-[3-(4-methyl-1-piperazinyl)propyl]-
	Phenothiazine-2-sulfonamide, N,N-dimethyl-10-[3-(4-methyl-1-piperazinyl)propyl]-
	Mazeptil
	RP 7843
	Sulfenazin
	SKF 5883
	Thioperazine
	Tioproperazin
	Vontil
	7843 R.P.
	Majeptyl
	Mazeptyl
	Megeptil
	Thioproperazin
	2-Dimethylsulfamido-(10-(3-1-methylpiperazinyl-4)propyl)-phenothiazine
	N,N-Dimethyl-10-[3-(4-methyl-1-piperazinyl)propyl]phenothiazine-2-sulfonamide
	Thiproperazine
	Cephalmin
Inchi:	InChI=1S/C22H30N4O2S2/c1-23(2)30(27,28)18-9-10-22-20(17-18)26(19-7-4-5-8-21(19)2
InchiKey:	VZYCZNZBPPHOFY-UHFFFAOYSA-N
Formula:	C22H30N4O2S2
SMILES:	CN1CCN(CCCN2c3ccccc3Sc3ccc(S(=O)(=O)N(C)C)cc32)CC1
Mol. weight [g/mol]:	446.63
CAS:	316-81-4

Physical Properties

Property code	Value	Unit	Source
ie	6.81 ± 0.07	eV	NIST Webbook
log10ws	-3.48		Crippen Method
logp	3.177		Crippen Method
mcvol	335.960	ml/mol	McGowan Method
rinpol	3528.00		NIST Webbook

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=C316814&Units=SI

Legend

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