MESORIDAZINE

Other names:	10H-Phenothiazine, 10-[2-(1-methyl-2-piperidinyl)ethyl]-2-(methylsulfinyl)-
	Phenothiazine, 10-[2-(1-methyl-2-piperidyl)ethyl]-2-(methylsulfinyl)-
	Lidanil
	Serentil
	Thioridazine thiomethyl sulfoxide
	Thioridazine-2-sulfoxide
	TPS 23
	Calodal
	Lidanar
	NC 123
	T-2-SO
	Thioridazien thiomethyl sulfoxide
	THD-2-SO
	10-(2(1-Methyl-2-piperidyl)ethyl)-2-(methylsulfinyl)phenothiazine
	10H-Phenothiazine, 2-methylthionyl-10-(2-(1-methylpiperidin-2-yl)ethyl)-
	Thioridazine monosulfoxide analog
	NSC 186066
	Thioridazine, sulfoxide
Inchi:	InChI=1S/C21H26N2OS2/c1-22-13-6-5-7-16(22)12-14-23-18-8-3-4-9-20(18)25-21-11-10-
InchiKey:	SLVMESMUVMCQIY-UHFFFAOYSA-N
Formula:	C21H26N2OS2
SMILES:	CN1CCCCC1CCN1c2ccccc2Sc2ccc(S(C)=O)cc21
Mol. weight [g/mol]:	386.59

Physical Properties

Property code	Value	Unit	Source
ie	7.22	eV	Cheméo Relay (1.0)
log10ws	-4.04		Cheméo Relay (1.0)
logp	4.901		Crippen Method
mcvol	296.040	ml/mol	McGowan Method
rinpol	3326.00		NIST Webbook
rinpol	3326.00		NIST Webbook
rinpol	3326.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5588330&Units=SI
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):	

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