Thioridazine

Other names:	10H-Phenothiazine, 10-[2-(1-methyl-2-piperidinyl)ethyl]-2-(methylthio)-
	Phenothiazine, 10-[2-(1-methyl-2-piperidyl)ethyl]-2-(methylthio)-
	Mallorol
	Malloryl
	Meleril
	Mellerets
	Mellerette
	Melleretten
	Melleril
	Sonapax
	Thioridazin
	Thioridazine, prolongatum
	TP-21
	Phenothiazine, 10-((1-methyl-2-piperidyl)ethyl)-2-(methylthio)-
	Mellarit
	2-Methylmercapto-10-(2-(N-methyl-2-piperidyl)ethyl)phenothiazine
	10-(2-(1-Methyl-2-piperidyl)ethyl)-2-(methylthio)phenothiazine
	Mellaril-S
	10H-Phenothiazine, 10-[2-(1-methyl-2-piperidyl)ethyl]-2-methylthio-
	(.+/-.)-Thioridazine
	dl-Thioridazine
	Melleril (liquid)
Inchi:	InChI=1S/C21H26N2S2/c1-22-13-6-5-7-16(22)12-14-23-18-8-3-4-9-20(18)25-21-11-10-1
InchiKey:	KLBQZWRITKRQQV-UHFFFAOYSA-N
Formula:	C21H26N2S2
SMILES:	CSc1ccc2c(c1)N(CCC1CCCCN1C)c1ccccc1S2
Mol. weight [g/mol]:	370.57
CAS:	50-52-2

Physical Properties

Property code	Value	Unit	Source
ie	7.00 ± 0.08	eV	NIST Webbook
ie	7.20 ± 0.05	eV	NIST Webbook
log10ws	-6.09		Crippen Method
logp	5.886		Crippen Method
mcvol	290.170	ml/mol	McGowan Method

rinpol	3100.00	NIST Webbook
rinpol	3117.00	NIST Webbook
rinpol	3080.00	NIST Webbook
rinpol	3105.00	NIST Webbook
rinpol	3070.00	NIST Webbook
rinpol	3104.00	NIST Webbook
rinpol	3114.00	NIST Webbook
rinpol	3125.00	NIST Webbook
rinpol	3117.00	NIST Webbook
rinpol	3135.00	NIST Webbook
rinpol	3125.00	NIST Webbook
rinpol	3105.00	NIST Webbook
rinpol	3080.00	NIST Webbook
rinpol	3114.00	NIST Webbook
rinpol	3114.00	NIST Webbook
rinpol	3105.00	NIST Webbook
rinpol	3094.00	NIST Webbook
rinpol	3114.00	NIST Webbook
rinpol	3120.00	NIST Webbook
rinpol	3116.00	NIST Webbook
rinpol	3100.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50522&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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