

Sulforidazine

Other names:	10H-Phenothiazine, 10-[2-(1-methyl-2-piperidiny)ethyl]-2-(methylsulfonyl)-Phenothiazine, 10-(2-(1-methyl-2-piperidyl)ethyl)-2-methylsulfonyl-Imagotan Inofal 10-(2-(1-Methyl-2-piperidyl)ethyl)-2-methylsulfonylphenothiazine Psychoson TPN-12 10-[2-(1-Methyl-2-piperidiny)ethyl]-2-methylsulfonylphenothiazine Thioridazine-2-sulfone 2-Methylsulfonyl-10-[2-(1-methyl-2-piperidyl)ethyl]phenothiazine
Inchi:	InChI=1S/C21H26N2O2S2/c1-22-13-6-5-7-16(22)12-14-23-18-8-3-4-9-20(18)26-21-11-1
InchiKey:	FLGCRGJDQJIJAW-UHFFFAOYSA-N
Formula:	C21H26N2O2S2
SMILES:	CN1CCCCC1CCN1c2ccccc2Sc2ccc(S(C)(=O)=O)cc21
Mol. weight [g/mol]:	402.57
CAS:	14759-06-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	4.567		Crippen Method
mcvol	301.910	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C14759069&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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