Triflupromazine

Other names:	10-[3-(Dimethylamino)propyl]-2-(trifluoromethyl)phenothiazine 10H-Phenothiazine-10-propanamine, N,N-dimethyl-2-(trifluoromethyl)- 2-(Trifluoromethyl)promazine Adazine Fluopromazine N,N-dimethyl-3-[2-(trifluoromethyl)phenothiazin-10-yl]propan-1-amine Phenothiazine, 10-[3-(dimethylamino)propyl]-2-(trifluoromethyl)- Psyquil Siquil Trifluopromazine Vesprin
Inchi:	InChI=1S/C18H19F3N2S/c1-22(2)10-5-11-23-14-6-3-4-7-16(14)24-17-9-8-13(12-15(17)2
InchiKey:	XSCGXQMFQXDFCW-UHFFFAOYSA-N
Formula:	C18H19F3N2S
SMILES:	CN(C)CCCN1c2ccccc2Sc2ccc(C(F)(F)F)cc21
Mol. weight [g/mol]:	352.42
CAS:	146-54-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Aqueous Solubility Prediction Method
logp	5.260		Crippen Method
mcvol	247.720	ml/mol	McGowan Method
rinpol	2220.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2238.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2238.00		NIST Webbook
rinpol	2239.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C146543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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