Fluphenazine M (amino-), monoacetylated

Other names: Trifluprомazine M (bis-nor-), acetylated
Inchi: InChI=1S/C18H17F3N2OS/c1-12(24)22-9-4-10-23-14-5-2-3-6-16(14)25-17-8-7-13(11-15
InchiKey: VDSDDOIKQFYIPK-UHFFFAOYSA-N
Formula: C18H17F3N2OS
SMILES: CC(O)=NCCCN1c2ccccc2Sc2ccc(C(F)(F)F)cc21
Mol. weight [g/mol]: 366.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	5.675		Crippen Method
mcvol	249.290	ml/mol	McGowan Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
rinpol	2765.00		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=R310333&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices