Trifluopromazine M (nor-), monoacetylated

Other names: Triflupromazine M (nor-), acetylated
Inchi: InChI=1S/C19H19F3N2OS/c1-13(25)23(2)10-5-11-24-15-6-3-4-7-17(15)26-18-9-8-14(12
InchiKey: XPSDEXXSOQHANR-UHFFFAOYSA-N
Formula: C19H19F3N2OS
SMILES: CC(=O)N(C)CCCN1c2ccccc2Sc2ccc(C(F)(F)F)cc21
Mol. weight [g/mol]: 380.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.38		Crippen Method
logp	5.177		Crippen Method
mcvol	263.380	ml/mol	McGowan Method
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310759&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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