Trifluopromazine M (nor-HO-), diacetylated

Other names: Triflupromazine M (nor-hydroxy-), acetylated
Inchi: InChI=1S/C21H21F3N2O3S/c1-13(27)25(3)9-4-10-26-17-7-6-16(29-14(2)28)12-20(17)30
InchiKey: ONGCYKGYTVQFEN-UHFFFAOYSA-N
Formula: C21H21F3N2O3S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccc(C(F)(F)F)cc1N2CCCN(C)C(C)=O
Mol. weight [g/mol]: 438.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	5.102		Crippen Method
mcvol	299.000	ml/mol	McGowan Method
rinpol	3120.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310764&Units=SI
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

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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