Trifluopromazine M (HO-), diacetylated

Inchi: InChI=1S/C21H23F3N2O2S/c1-4-25(3)10-5-11-26-17-8-7-16(28-14(2)27)13-20(17)29-19
InchiKey: RNOGQIRBNDWNOD-UHFFFAOYSA-N
Formula: C21H23F3N2O2S
SMILES: CCN(C)CCCN1c2ccc(OC(C)=O)cc2Sc2ccc(C(F)(F)F)cc21
Mol. weight [g/mol]: 424.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.92		Crippen Method
logp	5.575		Crippen Method
mcvol	297.430	ml/mol	McGowan Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook

Sources

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=R310744&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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