Homofenazine M (desalkyl-), monoacetylated

Inchi: InChI=1S/C23H26F3N3OS/c1-17(30)28-12-4-10-27(14-15-28)11-5-13-29-19-6-2-3-7-21(
InchiKey: SPZHMWDAWDUCGT-UHFFFAOYSA-N
Formula: C23H26F3N3OS
SMILES: CC(=O)N1CCCN(CCCN2c3ccccc3Sc3ccc(C(F)(F)F)cc32)CC1
Mol. weight [g/mol]: 449.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	5.252		Crippen Method
mcvol	318.860	ml/mol	McGowan Method
rinpol	3240.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310373&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