Flupenthixol M (desalkyl-dihydro-), monoacetylated

Inchi: InChI=1S/C23H25F3N2OS/c1-16(29)28-13-11-27(12-14-28)10-4-6-18-19-5-2-3-7-21(19)

InchiKey: PVXUUDCTMLHZFO-UHFFFAOYSA-N

Formula: C23H25F3N2OS

SMILES: CC(=O)N1CCN(CCCC2c3ccccc3Sc3ccc(C(F)(F)F)cc32)CC1

Mol. weight [g/mol]: 434.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	5.246		Crippen Method
mcvol	308.880	ml/mol	McGowan Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		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=R310313&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.