Levomepromazine M (HO-), monoacetylated

Inchi: InChI=1S/C21H26N2O3S/c1-14(12-22(3)4)13-23-16-8-6-7-9-20(16)27-21-11-19(26-15(2)
InchiKey: UUONPBYOPXKDSU-AWEZNQCLSA-N
Formula: C21H26N2O3S
SMILES: COc1cc2c(cc1OC(C)=O)Sc1ccccc1N2CC(C)CN(C)C
Mol. weight [g/mol]: 386.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	4.421		Crippen Method
mcvol	297.990	ml/mol	McGowan Method
rinpol	2747.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310388&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