Levomepromazine M (nor-HO-), diacetylated

Inchi: InChI=1S/C22H26N2O4S/c1-14(12-23(4)15(2)25)13-24-17-8-6-7-9-21(17)29-22-11-20(2
InchiKey: MLIMTTXCSZHVJM-AWEZNQCLSA-N
Formula: C22H26N2O4S
SMILES: COc1cc2c(cc1OC(C)=O)Sc1ccccc1N2CC(C)CN(C)C(C)=O
Mol. weight [g/mol]: 414.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	4.338		Crippen Method
mcvol	313.650	ml/mol	McGowan Method
rinpol	3220.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310402&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