Clotiazepam M (hydroxy-), acetylated

Inchi: InChI=1S/C18H17ClN2O3S/c1-4-12-8-14-17(20-9-16(23)21(3)18(14)25-12)13-6-5-11(7-1
InchiKey: QUKIBGRVEBWWEZ-UHFFFAOYSA-N
Formula: C18H17ClN2O3S
SMILES: CCc1cc2c(s1)N(C)C(=O)CN=C2c1ccc(OC(C)=O)cc1Cl
Mol. weight [g/mol]: 376.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.703		Crippen Method
mcvol	263.660	ml/mol	McGowan Method
rinpol	2870.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R312953&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices