Promethazine M (nor-HO-), diacetylated

Other names: Promethazine M (nor-hydroxy-), acetylated
Inchi: InChI=1S/C20H22N2O3S/c1-13(21(4)14(2)23)12-22-17-7-5-6-8-19(17)26-20-11-16(25-1
InchiKey: KMVWESWNNGFUJE-UHFFFAOYSA-N
Formula: C20H22N2O3S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CC(C)N(C)C(C)=O
Mol. weight [g/mol]: 370.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	4.081		Crippen Method
mcvol	279.600	ml/mol	McGowan Method
rinpol	3015.00		NIST Webbook
rinpol	3017.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310591&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