Promethazine M (nor-), monoacetylated

Other names: Promethazine M (nor-), acetylated
Inchi: InChI=1S/C18H20N2OS/c1-13(19(3)14(2)21)12-20-15-8-4-6-10-17(15)22-18-11-7-5-9-16
InchiKey: JCNNAQQGTJLYLB-UHFFFAOYSA-N
Formula: C18H20N2OS
SMILES: CC(=O)N(C)C(C)CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]: 312.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	4.156		Crippen Method
mcvol	243.980	ml/mol	McGowan Method
rinpol	2540.00		NIST Webbook
rinpol	2640.00		NIST Webbook
rinpol	2540.00		NIST Webbook
rinpol	2640.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310586&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