Promethazine M (HO-), monoacetylated

Other names: Promethazine M (hydroxy-), acetylated
Inchi: InChI=1S/C19H22N2O2S/c1-13(20(3)4)12-21-16-7-5-6-8-18(16)24-19-11-15(23-14(2)22)
InchiKey: RUHZYJBTFIIOKB-UHFFFAOYSA-N
Formula: C19H22N2O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2CC(C)N(C)C
Mol. weight [g/mol]: 342.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	4.165		Crippen Method
mcvol	263.940	ml/mol	McGowan Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310571&Units=SI

Legend

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

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