Promethazine M (bis-nor-), acetylated

Inchi: InChI=1S/C17H18N2OS/c1-12(18-13(2)20)11-19-14-7-3-5-9-16(14)21-17-10-6-4-8-15(17
InchiKey: IFFQWZYOBGHEDL-UHFFFAOYSA-N
Formula: C17H18N2OS
SMILES: CC(=O)NC(C)CN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]: 298.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.814		Crippen Method
mcvol	229.890	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R314479&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