Chlorpromazine M (bis-nor-), acetylated

Inchi: InChI=1S/C17H17ClN2OS/c1-12(21)19-9-4-10-20-14-5-2-3-6-16(14)22-17-8-7-13(18)11-
InchiKey: QZEAJJHJTPPDMU-UHFFFAOYSA-N
Formula: C17H17ClN2OS
SMILES: CC(=O)NCCCN1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]: 332.85

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	4.469		Crippen Method
mcvol	242.130	ml/mol	McGowan Method
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook
rinpol	2990.00		NIST Webbook

Sources

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=R310175&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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