

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
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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

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