Desmethylchloropromazine

Inchi: InChI=1S/C16H17ClN2S/c1-18-9-4-10-19-13-5-2-3-6-15(13)20-16-8-7-12(17)11-14(16)19
InchiKey: YHFXGBOUSIKGMZ-UHFFFAOYSA-N
Formula: C16H17ClN2S
SMILES: CNCCCN1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]: 304.84
CAS: 1225-64-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	4.552		Crippen Method
mcvol	226.470	ml/mol	McGowan Method
rinpol	2480.00		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=C1225645&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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