Chlorproethazine

Inchi: InChI=1S/C19H23ClN2S/c1-3-21(4-2)12-7-13-22-16-8-5-6-9-18(16)23-19-11-10-15(20)14
InchiKey: DBOUGBAQLIXZLV-UHFFFAOYSA-N
Formula: C19H23ClN2S
SMILES: CCN(CC)CCCN1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]: 346.92
CAS: 84-01-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	5.675		Crippen Method
mcvol	268.740	ml/mol	McGowan Method
rinpol	2617.00		NIST Webbook
rinpol	2617.00		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=C84015&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