

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)1
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
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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

Latest version available from:

<https://www.chemeo.com/cid/99-743-8/Chlorproethazine.pdf>

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