

# Chlorprothixene M (N-oxide)

**Inchi:** InChI=1S/C18H20ClNOS/c1-20(2,21)11-5-7-14-15-6-3-4-8-17(15)22-18-10-9-13(19)12-1  
**InchiKey:** JQBHJSFLNXPONK-UHFFFAOYSA-N  
**Formula:** C18H20ClNOS  
**SMILES:** C[N+](C)([O-])CCCC1c2ccccc2Sc2ccc(Cl)cc21  
**Mol. weight [g/mol]:** 333.88

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	5.291		Crippen Method
mcvol	250.540	ml/mol	McGowan Method
rinpole	2409.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R212269&Units=SI>

## Legend

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

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