

Phenothiazine, 10-(3'-aminopropyl)-2-chloro-

Inchi:	InChI=1S/C15H15ClN2S/c16-11-6-7-15-13(10-11)18(9-3-8-17)12-4-1-2-5-14(12)19-15/h
InchiKey:	ZTQZBABFEUDZFE-UHFFFAOYSA-N
Formula:	C15H15ClN2S
SMILES:	NCCCN1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]:	290.81
CAS:	2095-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	4.292		Crippen Method
mcvol	212.380	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2095172&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/93-504-9/Phenothiazine-10-3-aminopropyl-2-chloro.pdf>

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