

Norchlordiazepoxide

Inchi:	InChI=1S/C15H11ClN2O/c16-12-6-7-14-13(10-12)15(18(19)9-8-17-14)11-4-2-1-3-5-11/h
InchiKey:	YIXUNVZJCJYWIW-UHFFFAOYSA-N
Formula:	C15H11ClN2O
SMILES:	[O-][N+]1=C(c2ccccc2)c2cc(Cl)ccc2N=CC1
Mol. weight [g/mol]:	270.71
CAS:	16300-25-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	3.404		Crippen Method
mcvol	193.300	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=C16300257&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/57-636-3/Norchlordiazepoxide.pdf>

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