

Desmethylclomipramine

Other names:	Norclomipramine
Inchi:	InChI=1S/C18H21ClN2/c1-20-11-4-12-21-17-6-3-2-5-14(17)7-8-15-9-10-16(19)13-18(15)
InchiKey:	VPIXQGUBUKFLRF-UHFFFAOYSA-N
Formula:	C18H21ClN2
SMILES:	CNCCCN1c2ccccc2CCc2ccc(Cl)cc21
Mol. weight [g/mol]:	300.83
CAS:	303-48-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	4.186		Crippen Method
mcvol	238.300	ml/mol	McGowan Method

Sources

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=C303480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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