

N-methyl-n'-p-chlorobenzhydryl homopiperazine

Other names:	Homochlorcyclizine
Inchi:	InChI=1S/C19H23ClN2/c1-21-12-5-13-22(15-14-21)19(16-6-3-2-4-7-16)17-8-10-18(20)1
InchiKey:	WEUCDJCFJHYFRL-UHFFFAOYSA-N
Formula:	C19H23ClN2
SMILES:	CN1CCCN(C(c2ccccc2)c2ccc(Cl)cc2)CC1
Mol. weight [g/mol]:	314.85
CAS:	848-53-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	4.067		Crippen Method
mcvol	252.390	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C848533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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