

N-benzyl-n'-(beta-hydroxyethyl) homopiperazine

Inchi:	InChI=1S/C14H22N2O/c17-12-11-15-7-4-8-16(10-9-15)13-14-5-2-1-3-6-14/h1-3,5-6,17H
InchiKey:	KUJQTWKDKIOXGH-UHFFFAOYSA-N
Formula:	C14H22N2O
SMILES:	OCCN1CCCN(Cc2ccccc2)CC1
Mol. weight [g/mol]:	234.34
CAS:	23207-69-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	1.187		Crippen Method
mcvol	199.330	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=C23207694&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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