

3-(Benzylamino)quinuclidine

Inchi:	InChI=1S/C14H20N2/c1-2-4-12(5-3-1)10-15-14-11-16-8-6-13(14)7-9-16/h1-5,13-15H,6-1
InchiKey:	BMCRQEPTJNQZST-UHFFFAOYSA-N
Formula:	C14H20N2
SMILES:	c1ccc(CNC2CN3CCC2CC3)cc1
Mol. weight [g/mol]:	216.32
CAS:	6530-11-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	1.870		Crippen Method
mcvol	182.600	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=C6530116&Units=SI

Legend

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

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