

(3R)-(-)-1-Benzyl-3-aminopyrrolidine

Inchi:	InChI=1S/C11H16N2/c12-11-6-7-13(9-11)8-10-4-2-1-3-5-10/h1-5,11H,6-9,12H2/t11-/m0/
InchiKey:	HBVNLKQGRZPGRP-NSHDSACASA-N
Formula:	C11H16N2
SMILES:	NC1CCN(Cc2ccccc2)C1
Mol. weight [g/mol]:	176.26
CAS:	114715-39-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.220		Crippen Method
mcvol	151.190	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=C114715398&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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<https://www.chemeo.com/cid/86-119-5/3R-1-Benzyl-3-aminopyrrolidine.pdf>

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