

# (3S)-(+)-1-Benzyl-3-aminopyrrolidine

<b>Inchi:</b>	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-/m1/
<b>InchiKey:</b>	HBVNLKQGRZPGRP-LLVKDONJSA-N
<b>Formula:</b>	C11H16N2
<b>SMILES:</b>	NC1CCN(Cc2ccccc2)C1
<b>Mol. weight [g/mol]:</b>	176.26
<b>CAS:</b>	114715-38-7

## 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

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C114715387&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C114715387&amp;Units=SI</a>

## Legend

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

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