

# Adeptolon

<b>Inchi:</b>	InChI=1S/C16H20BrN3/c1-3-19(2)12-13-20(16-6-4-5-11-18-16)15-9-7-14(17)8-10-15/h4-
<b>InchiKey:</b>	IDDMFDHHCXRYQH-UHFFFAOYSA-N
<b>Formula:</b>	C16H20BrN3
<b>SMILES:</b>	CCN(C)CCN(c1ccc(Br)cc1)c1cccn1
<b>Mol. weight [g/mol]:</b>	334.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.934		Crippen Method
mcvol	236.220	ml/mol	McGowan Method
rinpol	2375.00		NIST Webbook

## Sources

<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=R535958&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R535958&amp;Units=SI</a>
<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>

## 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
<b>rinpol:</b>	Non-polar retention indices

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