

# 1,4-Dipentylisoquinoline

<b>Inchi:</b>	InChI=1S/C19H27N/c1-3-5-7-11-16-15-20-19(14-8-6-4-2)18-13-10-9-12-17(16)18/h9-10,
<b>InchiKey:</b>	UKODNDSPGMOPGN-UHFFFAOYSA-N
<b>Formula:</b>	C19H27N
<b>SMILES:</b>	CCCCC1cnc(CCCCC)c2cccc12
<b>Mol. weight [g/mol]:</b>	269.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	5.700		Crippen Method
mcvol	245.330	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook

## Sources

<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=R545376&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R545376&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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