

# 5-Isopentenylindole

<b>Inchi:</b>	InChI=1S/C13H15N/c1-10(2)3-4-11-5-6-13-12(9-11)7-8-14-13/h3,5-9,14H,4H2,1-2H3
<b>InchiKey:</b>	BDNMERUZUSYRO-UHFFFAOYSA-N
<b>Formula:</b>	C13H15N
<b>SMILES:</b>	CC(C)=CCc1ccc2[nH]ccc2c1
<b>Mol. weight [g/mol]:</b>	185.26

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.195		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpole	1767.00		NIST Webbook
rinpole	1767.00		NIST Webbook

## 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=R411911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R411911&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
<b>rinpole:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/30-617-3/5-Isopentenylindole.pdf>

Generated by Cheméo on 2024-04-30 07:23:32.471942017 +0000 UTC m=+16751061.392519337.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.