

3-(1H-Indol-3-ylmethyl)-1H-indole

Other names:	1H-Indole, 3,3'-methylenebis-
Inchi:	InChI=1S/C17H14N2/c1-3-7-16-14(5-1)12(10-18-16)9-13-11-19-17-8-4-2-6-15(13)17/h1-
InchiKey:	VFTRKSBEFQDZKX-UHFFFAOYSA-N
Formula:	C17H14N2
SMILES:	<chem>c1ccc2c(Cc3c[nH]c4ccccc34)c[nH]c2c1</chem>
Mol. weight [g/mol]:	246.31
CAS:	1968-05-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Crippen Method
logp	3.276		Crippen Method
mcvol	192.510	ml/mol	McGowan Method
rinpol	2700.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1968054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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