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: c1ccc2c(Cc3c[nH]c4ccccc34)c[nH]c2c1
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