

Bis(3-indolylethyl)amine

Inchi:	InChI=1S/C20H21N3/c1-3-7-19-17(5-1)15(13-22-19)9-11-21-12-10-16-14-23-20-8-4-2-6-
InchiKey:	IXLSYXSELOBCFE-UHFFFAOYSA-N
Formula:	C20H21N3
SMILES:	c1ccc2c(CCNCCc3c[nH]c4ccccc34)c[nH]c2c1
Mol. weight [g/mol]:	303.40
CAS:	94685-68-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	3.060		Crippen Method
mcvol	244.760	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94685684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/87-388-6/Bis-3-indolylethyl-amine.pdf>

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