

Histapyrrodine

Inchi: InChI=1S/C19H24N2/c1-3-9-18(10-4-1)17-21(19-11-5-2-6-12-19)16-15-20-13-7-8-14-20/
InchiKey: MXHODDGKGSGLDI-UHFFFAOYSA-N
Formula: C19H24N2
SMILES: c1ccc(CN(CCN2CCCC2)c2ccccc2)cc1
Mol. weight [g/mol]: 280.41
CAS: 493-80-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	3.789		Crippen Method
mcvol	240.150	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C493801&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/64-296-3/Histapyrrodine.pdf>

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