

Histapyrrodine M (N-desphenyl), acetylated

Inchi: InChI=1S/C15H22N2O/c1-14(18)17(12-11-16-9-5-6-10-16)13-15-7-3-2-4-8-15/h2-4,7-8H
InchiKey: DXRDHLJLGHMNQE-UHFFFAOYSA-N
Formula: C15H22N2O
SMILES: CC(=O)N(CCN1CCCC1)Cc1ccccc1
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	2.131		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R536446&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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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