Histapyrrodine M (oxo)

Inchi: InChI=1S/C19H22N2O/c22-19(20-13-7-8-14-20)16-21(18-11-5-2-6-12-18)15-17-9-3-1-4-
InchiKey: KOUAOKSOPBEEPX-UHFFFAOYSA-N
Formula: C19H22N2O
SMILES: O=C(CN(Cc1ccccc1)c1ccccc1)N1CCCC1
Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	3.316		Crippen Method
mcvol	241.720	ml/mol	McGowan Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook

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=R536466&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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