5-Hydroxy-5-methyl-2,3-bis-(1-pyrrolidinyl)-2-cycl

Inchi: InChI=1S/C14H22N2O2/c1-14(18)10-11(15-6-2-3-7-15)12(13(14)17)16-8-4-5-9-16/h18H
InchiKey: AQQYFYYRFLYWIQ-UHFFFAOYSA-N
Formula: C14H22N2O2
SMILES: CC1(O)CC(N2CCCC2)=C(N2CCCC2)C1=O
Mol. weight [g/mol]: 250.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	1.113		Crippen Method
mcvol	198.640	ml/mol	McGowan Method
ripol	3000.00		NIST Webbook
ripol	3000.00		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=R532499&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
ripol: Polar retention indices

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