11-Oxotetrahydro-rhombifoline

Inchi: InChI=1S/C14H20N2O2/c1-2-6-15-8-10-7-11(14(15)18)9-16-12(10)4-3-5-13(16)17/h2,10
InchiKey: LEIDJOZUXHDZKJ-UHFFFAOYSA-N
Formula: C14H20N2O2
SMILES: C=CCN1CC2CC(CN3C(=O)CCCC23)C1=O
Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	1.032		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		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=R205355&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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