11,12-seco-12,13-didehydromultiflorine

Inchi: InChI=1S/C15H22N2O/c1-2-3-5-16-9-12-7-13(11-16)15-8-14(18)4-6-17(15)10-12/h2,4,6,
InchiKey: QEFLZWOIQICVRH-UHFFFAOYSA-N
Formula: C15H22N2O
SMILES: C=CCCN1CC2CC(C1)C1CC(=O)C=CN1C2
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.671		Crippen Method
mcvol	202.560	ml/mol	McGowan Method
rinpol	2210.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2211.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R577734&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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