N-Formylangustifoline

Inchi: InChI=1S/C15H22N2O2/c1-2-3-14-13-6-11(9-17(14)10-18)8-16-5-4-12(19)7-15(13)16/h2
InchiKey: UUCCIWFXLFBXOP-UHFFFAOYSA-N
Formula: C15H22N2O2
SMILES: C=CCC1C2CC(CN1C=O)CN1CCC(=O)CC21
Mol. weight [g/mol]: 262.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	1.073		Crippen Method
mcvol	208.430	ml/mol	McGowan Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2367.00		NIST Webbook
rinpol	2363.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R264314&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

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