Dehydroangustifoline

Inchi: InChI=1S/C14H20N2O/c1-2-3-13-11-6-10(8-15-13)14-7-12(17)4-5-16(14)9-11/h2,7,10-11
InchiKey: PZTRDIUYRUKDJQ-GCZXYKMCSA-N
Formula: C14H20N2O
SMILES: C=CCC1NCC2CC1CN1CCC(=O)C=C21
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.329		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook
rinpol	2070.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R264136&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices