Isoangustifoline

Inchi: InChI=1S/C14H22N2O/c1-2-3-13-12-6-10(8-15-13)9-16-5-4-11(17)7-14(12)16/h2,10,12-1
InchiKey: SHZTWMVOBAEJMJ-UHFFFAOYSA-N
Formula: C14H22N2O
SMILES: C=CCC1NCC2CC1C1CC(=O)CCN1C2
Mol. weight [g/mol]: 234.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	1.204		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
rinpol	2051.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2033.00		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=R205439&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

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