3«alpha»-Nicotinoyloxytropane

Inchi: InChI=1S/C14H18N2O2/c1-16-11-4-5-12(16)8-13(7-11)18-14(17)10-3-2-6-15-9-10/h2-3,6
InchiKey: NHFDVEVAKLYKKT-ITGUQSILSA-N
Formula: C14H18N2O2
SMILES: CN1C2CCC1CC(OC(=O)c1cccnc1)C2
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.864		Crippen Method
mcvol	190.040	ml/mol	McGowan Method
rinpol	1953.00		NIST Webbook
rinpol	1952.00		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=R509583&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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