N-Acetyl Norapoatropine

Inchi: InChI=1S/C18H21NO3/c1-12(14-6-4-3-5-7-14)18(21)22-17-10-15-8-9-16(11-17)19(15)13
InchiKey: PHTYDHJIFIGMSQ-UHFFFAOYSA-N
Formula: C18H21NO3
SMILES: C=C(C(=O)OC1CC2CCC(C1)N2C(C)=O)c1ccccc1
Mol. weight [g/mol]: 299.36
CAS: 1094738-51-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	2.785		Crippen Method
mcvol	233.690	ml/mol	McGowan Method
rinpol	2528.70		NIST Webbook
rinpol	2528.70		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=C1094738518&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