

N-Acetyl norlittorine

Inchi: InChI=1S/C18H23NO4/c1-12(20)19-14-7-8-15(19)11-16(10-14)23-18(22)17(21)9-13-5-3
InchiKey: RQQNWNXACWZHKR-UHFFFAOYSA-N
Formula: C18H23NO4
SMILES: CC(=O)N1C2CCC1CC(OC(=O)C(O)Cc1cccc1)C2
Mol. weight [g/mol]: 317.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	1.675		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
rinpol	2710.20		NIST Webbook
rinpol	2710.20		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U415017&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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<https://www.cheméo.com/cid/99-452-1/N-Acetyl-norlittorine.pdf>

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