(1R,3a1S,11bS)-9-Hydroxy-10-methoxy-2,3a1,4,5,7 acetate

Inchi: InChI=1S/C18H21NO4/c1-10(20)23-15-4-3-11-5-6-19-9-12-7-14(21)16(22-2)8-13(12)17(

InchiKey: LSBMSYLHJUUWMU-UHFFFAOYSA-N

Formula: C18H21NO4

SMILES: COc1cc2c(cc1O)CN1CCC3=CCC(OC(C)=O)C2C31

Mol. weight [g/mol]: 315.36

CAS: 265992-98-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	2.334		Crippen Method
mcvol	233.000	ml/mol	McGowan Method
rinpol	2508.10		NIST Webbook
rinpol	2508.10		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C265992981&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices