

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

Inchi:
acetate

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:

LSBMSYLHJUWUMU-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
rinpola	2508.10		NIST Webbook
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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
rinpola:	Non-polar retention indices

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