

7-(Acetoxymethyl)-2,3,5,7a-tetrahydro-1H-pyrrolizin-1-yl-tiglate

InChI:
InChIKey:

InChI=1S/C15H21NO4/c1-4-10(2)15(18)20-13-6-8-16-7-5-12(14(13)16)9-19-11(3)17/h4-5

Formula:

C15H21NO4

SMILES:

CC=C(C)C(=O)OC1CCN2CC=C(COC(C)=O)C12

Mol. weight [g/mol]:

279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	1.442		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
rinpol	2062.10		NIST Webbook
rinpol	2062.10		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U415002&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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