

7-acetyl-9-(2-hydroxy-3-methylbutyryl)retronecine

Inchi:	InChI=1S/C15H23NO5/c1-9(2)14(18)15(19)20-8-11-4-6-16-7-5-12(13(11)16)21-10(3)17/
InchiKey:	OTEHYFUSZSWPPU-HSBZDZAISA-N
Formula:	C15H23NO5
SMILES:	CC(=O)OC1CCN2CC=C(COC(=O)C(O)C(C)C)C12
Mol. weight [g/mol]:	297.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.40		Crippen Method
logp	0.493		Crippen Method
mcvol	226.920	ml/mol	McGowan Method
rinpol	2024.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R240521&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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