

7-tigloyl-9-(2,3-dihydroxy propanoyl) retronecine

Inchi: InChI=1S/C16H25NO6/c1-3-10(2)15(20)23-13-5-7-17-6-4-11(14(13)17)9-22-16(21)12(19)
InchiKey: UCZOPSUTRUWZNY-SNTUAPAQSA-N
Formula: C16H25NO6
SMILES: CC=C(C)C(=O)OC1CCN2CCC(COC(=O)C(O)CO)C12
Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	-0.145		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
rinpol	2320.00		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=R227919&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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