3'-Acetylheliosupine

Inchi: InChI=1S/C22H33NO8/c1-7-13(2)19(25)31-17-9-11-23-10-8-16(18(17)23)12-29-20(26)22
InchiKey: LHYJPODIMQKZHJ-IBTXQZQRSA-N
Formula: C22H33NO8
SMILES: CC=C(C)C(=O)OC1CCN2CC=C(COC(=O)C(O)(C(C)OC(C)=O)C(C)(C)O)C12
Mol. weight [g/mol]: 439.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.77		Crippen Method
logp	0.875		Crippen Method
mcvol	334.560	ml/mol	McGowan Method
rinpol	2640.00		NIST Webbook
rinpol	2636.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R299508&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

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