uplandicine

Inchi: InChI=1S/C17H27NO7/c1-10(19)17(23,16(3,4)22)15(21)24-9-12-5-7-18-8-6-13(14(12)18
InchiKey: IHRIHUJNKKMIDN-NBCLGQJJSA-N
Formula: C17H27NO7
SMILES: CC(=O)O[C@@H]1CCN2CC=C(COC(=O)[C@](O)([C@H](C)O)C(C)(C)O)[C@H]12
Mol. weight [g/mol]: 357.40

Physical Properties

Property code	Value	Unit	Source
logp	-0.642		Crippen Method
mcvol	266.840	ml/mol	McGowan Method
rinpol	2337.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R240561&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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