Heliotrine (7S)

Inchi: InChI=1S/C16H27NO5/c1-10(2)16(20,11(3)21-4)15(19)22-9-12-5-7-17-8-6-13(18)14(12)1
InchiKey: LMFKRLGHEKVMNT-ZGMNHVEMSA-N
Formula: C16H27NO5
SMILES: COC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)C
Mol. weight [g/mol]: 313.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	0.327		Crippen Method
mcvol	245.310	ml/mol	McGowan Method
rinpol	2100.00		NIST Webbook
rinpol	2114.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R178228&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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