Indicine

Inchi: InChI=1S/C15H25NO5/c1-9(2)15(20,10(3)17)14(19)21-8-11-4-6-16-7-5-12(18)13(11)16/h
InchiKey: SFVVQRJOGUKCEG-UOFHRTMOSA-N
Formula: C15H25NO5
SMILES: CC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)O
Mol. weight [g/mol]: 299.36
CAS: 480-82-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	-0.327		Crippen Method
mcvol	231.220	ml/mol	McGowan Method
rinpol	2126.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2126.00		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=C480820&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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