Isocallimorphine

Inchi:	InChI=1S/C15H23NO5/c1-4-15(3,21-10(2)17)14(19)20-9-11-5-7-16-8-6-12(18)13(11)16/h
InchiKey:	WZYYIFYCXJFFSX-QNIGDANOSA-N
Formula:	C15H23NO5
SMILES:	CCC(C)(OC(C)=O)C(=O)OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]:	297.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	0.637		Crippen Method
mcvol	226.920	ml/mol	McGowan Method
rinpol	1977.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R178431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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