

Callimorphine

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/
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
rinpola	1965.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R178382&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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/41-887-2/Callimorphine.pdf>

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