3«beta»-Merresectine C

Inchi: InChI=1S/C25H35NO3/c1-16(2)6-8-18-12-20(13-19(24(18)27)9-7-17(3)4)25(28)29-23-14
InchiKey: MYEROKWORYNFGZ-NUNAXRQHSA-N
Formula: C25H35NO3
SMILES: CC(C)=CCc1cc(C(=O)OC2CC3CCC(C2)N3C)cc(CC=C(C)C)c1O
Mol. weight [g/mol]: 397.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.71		Crippen Method
logp	5.192		Crippen Method
mcvol	332.320	ml/mol	McGowan Method
rinpol	3070.00		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=R509672&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