

# 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
rinpole	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](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  
**rinpole:** Non-polar retention indices

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