

# Merresectine D

**Inchi:** InChI=1S/C21H29NO4/c1-13(2)5-6-14-9-15(10-19(25-4)20(14)23)21(24)26-18-11-16-7-8  
**InchiKey:** ONGAXCZYCQUMSY-PIIMJCKOSA-N  
**Formula:** C21H29NO4  
**SMILES:** COc1cc(C(=O)OC2CC3CCCC(C2)N3C)cc(CC=C(C)C)c1O  
**Mol. weight [g/mol]:** 359.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	3.691		Crippen Method
mcvol	286.130	ml/mol	McGowan Method
rinpole	2785.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R510088&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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>

## 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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