

# Methylpseudoecgonine

**Inchi:** InChI=1S/C17H21NO4/c1-18-12-8-9-14(18)15(13(10-12)17(20)21-2)22-16(19)11-6-4-3-5  
**InchiKey:** YBNSZTYCRZTRRX-FGZQJIAISA-N  
**Formula:** C17H21NO4  
**SMILES:** COC(=O)C1CC2CCC(C1OC(=O)c1cccc1)N2C  
**Mol. weight [g/mol]:** 303.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	1.868		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
rinsol	1473.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R510137&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  
**rinsol:** Non-polar retention indices

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