

# Californine-M (nor-demethylene) 3AC

**Inchi:** InChI=1S/C23H21NO7/c1-11(25)24-18-5-15-7-22(30-12(2)26)23(31-13(3)27)9-17(15)19  
**InchiKey:** FCMJLKXWLJDLDM-UHFFFAOYSA-N  
**Formula:** C23H21NO7  
**SMILES:** CC(=O)Oc1cc2c(cc1OC(C)=O)C1Cc3cc4c(cc3C(C2)N1C(C)=O)OCO4  
**Mol. weight [g/mol]:** 423.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	3.009		Crippen Method
mcvol	293.000	ml/mol	McGowan Method
rinpole	3350.00		NIST Webbook

## Sources

**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=R289031&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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