

# Californine-M (nor-) AC

**Inchi:** InChI=1S/C20H17NO5/c1-10(22)21-15-2-11-4-17-19(25-8-23-17)6-13(11)16(21)3-12-5-1  
**InchiKey:** HCMZTUUUKUXOFC-UHFFFAOYSA-N  
**Formula:** C20H17NO5  
**SMILES:** CC(=O)N1C2Cc3cc4c(cc3C1Cc1cc3c(cc12)OCO3)OCO4  
**Mol. weight [g/mol]:** 351.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.97		Crippen Method
logp	2.887		Crippen Method
mcvol	236.730	ml/mol	McGowan Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R289026&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

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