# Californine-M, (demethylene-) 2AC

**Inchi:** InChI=1S/C22H21NO6/c1-11(24)28-21-7-14-5-17-15-8-20-19(26-10-27-20)6-13(15)4-18(
**InchiKey:** VCHNAOXLVGELMF-UHFFFAOYSA-N
**Formula:** C22H21NO6
**SMILES:** CC(=O)Oc1cc2c(cc1OC(C)=O)C1Cc3cc4c(cc3C(C2)N1C)OCO4
**Mol. weight [g/mol]:** 395.41

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.19 | | Crippen Method |
| logp | 3.092 | | Crippen Method |
| mcvol | 277.340 | ml/mol | McGowan Method |
| rinpol | 3025.00 | | NIST Webbook |
| rinpol | 3025.00 | | NIST Webbook |
| rinpol | 3025.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R288969&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** 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
**rinpol:** Non-polar retention indices

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