Californine-M (nor-demethylene-methyl-) 2AC

Inchi: InChI=1S/C22H21NO6/c1-11(24)23-17-4-13-6-20-21(28-10-27-20)9-16(13)18(23)5-14-7-
InchiKey: MAFLBHBHOVGODB-UHFFFAOYSA-N
Formula: C22H21NO6
SMILES: COc1cc2c(cc1OC(C)=O)CC1c3cc4c(cc3CC2N1C(C)=O)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	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R289046&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.