Californine-M, (di-(demethylene-methyl-)), isomer-1, 2AC

Inchi: InChI=1S/C23H25NO6/c1-12(25)29-22-9-15-7-19-17-11-23(30-13(2)26)20(27-4)8-14(17)

InchiKey: BNWRIWAZUXHMOS-UHFFFAOYSA-N

Formula: C23H25NO6

SMILES: COc1cc2c(cc1OC(C)=O)CC1c3cc(OC(C)=O)c(OC)cc3CC2N1C

Mol. weight [g/mol]: 411.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.22		Crippen Method
logp	3.381		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
rinpol	3010.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R288994&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