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

Inchi: InChI=1S/C21H21NO5/c1-11(23)27-21-7-13-5-17-15-9-20-19(25-10-26-20)6-12(15)4-16(

InchiKey: BRYWXNQXMLXTOV-UHFFFAOYSA-N

Formula: C21H21NO5

SMILES: COc1cc2c(cc1OC(C)=O)CC1c3cc4c(cc3CC2N1C)OCO4

Mol. weight [g/mol]: 367.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.176		Crippen Method
mcvol	261.680	ml/mol	McGowan Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		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=R288974&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.