

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

Inchi:	InChI=1S/C21H21NO5/c1-11(23)27-21-9-15-12(6-18(21)24-3)4-16-14-8-20-19(25-10-26
InchiKey:	MZIBRQSEHYKJEA-UHFFFAOYSA-N
Formula:	C21H21NO5
SMILES:	COc1cc2c(cc1OC(C)=O)C1Cc3cc4c(cc3C(C2)N1C)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
rmpol	2920.00		NIST Webbook
rmpol	2920.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R288989&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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