Californine-M (nor-), acetylated

Inchi: InChI=1S/C20H17NO5/c1-10(22)21-15-2-11-4-17-19(25-8-23-17)6-13(11)16(21)3-12-5-1
InchiKey: HCMZTUUUKUXOFC-UHFFFAOYSA-N
Formula: C20H17NO5
SMILES: CC(=O)N1C2Cc3cc4c(cc3C1Cc1cc3c(cc12)OCO3)OCO4
Mol. weight [g/mol]: 351.36

Physical Properties

Property code	Value	Unit	Source
logp	2.887		Crippen Method
mcvol	236.730	ml/mol	McGowan Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook
rinpol	3090.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R289026&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices