

californine

Inchi: InChI=1S/C19H17NO4/c1-20-14-2-10-4-16-18(23-8-21-16)6-12(10)15(20)3-11-5-17-19(7)
InchiKey: PGINMPJZCWDQNT-UHFFFAOYSA-N
Formula: C19H17NO4
SMILES: CN1C2Cc3cc4c(cc3C1Cc1cc3c(cc12)OCO3)OCO4
Mol. weight [g/mol]: 323.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	2.970		Crippen Method
mcvol	221.070	ml/mol	McGowan Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook

Sources

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=R288954&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/47-526-6/californine.pdf>

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