

4'-Dihydroconsabatine

Inchi: InChI=1S/C20H31NO4/c1-13(2)4-5-14-12-20(24,9-8-18(14)22)19(23)25-17-10-15-6-7-16
InchiKey: WTJGJRJHdrydgx-BVQKRNHHSa-N
Formula: C₂₀H₃₁NO₄
SMILES: CC(C)=CCC1=CC(O)(C(=O)OC2CC3CCC(C2)N3C)CCC1O
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	2.323		Crippen Method
mcvol	280.640	ml/mol	McGowan Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R509850&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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