

Consabatine

Inchi: InChI=1S/C20H29NO4/c1-13(2)4-5-14-12-20(24,9-8-18(14)22)19(23)25-17-10-15-6-7-16
InchiKey: JMHTUVBKARXGPJ-HBNZNPKYSA-N
Formula: C20H29NO4
SMILES: CC(C)=CCC1=CC(O)(C(=O)OC2CC3CCC(C2)N3C)CCC1=O
Mol. weight [g/mol]: 347.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	2.531		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
rinpol	2482.00		NIST Webbook
rinpol	2482.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R510013&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

Latest version available from:

<https://www.chemeo.com/cid/30-661-4/Consabatine.pdf>

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