

QUINIDINE, AC

Inchi: InChI=1S/C23H26N2O4/c1-4-16-13-25-10-8-17(16)11-22(25)23(29-15(3)27)19-7-9-24-2
InchiKey: ZMTNCRMTTXKNE-HYJUJMFVSA-N
Formula: C23H26N2O4
SMILES: C=CC1CN2CCC1CC2C(OC(C)=O)c1ccnc2ccc(OC(C)=O)cc12
Mol. weight [g/mol]: 394.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Crippen Method
logp	3.661		Crippen Method
mcvol	300.530	ml/mol	McGowan Method
rinpola	2750.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R493542&Units=SI>
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>

Legend

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

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