QUINIDINE, AC

Inchi:	InChI=1S/C23H26N2O4/c1-4-16-13-25-10-8-17(16)11-22(25)23(29-15(3)27)19-7-9-24-21
InchiKey:	ZMTNCRMTTXYKNE-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
rinpol	2750.00		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=R493542&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

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