

QUINIDINE, M(N-OXIDE), AC

Inchi: InChI=1S/C22H26N2O4/c1-4-15-13-23-9-7-16(15)11-21(23)22(28-14(2)25)18-8-10-24(2)
InchiKey: PKNXGMPZBOFTH-CWFBCUTFSA-N
Formula: C22H26N2O4
SMILES: C=CC1CN2CCC1CC2C(OC(C)=O)c1cc[n+](O)c2ccc(OC)cc12
Mol. weight [g/mol]: 382.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.08		Crippen Method
logp	2.982		Crippen Method
mcvol	290.740	ml/mol	McGowan Method
rinpola	2935.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R255424&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/14-224-7/QUINIDINE-M-N-OXIDE-AC.pdf>

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