QUINIDINE, M(HO-), AC

Inchi: InChI=1S/C24H28N2O5/c1-5-16-13-26-9-7-17(16)10-21(26)24(31-15(3)28)18-6-8-25-20-
InchiKey: HNMOTJRWPNWTIX-PXPAFMLWSA-N
Formula: C24H28N2O5
SMILES: C=CC1CN2CCC1CC2C(OC(C)=O)c1ccnc2cc(OC(C)=O)c(OC)cc12
Mol. weight [g/mol]: 424.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	3.669		Crippen Method
mcvol	320.490	ml/mol	McGowan Method
rinpol	3185.00		NIST Webbook
rinpol	3185.00		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=R255419&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.