Quinoline-4-carboxylic acid, 2-methoxy, 2-(diethylaminoethyl)amide

Inchi: InChI=1S/C17H22N2O3/c1-4-19(5-2)10-11-22-17(20)14-12-16(21-3)18-15-9-7-6-8-13(14

InchiKey: DIFKSOYYWCMJRB-UHFFFAOYSA-N

Formula: C17H22N2O3

SMILES: CCN(CC)CCOC(=O)c1cc(OC)nc2ccccc12

Mol. weight [g/mol]: 302.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	2.742		Crippen Method
mcvol	240.440	ml/mol	McGowan Method
rinpol	2449.00		NIST Webbook
rinpol	2465.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R579349&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.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

rinpol: Non-polar retention indices

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