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

Inchi: InChI=1S/C21H30N2O3/c1-4-7-10-14-25-20-16-18(17-11-8-9-12-19(17)22-20)21(24)26-1

InchiKey: ZTOBHUWFUIMVNU-UHFFFAOYSA-N

Formula: C21H30N2O3

SMILES: CCCCCOc1cc(C(=O)OCCN(CC)CC)c2ccccc2n1

Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.74		Crippen Method
logp	4.302		Crippen Method
mcvol	296.800	ml/mol	McGowan Method
rinpol	2789.00		NIST Webbook
rinpol	2810.00		NIST Webbook
rinpol	2789.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R579309&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

rinpol: Non-polar retention indices