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

Inchi: InChI=1S/C22H32N2O3/c1-4-7-8-11-15-26-21-17-19(18-12-9-10-13-20(18)23-21)22(25)2

InchiKey: JHWSTGYIEBQFJA-UHFFFAOYSA-N

Formula: C22H32N2O3

SMILES: CCCCCCOc1cc(C(=O)OCCN(CC)CC)c2ccccc2n1

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.16		Crippen Method
logp	4.693		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
rinpol	2885.00		NIST Webbook
rinpol	2909.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R579334&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

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