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

Inchi: InChI=1S/C19H26N2O3/c1-4-12-23-18-14-16(15-9-7-8-10-17(15)20-18)19(22)24-13-11-2

InchiKey: WTKONSKOIJGRFG-UHFFFAOYSA-N

Formula: C19H26N2O3

SMILES: CCCOc1cc(C(=O)OCCN(CC)CC)c2ccccc2n1

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	3.522		Crippen Method
mcvol	268.620	ml/mol	McGowan Method
rinpol	2593.00		NIST Webbook
rinpol	2612.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R579354&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

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