

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

Inchi: InChI=1S/C20H28N2O3/c1-4-7-13-24-19-15-17(16-10-8-9-11-18(16)21-19)20(23)25-14-
InchiKey: LEHKDIADQAJSQP-UHFFFAOYSA-N
Formula: C20H28N2O3
SMILES: CCCCOC1CC(C(=O)OCCN(CC)CC)C2CCCC2N1
Mol. weight [g/mol]: 344.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.32		Crippen Method
logp	3.912		Crippen Method
mcvol	282.710	ml/mol	McGowan Method
rinpol	2693.00		NIST Webbook
rinpol	2710.00		NIST Webbook
rinpol	2693.00		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=R579314&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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