# 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)25-14-1

**InchiKey:** LEHKDIADQAJSQP-UHFFFAOYSA-N

**Formula:** C20H28N2O3

**SMILES:** CCCCOc1cc(C(=O)OCCN(CC)CC)c2ccccc2n1

**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/ci990307l

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

**rinpol:** Non-polar retention indices