

# 2H-benzo[a]quinolizine-3-carboxamide,n,n-diethyl ester carbonate

InChI: InChI=1S/C22H32N2O6/c1-6-23(7-2)21(25)16-13-24-9-8-14-10-19(27-3)20(28-4)11-15(12-13)22  
InChIKey: FDUXGGKAYKXHRK-UHFFFAOYSA-N

**Formula:** C22H32N2O6

**SMILES:** CCN(CC)C(=O)C1CN2CCc3cc(OC)c(OC)cc3C2CC1OC(=O)OC

**Mol. weight [g/mol]:** 420.50

**CAS:** 127851-81-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	2.643		Crippen Method
mcvol	321.940	ml/mol	McGowan Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C127851814&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

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