2H-benzo[a]quinolizine-3-carboxamide,n,n-diethy 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(1

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/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