2,6-Pyridinedicarbamic acid, 4-amino-3-nitro-, diethyl ester

Inchi: InChI=1S/C11H15N5O6/c1-3-21-10(17)14-7-5-6(12)8(16(19)20)9(13-7)15-11(18)22-4-2/h

InchiKey: CXVYHNPWNIILSK-UHFFFAOYSA-N

Formula: C11H15N5O6

SMILES: CCOC(O)=Nc1cc(N)c([N+](=O)[O-])c(N=C(O)OCC)n1

Mol. weight [g/mol]: 313.27

CAS: 16335-92-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	1.736		Crippen Method
mcvol	214.310	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16335925&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