

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/
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/ci9903071
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

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