2-Pyridinecarbamic acid, 4-(allylamino)-6-amino-5-nitro-, ethyl ester

Inchi: InChI=1S/C11H15N5O4/c1-3-5-13-7-6-8(15-11(17)20-4-2)14-10(12)9(7)16(18)19/h3,6H,

InchiKey: PCTZFFKVNHNSMK-UHFFFAOYSA-N

Formula: C11H15N5O4

SMILES: C=CCNc1cc(NC(=O)OCC)nc(N)c1[N+](=O)[O-]

Mol. weight [g/mol]: 281.27

CAS: 116659-54-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	1.738		Crippen Method
mcvol	202.570	ml/mol	McGowan Method

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=C116659542&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