Ethyl 6-amino-4-chloro-5-nitro-2-pyridinyl(benzyl)carba

Inchi: InChI=1S/C15H15ClN4O4/c1-2-24-15(21)19(9-10-6-4-3-5-7-10)12-8-11(16)13(20(22)23)c(N)n1

InchiKey: QGRAZLLKGHWNAH-UHFFFAOYSA-N

Formula: C15H15ClN4O4

SMILES: CCOC(=O)N(Cc1ccccc1)c1cc(Cl)c([N+](=O)[O-])c(N)n1

Mol. weight [g/mol]: 350.76

CAS: 116403-17-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.90		Crippen Method
logp	3.389		Crippen Method
mcvol	241.730	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116403179&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