

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)
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.cheméo.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

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