

4-Pyrimidineacetic acid, 6-amino-2-chloro-5-nitro-, ethyl ester

Inchi:	InChI=1S/C8H9ClN4O4/c1-2-17-5(14)3-4-6(13(15)16)7(10)12-8(9)11-4/h2-3H2,1H3,(H2,
InchiKey:	AECMFYPAWPTWNT-UHFFFAOYSA-N
Formula:	C8H9ClN4O4
SMILES:	CCOC(=O)Cc1nc(Cl)nc(N)c1[N+](=O)[O-]
Mol. weight [g/mol]:	260.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	0.726		Crippen Method
mcvol	166.860	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=B6010444&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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