Ethanol, 2-[(6-amino-2-chloro-5-nitro-4-pyrimidinyl)amino]-

Inchi: InChI=1S/C6H8ClN5O3/c7-6-10-4(8)3(12(14)15)5(11-6)9-1-2-13/h13H,1-2H2,(H3,8,9,10,

InchiKey: VJHSQGXRHONOAO-UHFFFAOYSA-N

Formula: C6H8ClN5O3

SMILES: Nc1nc(Cl)nc(NCCO)c1[N+](=O)[O-]

Mol. weight [g/mol]: 233.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.66		Crippen Method
logp	0.025		Crippen Method
mcvol	147.090	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=B6008442&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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