

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: VJHSQGXRHONAO-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.cheméo.com/doc/models/crippen_log10ws

Legend

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

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