Pyrimidine, 4,6-diamino-2-methyl-5-nitro-

Inchi: InChI=1S/C5H7N5O2/c1-2-8-4(6)3(10(11)12)5(7)9-2/h1H3,(H4,6,7,8,9)
InchiKey: SJJXPENCFKLUMR-UHFFFAOYSA-N
Formula: C5H7N5O2
SMILES: Cc1nc(N)c([N+](=O)[O-])c(N)n1
Mol. weight [g/mol]: 169.14
CAS: 3346-21-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.40		Crippen Method
logp	-0.142		Crippen Method
mcvol	114.890	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=C3346212&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