

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

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<https://www.chemeo.com/cid/40-961-0/Pyrimidine-4-6-diamino-2-methyl-5-nitro.pdf>

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