

4(1H)-Pyrimidinone, 6-amino-2-methyl-5-nitroso-

Other names:	4-Amino-6-hydroxy-2-methyl-5-nitrosopyrimidine 4-Pyrimidinol, 6-amino-2-methyl-5-nitroso- 4(3H)-Pyrimidinone, 6-amino-2-methyl-5-nitroso- 6-amino-2-methyl-5-nitroso-1H-pyrimidin-4-one
Inchi:	InChI=1S/C5H6N4O2/c1-2-7-4(6)3(9-11)5(10)8-2/h1H3,(H3,6,7,8,10)
InchiKey:	DRDJDNORXOOBHR-UHFFFAOYSA-N
Formula:	C5H6N4O2
SMILES:	<chem>Cc1nc(N)c(N=O)c(O)n1</chem>
Mol. weight [g/mol]:	154.13
CAS:	2209-72-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.42		Crippen Method
logp	0.471		Crippen Method
mcvol	104.910	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=C2209725&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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