

# 4,6-Pyrimidinediol, 5-nitro-, (keto form)

<b>Other names:</b>	5-nitropyrimidine-4,6-diol
<b>Inchi:</b>	InChI=1S/C4H3N3O4/c8-3-2(7(10)11)4(9)6-1-5-3/h1H,(H2,5,6,8,9)
<b>InchiKey:</b>	ABTLZAVJDRUDNG-UHFFFAOYSA-N
<b>Formula:</b>	C4H3N3O4
<b>SMILES:</b>	O=[N+](O)c1c(O)ncnc1O
<b>Mol. weight [g/mol]:</b>	157.08
<b>CAS:</b>	2164-83-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.75		Crippen Method
logp	-0.204		Crippen Method
mcvol	92.580	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2164832&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2164832&amp;Units=SI</a>

## Legend

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

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