

# 6-Chloro-2,4-dihydroxy-1,3-dimethylpyrimidine

<b>Other names:</b>	6-Chloro-1,3-dimethyluracil 1,3-Dimethyl-4-chlorouracil 2,4(1H,3H)-Pyrimidinedione, 6-chloro-1,3-dimethyl-
<b>Inchi:</b>	InChI=1S/C6H7ClN2O2/c1-8-4(7)3-5(10)9(2)6(8)11/h3H,1-2H3
<b>InchiKey:</b>	VATQPUHLFQHDBD-UHFFFAOYSA-N
<b>Formula:</b>	C6H7ClN2O2
<b>SMILES:</b>	Cn1c(Cl)cc(=O)n(C)c1=O
<b>Mol. weight [g/mol]:</b>	174.59
<b>CAS:</b>	6972-27-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	-0.263		Crippen Method
mcvol	115.580	ml/mol	McGowan Method

## Sources

<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=C6972276&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6972276&amp;Units=SI</a>
<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>

## 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

Latest version available from:

<https://www.chemeo.com/cid/28-706-7/6-Chloro-2-4-dihydroxy-1-3-dimethylpyrimidine.pdf>

Generated by Cheméo on 2024-04-23 14:26:01.39174588 +0000 UTC m=+16171610.312323193.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.