

# 6-Chlorouracil

<b>Other names:</b>	2,4(1H,3H)-Pyrimidinedione, 6-chloro-
<b>Inchi:</b>	InChI=1S/C4H3ClN2O2/c5-2-1-3(8)7-4(9)6-2/h1H,(H2,6,7,8,9)
<b>InchiKey:</b>	PKUFNWPSFCOSLU-UHFFFAOYSA-N
<b>Formula:</b>	C4H3ClN2O2
<b>SMILES:</b>	O=c1cc(Cl)[nH]c(=O)[nH]1
<b>Mol. weight [g/mol]:</b>	146.53
<b>CAS:</b>	4270-27-3

## Physical Properties

Property code	Value	Unit	Source
hsub	135.20 ± 2.00	kJ/mol	NIST Webbook
log10ws	0.56		Crippen Method
logp	-1.247		Crippen Method
mvol	87.400	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	134.30	kJ/mol	386.50	NIST Webbook

## 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=C4270273&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4270273&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>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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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