

2,4(1H,3H)-Pyrimidinedione, 6-chloro-3-methyl-

Other names:	Uracil, 6-chloro-3-methyl- 3-Methyl-6-chlorouracil 6-Chloro-3-methyluracil
Inchi:	InChI=1S/C5H5ClN2O2/c1-8-4(9)2-3(6)7-5(8)10/h2H,1H3,(H,7,10)
InchiKey:	SGLXGFAZAARYJY-UHFFFAOYSA-N
Formula:	C5H5ClN2O2
SMILES:	Cn1c(=O)cc(Cl)[nH]c1=O
Mol. weight [g/mol]:	160.56
CAS:	4318-56-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	-0.755		Crippen Method
mcvol	101.490	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	105.00 ± 6.00	kJ/mol	468.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4318563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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