

1-Methyl-6-chlorouracil

Inchi:	InChI=1S/C5H5ClN2O2/c1-8-3(6)2-4(9)7-5(8)10/h2H,1H3,(H,7,9,10)
InchiKey:	AOSGEKKSRYJBGW-UHFFFAOYSA-N
Formula:	C5H5ClN2O2
SMILES:	Cn1c(Cl)cc(=O)[nH]c1=O
Mol. weight [g/mol]:	160.56
CAS:	31737-09-4

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	109.00 ± 8.00	kJ/mol	441.00	NIST Webbook

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=C31737094&Units=SI

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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