Uracil, 1-methyl-

Other names:	1-Methyluracil
	2,4(1H,3H)-Pyrimidinedione, 1-methyl-
Inchi:	InChI=1S/C5H6N2O2/c1-7-3-2-4(8)6-5(7)9/h2-3H,1H3,(H,6,8,9)
InchiKey:	XBCXJKGHPABGSD-UHFFFAOYSA-N
Formula:	C5H6N2O2
SMILES:	Cn1ccc(=O)[nH]c1=O
Mol. weight [g/mol]:	126.11
CAS:	615-77-0

Physical Properties

Property code	Value	Unit	Source
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-0.80		Aqueous Solubility Prediction Method
log10ws	-0.81		Estimated Solubility Method
logp	-1.408		Crippen Method
mcvol	89.250	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	121.70 ± 4.00	kJ/mol	385.50	NIST Webbook
hsubt	112.50 ± 2.60	kJ/mol	398.00	NIST Webbook
hsubt	105.00 ± 8.00	kJ/mol	457.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

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