

2,4(1H,3H)-Pyrimidinedione, 3,6-dimethyl-

Other names:	Uracil, 3,6-dimethyl- 3,6-Dimethyl-2,4(1H,3H)-pyrimidinedione 3,6-Dimethyluracil
Inchi:	InChI=1S/C6H8N2O2/c1-4-3-5(9)8(2)6(10)7-4/h3H,1-2H3,(H,7,10)
InchiKey:	CFADSIBRSRZBQO-UHFFFAOYSA-N
Formula:	C6H8N2O2
SMILES:	Cc1cc(=O)n(C)c(=O)[nH]1
Mol. weight [g/mol]:	140.14
CAS:	19674-60-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	-1.100		Crippen Method
mcvol	103.340	ml/mol	McGowan Method

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=C19674603&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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