

4,6-DIMETHYL-2-PYRIMIDONE

Other names:	2(1H)-Pyrimidinone, 4,6-dimethyl- 4,6-Dimethyl-2-hydroxypyrimidine 4,6-Dimethyl-2-pyrimidinol 4,6-dimethylpyrimidin-2-ol
Inchi:	InChI=1S/C6H8N2O/c1-4-3-5(2)8-6(9)7-4/h3H,1-2H3,(H,7,8,9)
InchiKey:	WHEQVHAIRSPYDK-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	<chem>Cc1cc(C)[nH]c(=O)n1</chem>
Mol. weight [g/mol]:	124.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.49		Cheméo Relay (1.0)
logp	-0.095		Crippen Method
mcvol	97.470	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108792&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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

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