

4,6-Dimethyl-2-pyrimidone

Other names:	4,6-Dimethyl-2-hydroxypyrimidine 2(1H)-Pyrimidinone, 4,6-dimethyl- 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
CAS:	108-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.83		Crippen Method
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/17-039-0/4-6-Dimethyl-2-pyrimidone.pdf>

Generated by Cheméo on 2024-04-30 13:35:11.323869858 +0000 UTC m=+16773360.244447170.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.