

4(1H)-Pyrimidinone, 6-methyl-

Other names:	4-Pyrimidinol, 6-methyl- 4-Hydroxy-6-methylpyrimidine 6-Methyl-4(3H)-pyrimidinone 6-Methyl-4-oxopyrimidine 6-Methyl-4-pyrimidinol 6-methyl-1H-pyrimidin-4-one
Inchi:	InChI=1S/C5H6N2O/c1-4-2-5(8)7-3-6-4/h2-3H,1H3,(H,6,7,8)
InchiKey:	LHRIUKSRPHFASO-UHFFFAOYSA-N
Formula:	C5H6N2O
SMILES:	<chem>Cc1cc(O)ncn1</chem>
Mol. weight [g/mol]:	110.11
CAS:	3524-87-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	0.491		Crippen Method
mcvol	83.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3524876&Units=SI
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

Legend

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

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