

2(1H)-Pyridinone, 6-chloro-1-methyl-

Other names:	1-Methyl-6-chloro-pyrid-2-one 6-Chloro-1-methyl-2(1H)pyridinone
Inchi:	InChI=1S/C6H6ClNO/c1-8-5(7)3-2-4-6(8)9/h2-4H,1H3
InchiKey:	WTMIJNWKTCXRBK-UHFFFAOYSA-N
Formula:	C6H6ClNO
SMILES:	Cn1c(Cl)cccc1=O
Mol. weight [g/mol]:	143.57
CAS:	17228-63-6

Physical Properties

Property code	Value	Unit	Source
affp	918.50	kJ/mol	NIST Webbook
basg	885.50	kJ/mol	NIST Webbook
log10ws	-2.87		Crippen Method
logp	1.039		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17228636&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

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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