

2(1H)-Pyridinone, 3-acetyl-4-hydroxy-1,6-dimethyl-

Other names:	2(1H)-Pyridone, 3-acetyl-4-hydroxy-1,6-dimethyl-3-acetyl-4-hydroxy-1,6-dimethyl-2(1H)-pyridinone
Inchi:	InChI=1S/C9H11NO3/c1-5-4-7(12)8(6(2)11)9(13)10(5)3/h4,12H,1-3H3
InchiKey:	QUYIISZLCVRHGN-UHFFFAOYSA-N
Formula:	C9H11NO3
SMILES:	CC(=O)c1c(O)cc(C)n(C)c1=O
Mol. weight [g/mol]:	181.19
CAS:	7202-55-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	0.602		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
rinpol	1672.00		NIST Webbook

Sources

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=C7202553&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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