

2(1H)-Pyrimidinone

Other names:	1H-pyrimidin-2-one
Inchi:	InChI=1S/C4H4N2O/c7-4-5-2-1-3-6-4/h1-3H,(H,5,6,7)
InchiKey:	VTGOHKSTWXHQJK-UHFFFAOYSA-N
Formula:	C4H4N2O
SMILES:	Oc1ncccn1
Mol. weight [g/mol]:	96.09
CAS:	557-01-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.55		Crippen Method
logp	0.182		Crippen Method
mcvol	69.290	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C557017&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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<https://www.chemeo.com/cid/98-320-8/2-1H-Pyrimidinone.pdf>

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