

4(1H)-Pyrimidinone

Other names:	Deaminoisocytosine 4-Hydroxypyrimidine 4-Oxypyrimidine 4-Pyrimidinol NSC 1575 6-Hydroxypyrimidine 4-Oxypyrimidine NSC 157911 1H-pyrimidin-4-one
Inchi:	InChI=1S/C4H4N2O/c7-4-1-2-5-3-6-4/h1-3H,(H,5,6,7)
InchiKey:	DNCYBUMDUBHIJZ-UHFFFAOYSA-N
Formula:	C4H4N2O
SMILES:	O=c1cc[nH]cn1
Mol. weight [g/mol]:	96.09
CAS:	4562-27-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.12		Crippen Method
logp	-0.712		Crippen Method
mcvol	69.290	ml/mol	McGowan Method
tf	440.50 ± 0.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4562270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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