4(1H)-Pyrimidinone, 2-(methylthio)-

Other names:	2-(Methylthio)-4-pyrimidone
	2-Methylthiouracil
	4-Hydroxy-2-methylthiopyrimidine
	4-Pyrimidinol, 2-(methylthio)-
	2-(Methylthio)-4(1H)-pyrimidinone
	2-(methylthio)-1H-pyrimidin-4-one
Inchi:	InChI=1S/C5H6N2OS/c1-9-5-6-3-2-4(8)7-5/h2-3H,1H3,(H,6,7,8)
InchiKey:	UYHSQVMHSFXUOA-UHFFFAOYSA-N
Formula:	C5H6N2OS
SMILES:	CSc1nccc(O)n1
Mol. weight [g/mol]:	142.18
CAS:	5751-20-2

Physical Properties

Property code	Value	Unit	Source
ie	8.70	eV	NIST Webbook
log10ws	-1.29		Crippen Method
logp	0.904		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5751202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie:	Ionization energy
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/60-715-1/4-1H-Pyrimidinone-2-methylthio.pdf

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