2(1H)-Pyrimidinethione, 4,6-diamino-

Other names:	2-Mercapto-4,6-diaminopyrimidine
	4,6-Diamino-2-mercaptopyrimidine
	4,6-Diamino-2-thiopyrimidine
	4,6-Diamino-2-pyrimidinethiol
	4,6-Diamino-2-thiopyrimdine
	2-Thiol-4,6-diamino-pyrimidine
	4,6-diaminopyrimidine-2-thiol
Inchi:	InChI=1S/C4H6N4S/c5-2-1-3(6)8-4(9)7-2/h1H,(H5,5,6,7,8,9)
InchiKey:	QCAWOHUJKPKOMD-UHFFFAOYSA-N
Formula:	C4H6N4S
SMILES:	Nc1cc(N)[nH]c(=S)n1
Mol. weight [g/mol]:	142.18
CAS:	1004-39-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.57		Crippen Method
logp	-0.178		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=C1004393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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