

2(1H)-Pyrimidinethione, 4,5-diamino-

Other names:	2-Pyrimidinethiol, 4,5-diamino- 4,5-Diamino-2-pyrimidinethione
Inchi:	InChI=1S/C4H6N4S/c5-2-1-7-4(9)8-3(2)6/h1H,5H2,(H3,6,7,8,9)
InchiKey:	KDVXWCSUTDEXFF-UHFFFAOYSA-N
Formula:	C4H6N4S
SMILES:	<chem>N=c1[nH]c(S)ncc1N</chem>
Mol. weight [g/mol]:	142.18
CAS:	14623-58-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	-0.722		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

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=C14623586&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

Latest version available from:

<https://www.chemeo.com/cid/98-304-6/2-1H-Pyrimidinethione-4-5-diamino.pdf>

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