

4-Pyrimidinethiol, 5,6-diamino-

Other names:	5,6-diaminopyrimidine-4-thiol
Inchi:	InChI=1S/C4H6N4S/c5-2-3(6)7-1-8-4(2)9/h1H,5H2,(H3,6,7,8,9)
InchiKey:	LFJKVEOWXYKQGT-UHFFFAOYSA-N
Formula:	C4H6N4S
SMILES:	<chem>Nc1ncnc(S)c1N</chem>
Mol. weight [g/mol]:	142.18
CAS:	2846-89-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.78		Crippen Method
logp	-0.070		Crippen Method
mcvol	99.730	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2846891&Units=SI

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/31-413-8/4-Pyrimidinethiol-5-6-diamino.pdf>

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