

# 4,5-Pyrimidinediamine

<b>Other names:</b>	Pyrimidine, 4,5-diamino- 4,5-Diaminopyrimidine Pyrimidine-4,5-diamine
<b>Inchi:</b>	InChI=1S/C4H6N4/c5-3-1-7-2-8-4(3)6/h1-2H,5H2,(H2,6,7,8)
<b>InchiKey:</b>	PPAULTVPKLVII-UHFFFAOYSA-N
<b>Formula:</b>	C4H6N4
<b>SMILES:</b>	N=c1[nH]cncc1N
<b>Mol. weight [g/mol]:</b>	110.12
<b>CAS:</b>	13754-19-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	-1.011		Crippen Method
mcvol	83.380	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	502.20	K	4.30	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13754193&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13754193&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tbrp:</b>	Boiling point at reduced pressure

Latest version available from:

<https://www.cheméo.com/cid/80-700-5/4-5-Pyrimidinediamine.pdf>

Generated by Cheméo on 2024-04-20 10:43:43.322990841 +0000 UTC m=+15899072.243568181.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.