

# 1H-Pyrazolo[3,4-d]pyrimidin-4-amine

<b>Other names:</b>	4-Aminopyrazolo[3,4-d]pyrimidine 1H-Pyrazolo[3,4-d]pyrimidine, 4-amino- Pyrazoloadenine 4 APP 4-Aminopyrazole(3,4-d)pyrimidine 4-Aminopyrazolopyrimidine NSC 1393
<b>Inchi:</b>	InChI=1S/C5H5N5/c6-4-3-1-9-10-5(3)8-2-7-4/h1-2H,(H3,6,7,8,9,10)
<b>InchiKey:</b>	LHCPRYRLDOSKHK-UHFFFAOYSA-N
<b>Formula:</b>	C5H5N5
<b>SMILES:</b>	<chem>Nc1ncnc2[nH]ncc12</chem>
<b>Mol. weight [g/mol]:</b>	135.13
<b>CAS:</b>	2380-63-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	-0.547		Crippen Method
mvol	92.290	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2380634&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2380634&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>
<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>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume

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