

# 4-Amino-5-bromo-2-hydroxypyrimidine

<b>Other names:</b>	5-Bromocytosine 2(1H)-Pyrimidinone, 4-amino-5-bromo-
<b>Inchi:</b>	InChI=1S/C4H4BrN3O/c5-2-1-7-4(9)8-3(2)6/h1H,(H3,6,7,8,9)
<b>InchiKey:</b>	QFVKLKDEXOWFSL-UHFFFAOYSA-N
<b>Formula:</b>	C4H4BrN3O
<b>SMILES:</b>	<chem>Nc1nc(=O)[nH]cc1Br</chem>
<b>Mol. weight [g/mol]:</b>	190.00
<b>CAS:</b>	2240-25-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.68		Crippen Method
logp	-0.367		Crippen Method
mcpol	96.770	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	148.40 ± 1.50	kJ/mol	435.50	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2240257&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2240257&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.chemo.com/doc/models/crippen_log10ws">https://www.chemo.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>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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