

# Guanine

<b>Other names:</b>	6H-Purin-6-one, 2-amino-1,7-dihydro- C.I. Natural White 1 C.I. 75170 Dew Pearl Guanin Guanine enol Hypoxanthine, 2-amino- Mearlmaid Natural Pearl Essence Naturon Pathocidin Pearl Essence Stella Polaris 2-Amino-6-hydroxypurine 2-Aminohypoxanthine 2-Amino-1,7-dihydro-6H-purin-6-one 6H-Purin-6-one, 2-amino-1,9-dihydro- Natural White 1
<b>Inchi:</b>	InChI=1S/C5H5N5O/c6-5-9-3-2(4(11)10-5)7-1-8-3/h1H,(H4,6,7,8,9,10,11)
<b>InchiKey:</b>	UYTPUPDQBNUYGX-UHFFFAOYSA-N
<b>Formula:</b>	C5H5N5O
<b>SMILES:</b>	<chem>Nc1nc2nc[nH]c2c(=O)[nH]1</chem>
<b>Mol. weight [g/mol]:</b>	151.13
<b>CAS:</b>	73-40-5

## Physical Properties

Property code	Value	Unit	Source
affp	959.50	kJ/mol	NIST Webbook
basg	927.60	kJ/mol	NIST Webbook
chs	-2498.20 ± 0.79	kJ/mol	NIST Webbook
hfs	-183.90 ± 0.84	kJ/mol	NIST Webbook
ie	8.00 ± 0.20	eV	NIST Webbook
ie	8.24 ± 0.03	eV	NIST Webbook
ie	7.85	eV	NIST Webbook
log10ws	-0.30		Crippen Method
logp	-1.735		Crippen Method
mcvol	98.160	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	160.70	J/mol×K	298.00	NIST Webbook
cps	156.94	J/mol×K	296.70	NIST Webbook
hsubt	168.30 ± 0.60	kJ/mol	365.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C73405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C73405&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>chs:</b>	Standard solid enthalpy of combustion
<b>cps:</b>	Solid phase heat capacity
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>ie:</b>	Ionization energy
<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>ss:</b>	Solid phase molar entropy at standard conditions

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