

# 2(1H)-Pyrimidinone, 5-bromo-

<b>Other names:</b>	5-Bromo-2(1H)-pyrimidinone 5-Bromo-2-hydroxypyrimidine 5-Bromo-2-pyrimidinol 5-bromo-1H-pyrimidin-2-one
<b>Inchi:</b>	InChI=1S/C4H3BrN2O/c5-3-1-6-4(8)7-2-3/h1-2H,(H,6,7,8)
<b>InchiKey:</b>	VTUDATOSQGYWML-UHFFFAOYSA-N
<b>Formula:</b>	C4H3BrN2O
<b>SMILES:</b>	Oc1ncc(Br)cn1
<b>Mol. weight [g/mol]:</b>	174.98
<b>CAS:</b>	38353-06-9

## Physical Properties

Property code	Value	Unit	Source
ie	9.47 ± 0.05	eV	NIST Webbook
log10ws	-1.71		Crippen Method
logp	0.945		Crippen Method
mcvol	86.790	ml/mol	McGowan Method

## 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=C38353069&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38353069&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>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

Latest version available from:

<https://www.cheméo.com/cid/115-919-4/2-1H-Pyrimidinone-5-bromo.pdf>

Generated by Cheméo on 2024-04-28 19:51:24.835944223 +0000 UTC m=+16623133.756521544.

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