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

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38353069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume