

# 4,5-Dibromo-3(2H)-pyridazinone

<b>Other names:</b>	4,5-Dibromopyridazin-3-one 4,5-Dibromo-3[2H]-pyridazone
<b>Inchi:</b>	InChI=1S/C4H2Br2N2O/c5-2-1-7-8-4(9)3(2)6/h1H,(H,8,9)
<b>InchiKey:</b>	AGLQURQNVJVJNB-UHFFFAOYSA-N
<b>Formula:</b>	C4H2Br2N2O
<b>SMILES:</b>	O=c1[nH]ncc(Br)c1Br
<b>Mol. weight [g/mol]:</b>	253.88
<b>CAS:</b>	5788-58-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	0.813		Crippen Method
mcvol	104.290	ml/mol	McGowan Method

## Sources

<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=C5788589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5788589&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

<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/26-631-2/4-5-Dibromo-3-2H-pyridazinone.pdf>

Generated by Cheméo on 2024-05-03 01:06:48.335780081 +0000 UTC m=+16987657.256357394.

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