

# 4-Bromo-3,5-dimethylpyrazole-1-methanol

<b>Other names:</b>	4-bromo-3,5-dimethyl-1H-pyrazole-1-methanol
<b>Inchi:</b>	InChI=1S/C6H9BrN2O/c1-4-6(7)5(2)9(3-10)8-4/h10H,3H2,1-2H3
<b>InchiKey:</b>	ZPUHCXLBXSSWLL-UHFFFAOYSA-N
<b>Formula:</b>	C6H9BrN2O
<b>SMILES:</b>	Cc1nn(CO)c(C)c1Br
<b>Mol. weight [g/mol]:</b>	205.05
<b>CAS:</b>	94230-83-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	1.212		Crippen Method
mcvol	119.270	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=C94230838&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C94230838&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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

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