

# 1H-Pyrazole, 4-bromo-

<b>Other names:</b>	4-Bromopyrazole 4-bromo-1H-pyrazole 4-bromopyrazole Pyrazole, 4-bromo-
<b>Inchi:</b>	InChI=1S/C3H3BrN2/c4-3-1-5-6-2-3/h1-2H,(H,5,6)
<b>InchiKey:</b>	WVGCPEDBFHEHEZ-UHFFFAOYSA-N
<b>Formula:</b>	C3H3BrN2
<b>SMILES:</b>	Brc1cn[nH]c1
<b>Mol. weight [g/mol]:</b>	146.97
<b>CAS:</b>	2075-45-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	0.690		Crippen Method
mcvol	71.130	ml/mol	McGowan Method

## Sources

<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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Solubility, solution thermodynamics and preferential solvation for 4-bromopyrazole in mixed solvents of (methanol/ethanol + water) from T = (283.15 to 318.15) K:</b>	<a href="https://www.doi.org/10.1016/j.jct.2017.05.005">https://www.doi.org/10.1016/j.jct.2017.05.005</a> <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a> <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2075458&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2075458&amp;Units=SI</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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