

# 1H-Pyrazole, 4-phenyl-

<b>Other names:</b>	Pyrazole, 4-phenyl- 4-(C6H5)-pyrazole
<b>Inchi:</b>	InChI=1S/C9H8N2/c1-2-4-8(5-3-1)9-6-10-11-7-9/h1-7H,(H,10,11)
<b>InchiKey:</b>	GPGKNEKFDGOXPO-UHFFFAOYSA-N
<b>Formula:</b>	C9H8N2
<b>SMILES:</b>	<chem>c1ccc(-c2cn[nH]c2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	144.17
<b>CAS:</b>	10199-68-5

## Physical Properties

Property code	Value	Unit	Source
affp	906.00	kJ/mol	NIST Webbook
basg	871.80	kJ/mol	NIST Webbook
log10ws	-3.06		Crippen Method
logp	1.595		Crippen Method
mcvol	114.410	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=C10199685&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10199685&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>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<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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