

1H-Pyrazole, 1,5-dimethyl-

Other names:	Pyrazole, 1,5-dimethyl- 1,5-Dimethylpyrazole 1,5-Dimethyl-1H-pyrazole
Inchi:	InChI=1S/C5H8N2/c1-5-3-4-6-7(5)2/h3-4H,1-2H3
InchiKey:	LSZQMSSIUQNTDX-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	Cc1ccnn1C
Mol. weight [g/mol]:	96.13
CAS:	694-31-5

Physical Properties

Property code	Value	Unit	Source
affp	934.30	kJ/mol	NIST Webbook
basg	902.80	kJ/mol	NIST Webbook
log10ws	-3.00		Crippen Method
logp	0.729		Crippen Method
mcvol	81.810	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C694315&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/41-060-9/1H-Pyrazole-1-5-dimethyl.pdf>

Generated by Cheméo on 2024-04-20 07:05:15.361405934 +0000 UTC m=+15885964.281983249.

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