

1H-Pyrazole, 1,3-dimethyl-

Other names:	Pyrazole, 1,3-dimethyl- 1,3-Dimethylpyrazole 2,5-Dimethylpyrazole
Inchi:	InChI=1S/C5H8N2/c1-5-3-4-7(2)6-5/h3-4H,1-2H3
InchiKey:	NODLZCJDRXTSJO-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	Cc1ccn(C)n1
Mol. weight [g/mol]:	96.13
CAS:	694-48-4

Physical Properties

Property code	Value	Unit	Source
affp	933.90	kJ/mol	NIST Webbook
basg	902.30	kJ/mol	NIST Webbook
log10ws	-3.00		Crippen Method
logp	0.729		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	833.00		NIST Webbook
rinpol	833.00		NIST Webbook

Sources

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=C694484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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