Pyrazole, 1,4-dimethyl-

Other names:	1,4-Dimethylpyrazole
	1H-Pyrazole, 1,4-dimethyl-
Inchi:	InChI=1S/C5H8N2/c1-5-3-6-7(2)4-5/h3-4H,1-2H3
InchiKey:	SZQCPPRPWDXLMM-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	Cc1cnn(C)c1
Mol. weight [g/mol]:	96.13
CAS:	1072-68-0

Physical Properties

Property code	Value	Unit	Source
affp	928.40	kJ/mol	NIST Webbook
basg	896.80	kJ/mol	NIST Webbook
log10ws	-3.00		Crippen Method
logp	0.729		Crippen Method
mcvol	81.810	ml/mol	McGowan Method

Sources

Crippen Method:	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=C1072680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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