1H-Pyrazole, 3,4-dimethyl-

Other names:	3(5),4-Dimethylpyrazole
	Pyrazole, 3,4-dimethyl-
Inchi:	InChI=1S/C5H8N2/c1-4-3-6-7-5(4)2/h3H,1-2H3,(H,6,7)
InchiKey:	VQTVFIMEENGCJA-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	Cc1c[nH]nc1C
Mol. weight [g/mol]:	96.13
CAS:	2820-37-3

Physical Properties

Property code	Value	Unit	Source
affp	927.30	kJ/mol	NIST Webbook
basg	895.40	kJ/mol	NIST Webbook
log10ws	-1.41		Crippen Method
logp	0.545		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
tf	331.15 ± 1.50	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2820373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tf:	Normal melting (fusion) point