1H-Pyrazole, 1-methyl-

Other names:	1-methyl-1H-pyrazole
	1-methylpyrazole
	N-Methylpyrazole
	pyrazole, 1-methyl-
Inchi:	InChI=1S/C4H6N2/c1-6-4-2-3-5-6/h2-4H,1H3
InchiKey:	UQFQONCQIQEYPJ-UHFFFAOYSA-N
Formula:	C4H6N2
SMILES:	Cn1cccn1
Mol. weight [g/mol]:	82.10
CAS:	930-36-9

Physical Properties

Property code	Value	Unit	Source
affp	912.00	kJ/mol	NIST Webbook
basg	880.10	kJ/mol	NIST Webbook
log10ws	-2.53		Crippen Method
logp	0.420		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
rinpol	743.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	743.00		NIST Webbook
tb	400.20	K	NIST Webbook
tf	229.20	K	Vapour pressures of 1-methyl derivatives of benzimidazole, pyrazole and indole. The energy of the intermolecular hydrogen bond N-H...N

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures of 1-methyl derivatives of benzimidazole, pyrazole and indole. The energy of the intermolecular hydrogen bond N-H...N:	https://www.doi.org/10.1016/j.jct.2014.04.026

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point