1H-Imidazole, 4-methyl-

Other names:	Imidazole, 4-methyl-
	4(Or 5)-Methylimidazole
	4(5)-Methylimidazole
	4-Methylimidazole
	5-Methylimidazole
	4-Me-i
Inchi:	InChI=1S/C4H6N2/c1-4-2-5-3-6-4/h2-3H,1H3,(H,5,6)
InchiKey:	XLSZMDLNRCVEIJ-UHFFFAOYSA-N
Formula:	C4H6N2
SMILES:	Cc1c[nH]cn1
Mol. weight [g/mol]:	82.10
CAS:	822-36-6

Physical Properties

Property code	Value	Unit	Source
affp	952.80	kJ/mol	NIST Webbook
basg	920.90	kJ/mol	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.236		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
rinpol	1198.00		NIST Webbook
rinpol	1198.00		NIST Webbook
ripol	2165.00		NIST Webbook
ripol	2211.00		NIST Webbook
tb	536.20	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C822366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature