1H-Pyrazole, 3-methyl-

Other names:	3(5)-Methylpyrazole
	3-Methyl-1H-pyrazole
	3-methylpyrazole
	5-Methylpyrazole
	Pyrazole, 3(or 5)-methyl-
	Pyrazole, 5-methyl-
	pyrazole, 3-methyl-
Inchi:	InChI=1S/C4H6N2/c1-4-2-3-5-6-4/h2-3H,1H3,(H,5,6)
InchiKey:	XKVUYEYANWFIJX-UHFFFAOYSA-N
Formula:	C4H6N2
SMILES:	Cc1cc[nH]n1
Mol. weight [g/mol]:	82.10
CAS:	1453-58-3

Physical Properties

Property code	Value	Unit	Source
affp	906.00	kJ/mol	NIST Webbook
basg	874.20	kJ/mol	NIST Webbook
hfus	65.90	kJ/mol	Thermochemical studies of 3-methylpyrazole and 1,3,5-trimethylpyrazole
hvap	65.90 ± 2.00	kJ/mol	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.236		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
rinpol	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	930.00		NIST Webbook
tb	477.20	K	NIST Webbook

Sources

Thermochemical studies of 3-methylpyrazole and 1,3,5-trimethylpyrazole:	https://www.doi.org/10.1016/j.jct.2007.09.001
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1453583&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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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

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