1H-Pyrazole, 1,3,5-trimethyl-

Other names:	1,3,5-trimethylpyrazole
	pyrazole, 1,3,5-trimethyl-
Inchi:	InChI=1S/C6H10N2/c1-5-4-6(2)8(3)7-5/h4H,1-3H3
InchiKey:	HNOQAFMOBRWDKQ-UHFFFAOYSA-N
Formula:	C6H10N2
SMILES:	Cc1cc(C)n(C)n1
Mol. weight [g/mol]:	110.16
CAS:	1072-91-9

Physical Properties

Property code	Value	Unit	Source
affp	949.30	kJ/mol	NIST Webbook
basg	917.40	kJ/mol	NIST Webbook
hfus	61.70	kJ/mol	Thermochemical studies of 3-methylpyrazole and 1,3,5-trimethylpyrazole
log10ws	-3.48		Crippen Method
logp	1.037		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
ripol	2197.00		NIST Webbook
ripol	2197.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	101.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1072919&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure