Pyrazole, 3,4,4,5-tetramethyl-

Other names: 4H-Pyrazole,3,4,4,5-tetramethyl-
Inchi: InChI=1S/C7H12N2/c1-5-7(3,4)6(2)9-8-5/h1-4H3
InchiKey: AIHABYFCZQBWLH-UHFFFAOYSA-N
Formula: C7H12N2
SMILES: CC1=NN=C(C)C1(C)C
Mol. weight [g/mol]: 124.18
CAS: 19078-32-1

Physical Properties

Property code	Value	Unit	Source
gf	313.34	kJ/mol	Joback Method
hf	122.47	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
ie	10.12	eV	NIST Webbook
ie	9.57	eV	NIST Webbook
log10ws	-1.72		Crippen Method
logp	1.863		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	490.76	K	Joback Method
tc	726.83	K	Joback Method
tf	373.09	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.51	J/mol×K	490.76	Joback Method
cpg	274.22	J/mol×K	530.11	Joback Method
cpg	288.95	J/mol×K	569.45	Joback Method
cpg	302.80	J/mol×K	608.80	Joback Method
cpg	315.84	J/mol×K	648.14	Joback Method
cpg	328.18	J/mol×K	687.49	Joback Method

cpg	339.91	J/mol×K	726.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19078321&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume