1H-Pyrazole, 4,5-dihydro-3,5,5-trimethyl-

Other names:	2-Pyrazoline, 3,5,5-trimethyl-
	3,5,5-Trimethyl-2-pyrazoline
	3,5,5-Trimethylpyrazoline
	3,5,5-Trimethyl-«DELTA»[2]-pyrazoline
Inchi:	InChI=1S/C6H12N2/c1-5-4-6(2,3)8-7-5/h8H,4H2,1-3H3
InchiKey:	MEVTUZFUVAZEPY-UHFFFAOYSA-N
Formula:	C6H12N2
SMILES:	CC1=NNC(C)(C)C1
Mol. weight [g/mol]:	112.17
CAS:	3975-85-7

Physical Properties

Property code	Value	Unit	Source
gf	255.52	kJ/mol	Joback Method
hf	63.64	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.134		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	910.00		NIST Webbook
rinpol	910.00		NIST Webbook
tb	458.59	K	Joback Method
tc	690.08	K	Joback Method
tf	382.03	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.75	J/mol×K	458.59	Joback Method
cpg	231.50	J/mol×K	497.17	Joback Method
cpg	245.27	J/mol×K	535.75	Joback Method

cpg	258.18	J/mol×K	574.33	Joback Method
cpg	270.32	J/mol×K	612.91	Joback Method
cpg	281.78	J/mol×K	651.49	Joback Method
cpg	292.66	J/mol×K	690.08	Joback Method

Sources

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=C3975857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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