

5-Cyano-5-methyl-2-pyrrolidone

Inchi:	InChI=1S/C6H8N2O/c1-6(4-7)3-2-5(9)8-6/h2-3H2,1H3,(H,8,9)
InchiKey:	BXKKJJWDNAORNS-UHFFFAOYSA-N
Formula:	C6H8N2O
SMILES:	CC1(C#N)CCC(=O)N1
Mol. weight [g/mol]:	124.14
CAS:	86240-21-3

Physical Properties

Property code	Value	Unit	Source
gf	129.00	kJ/mol	Joback Method
hf	-26.46	kJ/mol	Joback Method
hfus	9.54	kJ/mol	Joback Method
hvap	49.54	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.179		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
tb	570.65	K	Joback Method
tc	824.57	K	Joback Method
tf	430.42	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.04	J/molxK	570.65	Joback Method
cpg	238.31	J/molxK	612.97	Joback Method
cpg	248.96	J/molxK	655.29	Joback Method
cpg	259.09	J/molxK	697.61	Joback Method
cpg	268.82	J/molxK	739.93	Joback Method
cpg	278.25	J/molxK	782.25	Joback Method
cpg	287.50	J/molxK	824.57	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C86240213&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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