

5-Methyl-2-pyrrolidinone

Other names:	5-Methyl-2-pyrrolidone 2-Pyrrolidinone, 5-methyl- «gamma»-Valerolactam
Inchi:	InChI=1S/C5H9NO/c1-4-2-3-5(7)6-4/h4H,2-3H2,1H3,(H,6,7)
InchiKey:	YVIVRJLWYJGJTJ-UHFFFAOYSA-N
Formula:	C5H9NO
SMILES:	CC1CCC(=O)N1
Mol. weight [g/mol]:	99.13
CAS:	108-27-0

Physical Properties

Property code	Value	Unit	Source
gf	-7.11	kJ/mol	Joback Method
hf	-185.94	kJ/mol	Joback Method
hfus	11.74	kJ/mol	Joback Method
hvap	37.99	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.285		Crippen Method
mcvol	82.000	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
tb	521.20	K	NIST Webbook
tc	673.97	K	Joback Method
tf	330.26	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.00	J/molxK	445.45	Joback Method
cpg	175.39	J/molxK	483.54	Joback Method
cpg	187.33	J/molxK	521.62	Joback Method
cpg	198.79	J/molxK	559.71	Joback Method
cpg	209.77	J/molxK	597.79	Joback Method
cpg	220.24	J/molxK	635.88	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=C108270&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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