

5-METHYLPYRROLIDIN-2-ONE

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

Physical Properties

Property code	Value	Unit	Source
hfus	11.74	kJ/mol	Joback Method
logp	0.285		Crippen Method
mcvol	82.000	ml/mol	McGowan Method
tb	521.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.00	J/mol×K	445.45	Joback Method
cpg	175.39	J/mol×K	483.54	Joback Method
cpg	187.33	J/mol×K	521.62	Joback Method
cpg	198.79	J/mol×K	559.71	Joback Method
cpg	209.77	J/mol×K	597.79	Joback Method
cpg	220.24	J/mol×K	635.88	Joback Method
cpg	230.18	J/mol×K	673.97	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C108270&Units=SI>

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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