2H-Azepin-2-one, hexahydro-7-methyl-

Other names:	«epsilon»-Methylcaprolactam
	6-Methyl-6-caprolactam
	7-Methylcaprolactam
	Hexahydro-7-methyl-2H-azepin-2-one
Inchi:	InChI=1S/C7H13NO/c1-6-4-2-3-5-7(9)8-6/h6H,2-5H2,1H3,(H,8,9)
InchiKey:	JAWSTIJAWZBKOU-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	CC1CCCCC(=O)N1
Mol. weight [g/mol]:	127.18
CAS:	1985-48-4

Physical Properties

Property code	Value	Unit	Source
chs	-4250.10 ± 1.30	kJ/mol	NIST Webbook
gf	-14.47	kJ/mol	Joback Method
hf	-239.54	kJ/mol	Joback Method
hfus	12.72	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.065		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	499.75	K	Joback Method
tc	738.91	K	Joback Method
tf	345.76	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.34	J/mol×K	499.75	Joback Method
cpg	262.59	J/mol×K	539.61	Joback Method
cpg	279.09	J/mol×K	579.47	Joback Method
cpg	294.79	J/mol×K	619.33	Joback Method

cpg	309.66	J/mol×K	659.19	Joback Method
cpg	323.66	J/mol×K	699.05	Joback Method
cpg	336.75	J/mol×K	738.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1985484&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
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