2-Piperidinone

Other names:	2-Piperidone
	«alpha»-Piperidone
	«delta»-Valerolactam
	Pentanoic acid, 5-amino-, lactam
	5-Pentanolactam
	Piperidon
	Piperidone-2
	Delta-valerolactam
	NSC 18894
	NSC 2305
	Valerolactim
Inchi:	InChI=1S/C5H9NO/c7-5-3-1-2-4-6-5/h1-4H2,(H,6,7)
InchiKey:	XUWHAWMETYGRKB-UHFFFAOYSA-N
Formula:	C5H9NO
SMILES:	O=C1CCCCN1
Mol. weight [g/mol]:	99.13
CAS:	675-20-7

Physical Properties

Property code	Value	Unit	Source
chs	-2947.20 ± 0.42	kJ/mol	NIST Webbook
gf	-11.50	kJ/mol	Joback Method
hf	-171.76	kJ/mol	Joback Method
hfus	8.57	kJ/mol	Joback Method
hvap	38.47	kJ/mol	Joback Method
ie	9.30	eV	NIST Webbook
ie	9.15 ± 0.02	eV	NIST Webbook
log10ws	-0.77		Crippen Method
logp	0.287		Crippen Method
mcvol	82.000	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
rinpol	1173.50		NIST Webbook
rinpol	1173.50		NIST Webbook
ripol	2060.00		NIST Webbook
ss	165.00	J/mol×K	NIST Webbook
ss	164.80	J/mol×K	NIST Webbook
tb	529.20	K	NIST Webbook

tc	692.75	K	Joback Method
tf	312.20 ± 0.50	K	NIST Webbook
tt	311.85 ± 0.05	K	NIST Webbook
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.54	J/mol×K	454.39	Joback Method
cpg	173.63	J/mol×K	494.12	Joback Method
cpg	230.64	J/mol×K	692.75	Joback Method
cpg	220.43	J/mol×K	653.02	Joback Method
cpg	209.61	J/mol×K	613.29	Joback Method
cpg	198.19	J/mol×K	573.57	Joback Method
cpg	186.19	J/mol×K	533.84	Joback Method
cps	144.20	J/mol×K	300.00	NIST Webbook
cps	189.80	J/mol×K	290.00	NIST Webbook
cps	208.30	J/mol×K	295.00	NIST Webbook
hfust	10.50	kJ/mol	311.90	NIST Webbook
hfust	10.49	kJ/mol	311.85	NIST Webbook
hfust	10.50	kJ/mol	311.85	NIST Webbook
hvapt	75.50	kJ/mol	302.50	NIST Webbook
sfust	33.70	J/mol×K	311.85	NIST Webbook
sfust	33.60	J/mol×K	311.85	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C675207&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

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume