2-Piperidinone, 1-methyl-

Other names:	2-Piperidone, 1-methyl-
	N-Methyl-«delta»-valerolactam
	N-Methyl-2-piperidinone
	N-Methyl-2-piperidone
	1-Methyl-2-piperidinone
	1-Methyl-2-piperidone
	1-Methylpiperidine-2-one
	1-Methylpiperidin-2-one
	N-Methylvalerolactam
	NSC 67384
Inchi:	InChI=1S/C6H11NO/c1-7-5-3-2-4-6(7)8/h2-5H2,1H3
InchiKey:	GGYVTHJIUNGKFZ-UHFFFAOYSA-N
Formula:	C6H11NO
SMILES:	CN1CCCCC1=O
Mol. weight [g/mol]:	113.16
CAS:	931-20-4

Physical Properties

Property code	Value	Unit	Source
affp	924.40	kJ/mol	NIST Webbook
basg	892.60	kJ/mol	NIST Webbook
chl	-3640.00 ± 0.40	kJ/mol	NIST Webbook
chl	-3635.00	kJ/mol	NIST Webbook
hvap	60.30 ± 0.90	kJ/mol	NIST Webbook
ie	8.92	eV	NIST Webbook
log10ws	-0.57		Crippen Method
logp	0.629		Crippen Method
mcvol	96.090	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	55.40	kJ/mol	363.00	NIST Webbook
hvapt	54.40 ± 3.10	kJ/mol	403.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	1.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C931204&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
tbrp:	Boiling point at reduced pressure