

# 2-Oxazolidinone,4-methyl-

<b>Inchi:</b>	InChI=1S/C4H7NO2/c1-3-2-7-4(6)5-3/h3H,2H2,1H3,(H,5,6)
<b>InchiKey:</b>	VAJFEOKPKHIPEN-UHFFFAOYSA-N
<b>Formula:</b>	C4H7NO2
<b>SMILES:</b>	CC1COC(=O)N1
<b>Mol. weight [g/mol]:</b>	101.10
<b>CAS:</b>	16112-59-7

## Physical Properties

Property code	Value	Unit	Source
gf	-101.65	kJ/mol	Joback Method
hf	-297.30	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	40.27	kJ/mol	Joback Method
ie	9.95	eV	NIST Webbook
log10ws	-0.53		Crippen Method
logp	0.115		Crippen Method
mcvol	73.780	ml/mol	McGowan Method
pc	5320.16	kPa	Joback Method
tb	449.52	K	Joback Method
tc	680.29	K	Joback Method
tf	345.56	K	Joback Method
vc	0.266	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.46	J/molxK	449.52	Joback Method
cpg	161.09	J/molxK	487.98	Joback Method
cpg	171.37	J/molxK	526.44	Joback Method
cpg	181.27	J/molxK	564.90	Joback Method
cpg	190.78	J/molxK	603.36	Joback Method
cpg	199.85	J/molxK	641.82	Joback Method
cpg	208.47	J/molxK	680.29	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C16112597&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16112597&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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