

# 2(3H)-Furanone, 3-acetyldihydro-3-methyl-

<b>Other names:</b>	«alpha»-Acetyl-«alpha»-methyl-gammabutyrolactone «alpha»-acetyl-«alpha»-methyl-«gamma»-butyrolactone
<b>Inchi:</b>	InChI=1S/C7H10O3/c1-5(8)7(2)3-4-10-6(7)9/h3-4H2,1-2H3
<b>InchiKey:</b>	VKDGCPFTXXDWQJ-UHFFFAOYSA-N
<b>Formula:</b>	C7H10O3
<b>SMILES:</b>	CC(=O)C1(C)CCOC1=O
<b>Mol. weight [g/mol]:</b>	142.15
<b>CAS:</b>	1123-19-9

## Physical Properties

Property code	Value	Unit	Source
gf	-298.51	kJ/mol	Joback Method
hf	-494.37	kJ/mol	Joback Method
hfus	10.61	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.529		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	523.72	K	Joback Method
tc	757.30	K	Joback Method
tf	348.17	K	Joback Method
vc	0.401	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.89	J/mol×K	523.72	Joback Method
cpg	264.96	J/mol×K	562.65	Joback Method
cpg	277.22	J/mol×K	601.58	Joback Method
cpg	288.75	J/mol×K	640.51	Joback Method
cpg	299.66	J/mol×K	679.44	Joback Method
cpg	310.06	J/mol×K	718.37	Joback Method
cpg	320.03	J/mol×K	757.30	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.50 ± 2.50	K	0.70	NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1123199&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1123199&amp;Units=SI</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>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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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