

# 2(3H)-Furanone, dihydro-5-methyl-

<b>Other names:</b>	«gamma»-Methyl-«gamma»-butyrolactone «gamma»-Pentalactone «gamma»-Valerolactone Pentanoic acid, 4-hydroxy-, «gamma»-lactone 4-Hydroxypentanoic acid lactone 4-Hydroxyvaleric acid lactone 4-Methyl-«gamma»-butyrolactone 4-Pentanolide 4-Valerolactone «gamma»-Pentanolactone «gamma»-Valerolakton Dihydro-5-methyl-2(3H)-furanone Valeric acid, 4-hydroxy-, gamma-lactone gamma-Valerolactone 5-Methyldihydrofuran-2(3H)-one 5-methyltetrahydrofuran-2-one Dihydro-5-methyl-2-furanone (.+/-)-«gamma»-Valerolactone (.+/-)-4-Methylbutyrolactone 5-Methyltetrahydro-2-furanone NSC 33700 Valeric acid, 4-hydroxy-, «gamma»-lactone Valerolactone 5-Methyldihydro-2(3H)-furanone Pentan-4-olide 2(3H)-Furanone, dihydro-5-methyl-, (.+/-)-
<b>Inchi:</b>	InChI=1S/C5H8O2/c1-4-2-3-5(6)7-4/h4H,2-3H2,1H3
<b>InchiKey:</b>	GAEKPEKOJKCEMS-UHFFFAOYSA-N
<b>Formula:</b>	C5H8O2
<b>SMILES:</b>	CC1CCC(=O)O1
<b>Mol. weight [g/mol]:</b>	100.12
<b>CAS:</b>	57129-69-8

## Physical Properties

Property code	Value	Unit	Source
gf	-180.94	kJ/mol	Joback Method

hf	-355.75		kJ/mol	Joback Method
hfus	10.13		kJ/mol	Joback Method
hvap	35.74		kJ/mol	Joback Method
log10ws	-0.78			Crippen Method
logp	0.712			Crippen Method
mcvol	77.890		ml/mol	McGowan Method
pc	4492.23		kPa	Joback Method
tb	479.20		K	NIST Webbook
tc	643.76		K	Joback Method
tf	251.80		K	Joback Method
vc	0.284		m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.05	J/mol×K	423.85	Joback Method
cpg	165.60	J/mol×K	460.50	Joback Method
cpg	176.71	J/mol×K	497.15	Joback Method
cpg	187.37	J/mol×K	533.80	Joback Method
cpg	197.57	J/mol×K	570.45	Joback Method
cpg	207.30	J/mol×K	607.10	Joback Method
cpg	216.54	J/mol×K	643.76	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.70	K	1.70	NIST Webbook

## Sources

- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>
- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57129698&Units=SI>
- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)
- Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

# 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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