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

Other names:	«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
Inchi:	InChI=1S/C5H8O2/c1-4-2-3-5(6)7-4/h4H,2-3H2,1H3
InchiKey:	GAEKPEKOJKCEMS-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC1CCC(=O)O1
Mol. weight [g/mol]:	100.12
CAS:	108-29-2

Physical Properties

Property code	Value	Unit	Source
chl	-2649.60 ± 0.80	kJ/mol	NIST Webbook
gf	-180.94	kJ/mol	Joback Method

hf	-406.50 ± 1.10	kJ/mol	NIST Webbook
hfl	-461.30 ± 1.00	kJ/mol	NIST Webbook
hfus	10.13	kJ/mol	Joback Method
hvap	53.90 ± 0.20	kJ/mol	NIST Webbook
hvap	54.80 ± 0.40	kJ/mol	NIST Webbook
hvap	54.80	kJ/mol	NIST Webbook
hvap	54.80 ± 0.40	kJ/mol	NIST Webbook
log10ws	-0.78		Crippen Method
logp	0.712		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
rinpol	965.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	962.30		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	953.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	950.00		NIST Webbook

rinpol	965.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	914.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1614.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1589.00		NIST Webbook
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ripol	1617.00		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1605.00		NIST Webbook
tb	480.70	K	NIST Webbook
tc	643.76	K	Joback Method
tf	251.80	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.30	J/mol×K	607.10	Joback Method
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	216.54	J/mol×K	643.76	Joback Method
hvapt	53.50	kJ/mol	395.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108292&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume