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

Other names:	2,3-Dihydro-5-methyl-2-furanone
	2,3-Dihydro-5-methylfuran-2-one
	2-Oxo-5-methyl-2,3-dihydrofuran
	3-Pentenoic acid, 4-hydroxy-, «gamma»-lactone
	4-Hydroxy-3-pentenoic acid «gamma»-lactone
	4-Hydroxypent-3-enoic acid lactone
	5-Methyl-2(3H)-furanone («alpha»-angelicalactone)
	5-methyl-2(3H)-furanone
	5-methylfuran-2(3H)-one
	Angelica lactone
	NSC 654
	Penten-3-oic acid, 4-hydroxy-, «gamma»-lactone
	«alpha»-Angelica lactone
	«beta»,«gamma»-Angelica lactone
	«delta»2-Angelica lactone
	«gamma»-Methyl-«beta»,«gamma»-crotonolactone
Inchi:	InChI=1S/C5H6O2/c1-4-2-3-5(6)7-4/h2H,3H2,1H3
InchiKey:	QOTQFLOTGBBMEX-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	CC1=CCC(=O)O1
Mol. weight [g/mol]:	98.10
CAS:	591-12-8

Physical Properties

Property code	Value	Unit	Source
gf	-152.90	kJ/mol	Joback Method
hf	-289.10	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	37.00	kJ/mol	Joback Method
ie	9.62 ± 0.05	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	0.837		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
rinpol	830.10		NIST Webbook
rinpol	830.10		NIST Webbook
rinpol	830.10		NIST Webbook

rinpol	885.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	865.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	836.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	901.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1429.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1430.00		NIST Webbook
tb	432.66	K	Joback Method
tc	656.90	K	Joback Method
tf	269.32	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.67	J/mol×K	432.66	Joback Method
cpg	149.00	J/mol×K	470.03	Joback Method
cpg	157.97	J/mol×K	507.41	Joback Method
cpg	166.57	J/mol×K	544.78	Joback Method
cpg	174.79	J/mol×K	582.15	Joback Method
cpg	182.62	J/mol×K	619.53	Joback Method
cpg	190.05	J/mol×K	656.90	Joback Method
hvapt	40.30	kJ/mol	383.00	NIST Webbook

rhol	1099.32	kg/m3	288.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhol	1093.94	kg/m3	293.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhol	1088.55	kg/m3	298.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhol	1083.16	kg/m3	303.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhol	1077.77	kg/m3	308.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhol	1072.38	kg/m3	313.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhol	1066.98	kg/m3	318.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhol	1061.58	kg/m3	323.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	329.20	K	1.60	NIST Webbook
tbrp	329.00	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water:	https://www.doi.org/10.1021/acs.jced.8b01146
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume