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

Other names:	«beta»-Angelica lactone
	«alpha»,«beta»-Angelica lactone
	«DELTA»1-Angelica lactone
	«gamma»-Methyl-«delta»,«alpha»,«beta»-butenolide
	2-Penten-4-olide
	2-Pentenoic acid, 4-hydroxy-, «gamma»-lactone
	4-Hydroxy-2-pentenoic acid «gamma»-lactone
	5-Methyl-2(5H)-furanone
	«gamma»-Methyl-«alpha»,«beta»-crotonolactone
	4-Hydroxypent-2-enoic acid lactone
	5-Methyl-5H-furan-2-one
	4-Methyl-2-buten-4-olide
	NSC 655
	4-methyl-2-butenoic acid «gamma»-lactone
	5-Methyl-2(5H)-furanone («beta»-angelica lactone)
	Pent-2-en-4-olide
	5-methylfuran-2(5H)-one
Inchi:	InChI=1S/C5H6O2/c1-4-2-3-5(6)7-4/h2-4H,1H3
InchiKey:	BGLUXFNVVSVEET-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	CC1C=CC(=O)O1
Mol. weight [g/mol]:	98.10
CAS:	591-11-7

Physical Properties

Property code	Value	Unit	Source
gf	-150.98	kJ/mol	Joback Method
hf	-297.97	kJ/mol	Joback Method
hfus	11.35	kJ/mol	Joback Method
hvap	36.03	kJ/mol	Joback Method
ie	10.12 ± 0.05	eV	NIST Webbook
log10ws	-0.64		Crippen Method
logp	0.488		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	938.00		NIST Webbook
rinpol	934.00		NIST Webbook

rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	938.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	914.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1658.00		NIST Webbook
tb	423.01	K	Joback Method
tc	645.30	K	Joback Method
tf	252.56	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.96	J/mol×K	608.25	Joback Method
cpg	140.46	J/mol×K	423.01	Joback Method
cpg	150.58	J/mol×K	460.06	Joback Method
cpg	160.30	J/mol×K	497.11	Joback Method
cpg	169.61	J/mol×K	534.16	Joback Method
cpg	178.50	J/mol×K	571.20	Joback Method
cpg	194.99	J/mol×K	645.30	Joback Method
hvapt	48.20	kJ/mol	418.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591117&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

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
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