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

Other names:	1,4-Heptanolide
	4-Heptanolide
	4-Hydroxyheptanoic acid lactone
	4-Hydroxyheptanoic acid, «gamma»-lactone
	5-Propyldihydro-2(3H)-furanone
	Heptan-4-olide
	Heptanoic acid, 4-hydroxy-, «gamma»-lactone
	Heptanolide-4,1
	NSC 46097
	dihydro-5-propyl-2(3H)-furanone
	«gamma»-Heptalactone
	«gamma»-Heptanolactone
	«gamma»-Heptanolide
	«gamma»-Propiobutyrolactone
	«gamma»-Propyl-«gamma»-butyrolactone
Inchi:	InChI=1S/C7H12O2/c1-2-3-6-4-5-7(8)9-6/h6H,2-5H2,1H3
InchiKey:	VLSVVMPLPMNWBH-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCCC1CCC(=O)O1
Mol. weight [g/mol]:	128.17
CAS:	105-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-164.10	kJ/mol	Joback Method
hf	-397.03	kJ/mol	Joback Method
hfus	15.31	kJ/mol	Joback Method
hvap	62.30 ± 0.30	kJ/mol	NIST Webbook
log10ws	-1.62		Crippen Method
logp	1.492		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	1128.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1172.00		NIST Webbook

rinpol	1113.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1163.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1803.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1766.00		NIST Webbook
tb	469.61	K	Joback Method
tc	683.50	K	Joback Method
tf	274.34	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.28	J/mol×K	469.61	Joback Method
cpg	248.59	J/mol×K	505.26	Joback Method
cpg	262.27	J/mol×K	540.91	Joback Method
cpg	275.34	J/mol×K	576.56	Joback Method
cpg	287.80	J/mol×K	612.21	Joback Method
cpg	299.62	J/mol×K	647.86	Joback Method
cpg	310.83	J/mol×K	683.50	Joback Method

pvap	0.02	kPa	313.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.01	kPa	302.80	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.02	kPa	308.00	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	7.29e-03	kPa	298.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.03	kPa	318.00	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.05	kPa	323.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.07	kPa	328.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.09	kPa	333.00	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.13	kPa	338.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.18	kPa	343.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones

pvap	0.24	kPa	348.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.32	kPa	353.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.44	kPa	358.40	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.57	kPa	363.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vapourization of a series of the c-lactones:	https://www.doi.org/10.1016/j.jct.2008.02.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105215&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap:	Vapor 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