

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

Other names:	.gamma.-caprolactone 2(3H)-Furanone-5-ethylidihydro-5 4-Ethyl-4-butanolide 4-Ethylbutanolide 4-Hexanolide 4-Hydroxyhexanoic acid lactone 4-ethylbutanolide («gamma»-hexalactone) 5-Ethylidihydrofuran-2(3H)-one 5-Ethyltetrahydro-2-furanone 5-ethylidihydro-2(3H)-furanone 6-Caprolactone Dihydro-5-ethyl-2(3H)-furanone Furan-2-one (3 H) 5-ethyl(dihydro) Hexan-4-olide Hexanoic acid, 4-hydroxy-, lactone Hexanoic acid, 4-hydroxy-, «gamma»-lactone Hexanolide-1,4 NSC 134769 NSC 24255 Tonkalide Toukalide hexa-4-olide «gamma»-Caprolactone «gamma»-Ethyl-n-butyrolactone «gamma»-Ethyl-«gamma»-butyrolactone «gamma»-Ethylbutyrolactone «gamma»-Hexalactone «gamma»-Hexanolactone
Inchi:	InChI=1S/C6H10O2/c1-2-5-3-4-6(7)8-5/h5H,2-4H2,1H3
InchiKey:	JBFH TYHTHYHCDJ-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CCC1CCC(=O)O1
Mol. weight [g/mol]:	114.14
CAS:	695-06-7

Physical Properties

Property code	Value	Unit	Source
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gf	-172.52	kJ/mol	Joback Method
hf	-376.39	kJ/mol	Joback Method
hfus	12.72	kJ/mol	Joback Method
h _{vap}	57.20 ± 0.30	kJ/mol	NIST Webbook
h _{vap}	55.30 ± 0.60	kJ/mol	NIST Webbook
log ₁₀ ws	-1.20		Crippen Method
logp	1.102		Crippen Method
m _{cvol}	91.980	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1013.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1006.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1055.20		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1009.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1068.00		NIST Webbook

ripol	1003.00	NIST Webbook
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ripol	1690.00		NIST Webbook
ripol	1683.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1694.00		NIST Webbook
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ripol	1717.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	1745.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1715.00		NIST Webbook
ripol	1682.00		NIST Webbook
tb	492.20	K	NIST Webbook
tc	663.70	K	Joback Method
tf	263.07	K	Joback Method
vc	0.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.05	J/molxK	446.73	Joback Method
cpg	206.06	J/molxK	482.89	Joback Method
cpg	263.02	J/molxK	663.70	Joback Method
cpg	252.73	J/molxK	627.54	Joback Method
cpg	241.89	J/molxK	591.38	Joback Method
cpg	218.55	J/molxK	519.05	Joback Method
cpg	230.49	J/molxK	555.22	Joback Method
hvapt	57.40	kJ/mol	298.15	Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography
pvap	0.70	kPa	353.30	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.17	kPa	328.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.13	kPa	323.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.23	kPa	333.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.31	kPa	338.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones

pvap	0.41	kPa	343.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.54	kPa	348.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.62	kPa	350.90	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.07	kPa	283.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.13	kPa	293.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.22	kPa	303.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.36	kPa	312.90	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.56	kPa	323.30	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.86	kPa	333.30	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	1.37	kPa	343.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone

pvap	0.07	kPa	315.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	6.43e-03	kPa	284.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	7.33e-03	kPa	285.30	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	9.98e-03	kPa	288.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.01	kPa	290.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.01	kPa	293.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.02	kPa	295.30	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.02	kPa	298.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.03	kPa	300.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.03	kPa	303.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones

pvap	0.04	kPa	305.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.05	kPa	308.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.05	kPa	310.10	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.07	kPa	313.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	6.12e-03	kPa	283.30	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
pvap	0.09	kPa	318.20	Vapour pressures and enthalpies of vapourization of a series of the c-lactones
rhoI	1029.16	kg/m3	288.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	998.23	kg/m3	323.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1002.65	kg/m3	318.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1011.49	kg/m3	308.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water

rhoI	1015.91	kg/m3	303.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1020.33	kg/m3	298.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1024.74	kg/m3	293.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1007.07	kg/m3	313.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C695067&Units=SI
Vapour pressures and enthalpies of vapourization of a series of the lactones:	https://www.doi.org/10.1016/j.jct.2008.02.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water:	https://www.doi.org/10.1021/acs.jced.8b01146
Vapor pressure data of e-caprolactone, d-hexalactone, and gamma-butyrolactone:	https://www.doi.org/10.1016/j.jct.2007.09.008
Vapor pressures and enthalpies of vaporization of a series of .gamma. and delta.lactones by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2014.01.016
McGowan Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
Phase behaviour of binary systems of lactones in carbon dioxide:	https://www.doi.org/10.1016/j.jct.2009.07.003

Legend

cp _g :	Ideal gas heat capacity
g _f :	Standard Gibbs free energy of formation
h _f :	Enthalpy of formation at standard conditions
h _{fus} :	Enthalpy of fusion at standard conditions
h _{vap} :	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
mcpvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
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

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