

2H-Pyran-2-one, tetrahydro-6-methyl-

Other names:	.delta.-caprolactone 2H-Pyran-2-one, 6-methyl, tetrahydro 5-Hexanolide 5-Hydroxyhexanoic acid lactone <<delta>>-Hexalactone Hexanoic acid, 5-hydroxy-, lactone Hexanoic acid, 5-hydroxy-, «delta»-lactone delta-Hexalactone tetrahydro-6-methyl-2H-pyran-2-one «delta»-Caprolactone «delta»-Hexalactone «delta»-Hexanolactone «delta»-Hexanolide «delta»-Methyl-«delta»-valerolactone
Inchi:	InChI=1S/C6H10O2/c1-5-3-2-4-6(7)8-5/h5H,2-4H2,1H3
InchiKey:	RZTOWFMDBDPERY-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC1CCCC(=O)O1
Mol. weight [g/mol]:	114.14
CAS:	823-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-184.62	kJ/mol	Joback Method
hf	-382.55	kJ/mol	Joback Method
hfus	10.62	kJ/mol	Joback Method
hvap	58.10	kJ/mol	NIST Webbook
hvap	60.90 ± 0.10	kJ/mol	NIST Webbook
log10ws	-1.20		Crippen Method
logp	1.102		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	1084.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1049.00		NIST Webbook
rinpol	1084.00		NIST Webbook

ripol	1084.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1798.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1772.00		NIST Webbook
ripol	1786.00		NIST Webbook
ripol	1792.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1789.00		NIST Webbook
tb	451.00	K	Joback Method
tc	676.91	K	Joback Method
tf	259.55	K	Joback Method
vc	0.333	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.86	J/mol×K	451.00	Joback Method
cpg	267.01	J/mol×K	676.91	Joback Method
cpg	256.02	J/mol×K	639.26	Joback Method
cpg	232.15	J/mol×K	563.96	Joback Method
cpg	219.30	J/mol×K	526.30	Joback Method
cpg	205.87	J/mol×K	488.65	Joback Method
cpg	244.40	J/mol×K	601.61	Joback Method
pvap	0.35	kPa	343.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone

pvap	5.00e-03	kPa	283.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.01	kPa	293.20	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.03	kPa	303.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.05	kPa	313.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.56	kPa	353.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.10	kPa	323.20	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	0.19	kPa	333.10	Vapour pressure data of e-caprolactone, d-hexalactone, and c-caprolactone
pvap	3.80e-03	kPa	283.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	3.58e-03	kPa	283.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	4.49e-03	kPa	285.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	5.52e-03	kPa	288.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	5.81e-03	kPa	288.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	5.57e-03	kPa	288.40	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	8.61e-03	kPa	293.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	8.93e-03	kPa	293.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	298.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	298.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.42	kPa	348.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	303.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.03	kPa	308.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	0.03	kPa	308.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.04	kPa	313.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.04	kPa	313.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.06	kPa	318.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.09	kPa	323.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.12	kPa	328.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.12	kPa	328.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.17	kPa	333.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.19	kPa	335.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.24	kPa	338.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	0.23	kPa	338.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.31	kPa	343.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.42	kPa	348.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	303.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.53	kPa	352.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
rhoI	1053.81	kg/m ³	288.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1023.51	kg/m ³	323.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1032.15	kg/m ³	313.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1036.48	kg/m ³	308.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1040.81	kg/m ³	303.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water

rhoI	1045.14	kg/m3	298.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1049.47	kg/m3	293.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water
rhoI	1027.82	kg/m3	318.15	Thermal and Volumetric Properties of Five Lactones at Infinite Dilution in Water

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Vapour pressure data of e-caprolactone, d-hexalactone, and P-hexalactone	https://www.doi.org/10.1016/j.jct.2007.09.008
Phase behaviour of binary systems of lactones in carbon dioxide:	https://www.doi.org/10.1016/j.jct.2009.07.003
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C823223&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of d-lactones:	https://www.doi.org/10.1016/j.jct.2006.06.010

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
rhoI:	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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