

2H-Pyran-2-one, tetrahydro-

Other names:	.delta.-valerolactone 1-Oxacyclohexan-2-one 5-Hydroxypentanoic acid «delta»-lactone 5-Hydroxypentanoic acid Â«deltaÂ»-lactone 5-Pentanolide 5-Valerolactone Cyclopentanolide Delta-valerolactone NSC 6247 Pentan-5-olide Pentanoic acid, 5-hydroxy-, «delta»-lactone Pentanoic acid, 5-hydroxy-, Â«deltaÂ»-lactone Tetrahydro-2-pyranone Tetrahydro-2H-pyran-2-one Tetrahydropyran-2-one Valeric acid, «delta»-hydroxy-, «delta»-lactone Valeric acid, Â«deltaÂ»-hydroxy-, Â«deltaÂ»-lactone oxan-2-one valeric acid, .delta.-hydroxy-, lactone «delta»-Pentalactone «delta»-Valerolactone «delta»-Valeryllactone Â«deltaÂ»-Pentalactone Â«deltaÂ»-Valerolactone Â«deltaÂ»-Valeryllactone
Inchi:	InChI=1S/C5H8O2/c6-5-3-1-2-4-7-5/h1-4H2
InchiKey:	OZJPLYNZGCXSJM-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	O=C1CCCCO1
Mol. weight [g/mol]:	100.12
CAS:	542-28-9

Physical Properties

Property code	Value	Unit	Source
chl	-2673.30 ± 0.50	kJ/mol	NIST Webbook
gf	-185.33	kJ/mol	Joback Method

hf	-379.60 ± 0.90		kJ/mol	NIST Webbook
hf	-376.00 ± 3.00		kJ/mol	NIST Webbook
hfl	-436.00 ± 3.00		kJ/mol	NIST Webbook
hfl	-437.60 ± 0.80		kJ/mol	NIST Webbook
hfus	6.96		kJ/mol	Joback Method
hvap	36.22		kJ/mol	Joback Method
log10ws	-0.67			Crippen Method
logp	0.714			Crippen Method
mcvol	77.890		ml/mol	McGowan Method
pc	4862.97		kPa	Joback Method
rinpol	991.00			NIST Webbook
rinpol	961.00			NIST Webbook
rinpol	961.00			NIST Webbook
rinpol	1010.00			NIST Webbook
rinpol	954.00			NIST Webbook
rinpol	991.00			NIST Webbook
rinpol	965.00			NIST Webbook
ripol	1780.00			NIST Webbook
ripol	1784.00			NIST Webbook
ripol	1785.00			NIST Webbook
ripol	1786.00			NIST Webbook
ripol	1730.00			NIST Webbook
sl	219.00		J/mol×K	NIST Webbook
sl	219.00		J/mol×K	NIST Webbook
sl	219.00		J/mol×K	NIST Webbook
tb	492.20		K	NIST Webbook
tc	662.42		K	Joback Method
tf	262.80 ± 0.60		K	NIST Webbook
tt	262.82 ± 0.02		K	NIST Webbook
tt	262.82 ± 0.02		K	NIST Webbook
tt	262.82 ± 0.02		K	NIST Webbook
vc	0.278		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.21	J/mol×K	624.15	Joback Method
cpg	186.47	J/mol×K	547.60	Joback Method
cpg	197.12	J/mol×K	585.88	Joback Method
cpg	216.74	J/mol×K	662.42	Joback Method
cpg	151.33	J/mol×K	432.79	Joback Method

cpg	163.57	J/molxK	471.06	Joback Method
cpg	175.28	J/molxK	509.33	Joback Method
cpl	171.60	J/molxK	298.15	NIST Webbook
cpl	171.60	J/molxK	298.15	NIST Webbook
cpl	171.60	J/molxK	298.15	NIST Webbook
dvisc	0.0021191	Paxs	318.15	Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K
dvisc	0.0023130	Paxs	313.15	Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K
dvisc	0.0024957	Paxs	308.15	Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K
dvisc	0.0027577	Paxs	303.15	Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K
hfust	10.53	kJ/mol	263.00	NIST Webbook
hvapt	48.60	kJ/mol	387.50	NIST Webbook
hvapt	52.40 ± 0.20	kJ/mol	410.50	NIST Webbook
pvap	0.02	kPa	303.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.44	kPa	349.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	0.46	kPa	350.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.46	kPa	351.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	2.83e-03	kPa	278.40	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	4.19e-03	kPa	283.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	4.03e-03	kPa	283.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	4.41e-03	kPa	283.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	6.85e-03	kPa	288.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	6.80e-03	kPa	288.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	6.56e-03	kPa	288.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	6.54e-03	kPa	288.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	7.83e-03	kPa	290.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	9.87e-03	kPa	293.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	293.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	294.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	297.90	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	298.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	299.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	303.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.49	kPa	352.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	304.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	0.03	kPa	307.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.03	kPa	307.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.03	kPa	308.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.04	kPa	309.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.05	kPa	313.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.05	kPa	313.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.05	kPa	313.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.05	kPa	313.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.05	kPa	313.20	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	0.06	kPa	318.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.07	kPa	318.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.10	kPa	323.10	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	0.09	kPa	323.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.12	kPa	328.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.14	kPa	328.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.12	kPa	328.40	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.16	kPa	333.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.18	kPa	333.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	0.18	kPa	333.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.23	kPa	338.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.22	kPa	338.20	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	0.32	kPa	343.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.30	kPa	343.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.51	kPa	353.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.41	kPa	348.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.30	kPa	343.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
speedsl	1498.63	m/s	318.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones

speedsl	1516.01	m/s	313.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1533.45	m/s	308.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1551.27	m/s	303.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1569.16	m/s	298.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1587.22	m/s	293.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones
speedsl	1481.50	m/s	323.15	A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.20	K	0.07	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	3.59800e+01
Coeff. B	-1.07999e+04
Coeff. C	-5.63340e+01
Temperature range (K), min.	358.92
Temperature range (K), max.	408.48

Sources

- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- The Yaws Handbook of Vapor Pressure:** <https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
- A comparative study on the interactions of [bmim][NTf2] ionic liquid with selected four- to seven-membered-ring lactones:** <https://www.doi.org/10.1016/j.jct.2016.12.032>
- Joback Method:** https://en.wikipedia.org/wiki/Joback_method
- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C542289&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>
- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>
- Volumetric and transport properties of binary liquid mixtures of N-methylacetamide with lactones at temperatures (303.15 to 318.15) K:** <https://www.doi.org/10.1016/j.jct.2008.05.004>

Legend

- chl:** Standard liquid enthalpy of combustion
- cpg:** Ideal gas heat capacity
- cpl:** Liquid phase heat capacity
- dvisc:** Dynamic viscosity
- gf:** Standard Gibbs free energy of formation
- hf:** Enthalpy of formation at standard conditions
- hfl:** Liquid phase enthalpy of formation at standard conditions
- hfus:** Enthalpy of fusion at standard conditions
- hfust:** Enthalpy of fusion at a given temperature
- hvap:** 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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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