

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

Other names:	5-Hydroxyoctanoic acid lactone 5-Hydroxyoctanoic acid «delta»-lactone 5-Octanolide 5-octanolide («delta»-octalactone) D-octanolactone Octanoic acid, 5-hydroxy-, «delta»-lactone tetrahydro-6-propyl-2H-pyran-2-one «beta»-Octalactone «delta»-Octalactone «delta»-Octanolactone «delta»-Octanolide «delta»-Propylvalerolactone
Inchi:	InChI=1S/C8H14O2/c1-2-4-7-5-3-6-8(9)10-7/h7H,2-6H2,1H3
InchiKey:	FYTRVXSHONWYNE-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CCCC1CCCC(=O)O1
Mol. weight [g/mol]:	142.20
CAS:	698-76-0

Physical Properties

Property code	Value	Unit	Source
gf	-167.78	kJ/mol	Joback Method
hf	-423.83	kJ/mol	Joback Method
hfus	15.80	kJ/mol	Joback Method
hvap	67.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.04		Crippen Method
logp	1.882		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1289.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1252.00		NIST Webbook

rinpol	1241.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1295.00	NIST Webbook
rinpol	1266.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1283.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1298.00	NIST Webbook
rinpol	1302.00	NIST Webbook
rinpol	1288.00	NIST Webbook
rinpol	1287.00	NIST Webbook
rinpol	1306.00	NIST Webbook
rinpol	1292.00	NIST Webbook
rinpol	1268.00	NIST Webbook
ripol	1964.00	NIST Webbook
ripol	1955.00	NIST Webbook
ripol	1988.00	NIST Webbook
ripol	1977.00	NIST Webbook
ripol	1966.00	NIST Webbook
ripol	1977.00	NIST Webbook
ripol	1929.00	NIST Webbook
ripol	1941.00	NIST Webbook
ripol	1976.00	NIST Webbook
ripol	1988.00	NIST Webbook
ripol	1988.00	NIST Webbook
ripol	1948.00	NIST Webbook
ripol	1956.00	NIST Webbook
ripol	2002.00	NIST Webbook
ripol	1985.00	NIST Webbook
ripol	1986.00	NIST Webbook

ripol	1989.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1947.00		NIST Webbook
ripol	1990.00		NIST Webbook
ripol	1985.00		NIST Webbook
ripol	1989.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1967.00		NIST Webbook
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ripol	1947.00		NIST Webbook
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ripol	1988.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	1977.00		NIST Webbook
ripol	1977.00		NIST Webbook
ripol	1973.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1965.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1929.00		NIST Webbook
tb	496.76	K	Joback Method
tc	715.62	K	Joback Method
tf	282.09	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	364.77	J/mol×K	715.62	Joback Method
cpg	352.13	J/mol×K	679.14	Joback Method
cpg	338.71	J/mol×K	642.67	Joback Method
cpg	324.53	J/mol×K	606.19	Joback Method
cpg	309.58	J/mol×K	569.71	Joback Method
cpg	293.89	J/mol×K	533.24	Joback Method
cpg	277.44	J/mol×K	496.76	Joback Method
hvapt	66.60	kJ/mol	298.15	Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography
pvap	7.69e-03	kPa	313.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	8.76e-03	kPa	314.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	318.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	323.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.03	kPa	328.40	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	5.97e-03	kPa	309.80	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.04	kPa	335.70	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	0.05	kPa	338.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.07	kPa	343.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.10	kPa	348.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.13	kPa	353.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	5.24e-03	kPa	308.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	4.41e-03	kPa	306.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	3.44e-03	kPa	303.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	2.24e-03	kPa	298.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	1.37e-03	kPa	293.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	8.80e-04	kPa	288.30	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap

0.04

kPa

333.40

Vapour
pressures and
enthalpies of
vaporization of a
series of
d-lactones

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C698760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
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
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

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