

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

Other names:	5-Decanolide 5-Hydroxy decanoic acid, lactone 5-Hydroxydecanoic acid «delta»-lactone 5-Hydroxydecanoic lactone 5-Pentyl-5-pentanolide 5-decanolide («delta»-decalactone) <«delta»>-decalactone A13-36028 Amyl-«delta»-valerolactone Decanoic acid, 5-hydroxy-, «delta»-lactone Decanolide-1,5 decan-5-olide tetrahydro-6-pentyl-2H-pyran-2-one «delta»-Amylvalerolactone «delta»-Decalactone «delta»-Decanolactone «delta»-Decanolide
Inchi:	InChI=1S/C10H18O2/c1-2-3-4-6-9-7-5-8-10(11)12-9/h9H,2-8H2,1H3
InchiKey:	GHBSPIPJMLAMEP-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCCCC1CCCC(=O)O1
Mol. weight [g/mol]:	170.25
CAS:	705-86-2

Physical Properties

Property code	Value	Unit	Source
gf	-150.94	kJ/mol	Joback Method
hf	-465.11	kJ/mol	Joback Method
hfus	20.98	kJ/mol	Joback Method
hvap	74.20 ± 0.30	kJ/mol	NIST Webbook
hvap	63.00 ± 1.50	kJ/mol	NIST Webbook
log10ws	-2.88		Crippen Method
logp	2.662		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1504.00		NIST Webbook

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rinpol	1474.00	NIST Webbook
rinpol	1496.00	NIST Webbook
rinpol	1481.00	NIST Webbook
rinpol	1491.00	NIST Webbook
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ripol	2178.00		NIST Webbook
ripol	2198.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2206.00		NIST Webbook
ripol	2215.00		NIST Webbook
ripol	2163.00		NIST Webbook
tb	542.52	K	Joback Method
tc	754.33	K	Joback Method
tf	304.63	K	Joback Method
vc	0.556	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.99	J/mol×K	542.52	Joback Method
cpg	389.20	J/mol×K	577.82	Joback Method
cpg	406.54	J/mol×K	613.12	Joback Method
cpg	423.01	J/mol×K	648.42	Joback Method
cpg	438.59	J/mol×K	683.72	Joback Method
cpg	453.30	J/mol×K	719.02	Joback Method
cpg	467.14	J/mol×K	754.33	Joback Method

hvapt	75.50	kJ/mol	298.15	Vapor pressures and enthalpies of vaporization of a series of .gamma. and .delta.-lactones by correlation gas chromatography
hvapt	57.70 ± 0.80	kJ/mol	376.00	NIST Webbook
pvap	2.57e-03	kPa	325.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	9.60e-04	kPa	313.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	1.23e-03	kPa	316.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	1.50e-03	kPa	318.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	1.81e-03	kPa	320.60	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	2.07e-03	kPa	322.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	2.26e-03	kPa	323.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	6.70e-04	kPa	309.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	3.38e-03	kPa	328.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	3.90e-03	kPa	330.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	4.92e-03	kPa	333.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	5.98e-03	kPa	335.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	7.21e-03	kPa	337.80	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	8.54e-03	kPa	340.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	343.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	345.40	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.01	kPa	348.00	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	348.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

pvap	0.02	kPa	350.50	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	353.10	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	353.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.02	kPa	355.40	Vapour pressures and enthalpies of vaporization of a series of d-lactones
pvap	0.03	kPa	358.20	Vapour pressures and enthalpies of vaporization of a series of d-lactones

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C705862&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:	https://www.doi.org/10.1016/j.jct.2014.01.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
chromatography:	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

h_{vap}:	Enthalpy of vaporization at standard conditions
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
p_{vap}:	Vapor pressure
ri_{npol}:	Non-polar retention indices
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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