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

Other names:	5-Acetyldihydro-2(3H)-furanone
	4-Hydroxy-5-ketohexanoic acid lactone
	Solerone
	Hexanoic acid, 4-hydroxy-5-oxo-, lactone
	5-acetyldihydrofuran-2(3H)-one
Inchi:	InChI=1S/C6H8O3/c1-4(7)5-2-3-6(8)9-5/h5H,2-3H2,1H3
InchiKey:	AHLDCEZSQNGEFT-UHFFFAOYSA-N
Formula:	C6H8O3
SMILES:	CC(=O)C1CCC(=O)O1
Mol. weight [g/mol]:	128.13
CAS:	29393-32-6

Physical Properties

Property code	Value	Unit	Source
gf	-301.44	kJ/mol	Joback Method
hf	-488.97	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	44.71	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	0.281		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
rinpol	1299.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2013.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2013.00		NIST Webbook
tb	500.60	K	Joback Method
tc	728.46	K	Joback Method
tf	313.00	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.14	J/mol×K	500.60	Joback Method
cpg	221.35	J/mol×K	538.58	Joback Method
cpg	232.98	J/mol×K	576.55	Joback Method
cpg	244.01	J/mol×K	614.53	Joback Method
cpg	254.44	J/mol×K	652.50	Joback Method
cpg	264.24	J/mol×K	690.48	Joback Method
cpg	273.42	J/mol×K	728.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29393326&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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