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

Physical Properties

Property code	Value	Unit	Source
hf	-517.22	kJ/mol	Cheméo Relay (1.0)
hfus	14.32	kJ/mol	Joback Method
hvap	61.10	kJ/mol	Cheméo Relay (1.0)
ie	9.97	eV	Cheméo Relay (1.0)
logp	0.281		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
rinpol	1299.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2013.00		NIST Webbook
ripol	2096.00		NIST Webbook
tb	524.24	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29393326&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature