2(3H)-Furanone, 5-ethyldihydro-5-methyl-

Other names:	«gamma»-Methyl-«gamma»-caprolactone
	«gamma»-Methyl-«gamma»-ethylbutyrolactone
	4-Hydroxy-4-methylhexanoic acid lactone
	4-Methyl-4-hexanolide
	4-Methyl-4-hydroxyhexanoic acid lactone
	Hexanoic acid, 4-hydroxy-4-methyl-, «gamma»-lactone
Inchi:	InChI=1S/C7H12O2/c1-3-7(2)5-4-6(8)9-7/h3-5H2,1-2H3
InchiKey:	MJFDQFVZHVJKFU-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCC1(C)CCC(=O)O1
Mol. weight [g/mol]:	128.17
CAS:	2865-82-9

Physical Properties

Property code	Value	Unit	Source
gf	-169.59	kJ/mol	Joback Method
hf	-381.79	kJ/mol	Joback Method
hfus	9.01	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.492		Crippen Method
mcvol	106.070	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1666.00		NIST Webbook
tb	469.85	K	Joback Method
tc	693.32	K	Joback Method
tf	298.24	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.88	J/mol×K	469.85	Joback Method
cpg	249.25	J/mol×K	507.10	Joback Method
cpg	262.72	J/mol×K	544.34	Joback Method
cpg	275.40	J/mol×K	581.59	Joback Method
cpg	287.36	J/mol×K	618.83	Joback Method
cpg	298.70	J/mol×K	656.08	Joback Method
cpg	309.50	J/mol×K	693.32	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2865829&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