2(3H)-Furanone, dihydro-5,5-dimethyl-

Other names:	4-Methylpentan-4-olide
	Isocaprolactone
	«gamma»-Isocaprolactone
	«gamma»-Methyl-«gamma»-valerolactone
	«gamma»,«gamma»-Dimethyl-«gamma»-butyrolactone
	«gamma»,«gamma»-Dimethylbutyrolactone
	Dihydro-5,5-dimethyl-2(3H)-furanone
	Tetrahydro-5,5-dimethyl-2-furanone
	4-Methyl-4-hydroxypentanoic acid lactone
	4-Methyl-4-pentanolide
	4,4-dimethylbutan-4-olide
	5,5-Dimethyldihydrofuran-2(3H)-one
	Pentanoic acid 4-hydroxy 4-methyl-«gamma»-lactone
	Valeric acid, 4-hydroxy-4-methyl-, g-lactone
	5,5-Dimethyldihydro-2(3H)-furanone
Inchi:	InChI=1S/C6H10O2/c1-6(2)4-3-5(7)8-6/h3-4H2,1-2H3
InchiKey:	NPHAVLULUWJQAS-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC1(C)CCC(=O)O1
Mol. weight [g/mol]:	114.14
CAS:	3123-97-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.01	kJ/mol	Joback Method
hf	-361.15	kJ/mol	Joback Method
hfus	6.42	kJ/mol	Joback Method
hvap	36.81	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.102		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	991.70		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1628.00		NIST Webbook
tb	446.97	K	Joback Method
tc	673.94	K	Joback Method

tf	286.97	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.12	J/mol×K	636.11	Joback Method
cpg	193.83	J/mol×K	446.97	Joback Method
cpg	207.04	J/mol×K	484.80	Joback Method
cpg	219.39	J/mol×K	522.63	Joback Method
cpg	230.96	J/mol×K	560.45	Joback Method
cpg	241.84	J/mol×K	598.28	Joback Method
cpg	261.89	J/mol×K	673.94	Joback Method
hvapt	52.70	kJ/mol	395.50	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3123975&Units=SI

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

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