2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (.+/-.)-

Other names: (+/-)-Pantoyl lactone
(±)-dihydro-3-hydroxy-4,4-dimethylfuran-2(3H)-one
2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-
2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (±)-
2,4-Dihydroxy-3,3-dimethylbutanoic acid «gamma»-lactone
2-hydroxy-3,3-dimethyl-.gamma.-butyrolactone
3-Hydroxy-4,4-dimethyldihydro-2(3H)-furanone
3-hydroxy-4,4-dimethyl-2-tetrahydrofuranone
DL-Pantoic acid «gamma»-lactone
Dihydro-3-hydroxy-4,4-dimethyl-2(3H)-furanone
RS-pantolactone
dl-pantolactone

Inchi: InChI=1S/C6H10O3/c1-6(2)3-9-5(8)4(6)7/h4,7H,3H2,1-2H3

InchiKey: SERHXTVXHNVDKA-UHFFFAOYSA-N

Formula: C6H10O3

SMILES: CC1(C)COC(=O)C1O

Mol. weight [g/mol]: 130.14

CAS: 79-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-322.54	kJ/mol	Joback Method
hf	-533.72	kJ/mol	Joback Method
hfus	11.58	kJ/mol	Joback Method
hvap	53.18	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	-0.070		Crippen Method
mcvol	97.850	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	1031.80		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2034.00		NIST Webbook
ripol	2034.00		NIST Webbook
tb	534.48	K	Joback Method
tc	745.23	K	Joback Method
tf	343.55	K	Joback Method

vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.67	J/mol×K	534.48	Joback Method
cpg	253.86	J/mol×K	569.60	Joback Method
cpg	264.47	J/mol×K	604.73	Joback Method
cpg	274.55	J/mol×K	639.85	Joback Method
cpg	284.18	J/mol×K	674.98	Joback Method
cpg	293.41	J/mol×K	710.10	Joback Method
cpg	302.32	J/mol×K	745.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic Properties of Mixtures Containing Precursors of Vitamin B5:	https://www.doi.org/10.1021/je020060f
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