Pantolactone

Other names:	(D)-Pantolactone
	(R)-(-)-Pantolactone
	(R)-3-hydroxy-4,4-dimethyldihydrofuran-2(3H)-one
	(R)-pantolactone
	2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (3R)-
	2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, (R)-
	2(3H)-Furanone, dihydro-3-hydroxy-4,4-dimethyl-, D-(-)-
	2-hydroxy-3,3-dimethyl-«gamma»-butyrolactone
	D(-)-2-Hydroxy-3,3-dimethyl-«gamma»-butyrolactone
	D-(-)-Pantoic acid lactone
	D-(-)-Pantolactone
	D-(-)-Pantolyl lactone
	D-(-)-Pantoyl lactone
	D-(-)-«alpha»Hydroxy-«beta»,«beta»-dimethyl-«gamma»-butyrolactone
	D-pantolactone
	Dihydro-3-hydroxy-4,4-dimethyl-2(3H)-furanone, R-(-)-pantolactone
	Dihydro-3-hydroxy-4,4-dimethyl-2(3H)-furanone, pantolactone
	Pantolyl lactone
	Pantothenic lactone
	Pantoyl lactone
	«alpha»-hydroxy-«beta»,«beta»-dimethyl-«gamma»-butyrolactone
Inchi:	InChI=1S/C6H10O3/c1-6(2)3-9-5(8)4(6)7/h4,7H,3H2,1-2H3/t4-/m1/s1
InchiKey:	SERHXTVXHNVDKA-SCSAIBSYSA-N
Formula:	C6H10O3
SMILES:	CC1(C)COC(=O)C1O
Mol. weight [g/mol]:	130.14
CAS:	599-04-2

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
ripol	2034.00		NIST Webbook
ripol	1998.00		NIST Webbook
ripol	1998.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2077.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2051.00		NIST Webbook
ripol	2006.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2028.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.20	K	2.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and Modeling Studies on the Solubility of d-Pantolactone in Four Pure Solvents and Ethanol Water Mixtures:	https://www.doi.org/10.1021/je500996n
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=C599042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume