2(3H)-Furanone, dihydro-4-methyl-

Other names:	«beta»-Methyl-«gamma»-butyro-lactone
	3-Methyl-4-butanolide
	3-Methylbutanolide
	Dihydro-4-methyl-2(3H)-furanone
	4-Methyldihydro-2(3H)-furanone
Inchi:	InChI=1S/C5H8O2/c1-4-2-5(6)7-3-4/h4H,2-3H2,1H3
InchiKey:	ALZLTHLQMAFAPA-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC1COC(=O)C1
Mol. weight [g/mol]:	100.12
CAS:	1679-49-8

Physical Properties

Property code	Value	Unit	Source
gf	-180.94	kJ/mol	Joback Method
hf	-355.75	kJ/mol	Joback Method
hfus	10.13	kJ/mol	Joback Method
hvap	35.74	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.569		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	913.00		NIST Webbook
tb	423.85	K	Joback Method
tc	643.76	K	Joback Method
tf	251.80	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.05	J/mol×K	423.85	Joback Method
cpg	165.60	J/mol×K	460.50	Joback Method
cpg	176.71	J/mol×K	497.15	Joback Method
cpg	187.37	J/mol×K	533.80	Joback Method
cpg	197.57	J/mol×K	570.45	Joback Method
cpg	207.30	J/mol×K	607.10	Joback Method
cpg	216.54	J/mol×K	643.76	Joback Method

Sources

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=C1679498&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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