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

Other names:	«alpha»-Methyl-«gamma»-butyrolactone
	«alpha»-Methylbutyrolactone
	2-Methyl-«gamma»-butyrolactone
	2-Methyl-4-butanolide
	2-Methylbutanolide
	4-Hydroxy-2-methylbutanoic acid lactone
	4-Hydroxy-2-methylbutyric acid lactone
	3-Methyldihydro-2(3H)-furanone
	3-Methyldihydrofuran-2(3H)-one
	Dihydro-3-methyl-2(3H)-furanone
	3-methyl-tetrahydro-2-furanon
	3-Methyl-dihydrofuranone
	alpha-methyl-«gamma»-butyrolactone
Inchi:	InChI=1S/C5H8O2/c1-4-2-3-7-5(4)6/h4H,2-3H2,1H3
InchiKey:	QGLBZNZGBLRJGS-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	CC1CCOC1=O
Mol. weight [g/mol]:	100.12
CAS:	1679-47-6

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	948.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	957.40		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1582.00		NIST Webbook

ripol	1587.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1557.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.70	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1679476&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume