(S)-dihydro-4-methylfuran-2(3H)-one

Other names: (S)-(-)-3-Methyl-«gamma»-butyrolactone
Inchi: InChI=1S/C5H8O2/c1-4-2-5(6)7-3-4/h4H,2-3H2,1H3/t4-/m1/s1
InchiKey: ALZLTHLQMAFAPA-SCSAIBSYSA-N
Formula: C5H8O2
SMILES: CC1COC(=O)C1
Mol. weight [g/mol]: 100.12
CAS: 64190-48-3

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
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	376.70	K	4.50	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=C64190483&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume