4-Hydroxy-5-methyl-3(2H)furanone

Inchi: InChI=1S/C5H8O3/c1-3-5(7)4(6)2-8-3/h3,5,7H,2H2,1H3
InchiKey: KTKGSSUXUIUZDA-UHFFFAOYSA-N
Formula: C5H8O3
SMILES: CC1OCC(=O)C1O
Mol. weight [g/mol]: 116.12

Physical Properties

Property code	Value	Unit	Source
gf	-325.47	kJ/mol	Joback Method
hf	-528.32	kJ/mol	Joback Method
hfus	15.29	kJ/mol	Joback Method
hvap	52.11	kJ/mol	Joback Method
log10ws	0.34		Crippen Method
logp	-0.665		Crippen Method
mcvol	83.760	ml/mol	McGowan Method
pc	4869.76	kPa	Joback Method
ripol	1462.00		NIST Webbook
ripol	1462.00		NIST Webbook
tb	511.36	K	Joback Method
tc	716.88	K	Joback Method
tf	308.38	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.04	J/mol×K	511.36	Joback Method
cpg	210.49	J/mol×K	545.61	Joback Method
cpg	220.51	J/mol×K	579.87	Joback Method
cpg	230.10	J/mol×K	614.12	Joback Method
cpg	239.26	J/mol×K	648.37	Joback Method
cpg	247.95	J/mol×K	682.62	Joback Method
cpg	256.18	J/mol×K	716.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R616403&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume