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

Inchi: InChI=1S/C6H8O2/c1-4-5(2)8-3-6(4)7/h3H2,1-2H3
InchiKey: ZKDVDJRTCAKLQZ-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1=C(C)C(=O)CO1
Mol. weight [g/mol]: 112.13

Physical Properties

Property code	Value	Unit	Source
gf	-154.11	kJ/mol	Joback Method
hf	-321.21	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	39.89	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.880		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
rinpol	1020.00		NIST Webbook
tb	460.52	K	Joback Method
tc	682.96	K	Joback Method
tf	293.11	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.82	J/mol×K	460.52	Joback Method
cpg	188.25	J/mol×K	497.59	Joback Method
cpg	198.29	J/mol×K	534.67	Joback Method
cpg	207.94	J/mol×K	571.74	Joback Method
cpg	217.18	J/mol×K	608.81	Joback Method
cpg	226.00	J/mol×K	645.89	Joback Method
cpg	234.39	J/mol×K	682.96	Joback Method

Sources

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=R225077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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