3-hydroxy-4,5-dimethyl-3(2H)-furanone

Inchi: InChI=1S/C6H8O3/c1-3-4(2)9-6(8)5(3)7/h5,7H,1-2H3
InchiKey: DFCKRIQJSYAFQG-UHFFFAOYSA-N
Formula: C6H8O3
SMILES: CC1=C(C)C(O)C(=O)O1
Mol. weight [g/mol]: 128.13

Physical Properties

Property code	Value	Unit	Source
gf	-298.64	kJ/mol	Joback Method
hf	-493.78	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.198		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
tb	548.03	K	Joback Method
tc	754.77	K	Joback Method
tf	349.69	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.64	J/mol×K	548.03	Joback Method
cpg	231.11	J/mol×K	582.49	Joback Method
cpg	240.20	J/mol×K	616.94	Joback Method
cpg	248.92	J/mol×K	651.40	Joback Method
cpg	257.23	J/mol×K	685.86	Joback Method
cpg	265.12	J/mol×K	720.32	Joback Method
cpg	272.59	J/mol×K	754.77	Joback Method

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=R390666&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume