3(2H)-Furanone, 2-acetyl-4-hydroxy

Inchi: InChI=1S/C6H6O4/c1-3(7)6-5(9)4(8)2-10-6/h2,6,8H,1H3
InchiKey: ZCFLPKHCTMEWQM-UHFFFAOYSA-N
Formula: C6H6O4
SMILES: CC(=O)C1OC=C(O)C1=O
Mol. weight [g/mol]: 142.11

Physical Properties

Property code	Value	Unit	Source
gf	-417.93	kJ/mol	Joback Method
hf	-594.89	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	62.34	kJ/mol	Joback Method
log10ws	-0.16		Crippen Method
logp	-0.057		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
rinpol	1093.00		NIST Webbook
tb	596.92	K	Joback Method
tc	810.49	K	Joback Method
tf	387.10	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.96	J/mol×K	596.92	Joback Method
cpg	241.83	J/mol×K	632.52	Joback Method
cpg	250.24	J/mol×K	668.11	Joback Method
cpg	258.17	J/mol×K	703.71	Joback Method
cpg	265.61	J/mol×K	739.30	Joback Method
cpg	272.56	J/mol×K	774.90	Joback Method
cpg	278.99	J/mol×K	810.49	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=R74654&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