5-Ethyl-4-hydroxy-2-methyl-3(2H)-furanone, acetate

Other names: 2-Ethyl-4-hydroxy-5-methyl-3(2H)-furanone, acetate
Inchi: InChI=1S/C9H12O4/c1-4-7-8(11)9(5(2)12-7)13-6(3)10/h7H,4H2,1-3H3
InchiKey: GTIGIDDMNIPUBG-UHFFFAOYSA-N
Formula: C9H12O4
SMILES: CCC1OC(C)=C(OC(C)=O)C1=O
Mol. weight [g/mol]: 184.19

Physical Properties

Property code	Value	Unit	Source
gf	-370.48	kJ/mol	Joback Method
hf	-648.27	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	55.41	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.159		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1330.50		NIST Webbook
rinpol	1330.50		NIST Webbook
tb	600.78	K	Joback Method
tc	818.33	K	Joback Method
tf	394.84	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.49	J/mol×K	600.78	Joback Method
cpg	360.92	J/mol×K	637.04	Joback Method
cpg	373.71	J/mol×K	673.30	Joback Method
cpg	385.83	J/mol×K	709.56	Joback Method
cpg	397.27	J/mol×K	745.82	Joback Method
cpg	407.98	J/mol×K	782.08	Joback Method
cpg	417.96	J/mol×K	818.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352320&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume