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

Other names: Furaneol acetate
Inchi: InChI=1S/C8H10O4/c1-4-7(10)8(5(2)11-4)12-6(3)9/h4H,1-3H3
InchiKey: VPKIUOQJQJVLRW-UHFFFAOYSA-N
Formula: C8H10O4
SMILES: CC(=O)OC1=C(C)OC(C)C1=O
Mol. weight [g/mol]: 170.16

Physical Properties

Property code	Value	Unit	Source
gf	-378.90	kJ/mol	Joback Method
hf	-627.63	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	53.19	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	0.769		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
ripol	1968.00		NIST Webbook
ripol	1968.00		NIST Webbook
tb	577.90	K	Joback Method
tc	799.39	K	Joback Method
tf	383.57	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.59	J/mol×K	577.90	Joback Method
cpg	313.06	J/mol×K	614.82	Joback Method
cpg	324.99	J/mol×K	651.73	Joback Method
cpg	336.32	J/mol×K	688.65	Joback Method
cpg	347.04	J/mol×K	725.56	Joback Method
cpg	357.11	J/mol×K	762.48	Joback Method
cpg	366.49	J/mol×K	799.39	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=R327252&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume