2(3H)-Furanone, dihydro-5,5-dimethyl-4-(3-oxobutyl)-

Inchi: InChI=1S/C10H16O3/c1-7(11)4-5-8-6-9(12)13-10(8,2)3/h8H,4-6H2,1-3H3
InchiKey: AWQSAIIDOMEEOD-UHFFFAOYSA-N
Formula: C10H16O3
SMILES: CC(=O)CCC1CC(=O)OC1(C)C
Mol. weight [g/mol]: 184.23
CAS: 4436-81-1

Physical Properties

Property code	Value	Unit	Source
chs	-5451.30	kJ/mol	NIST Webbook
gf	-280.96	kJ/mol	Joback Method
hf	-576.63	kJ/mol	Joback Method
hfs	-773.20	kJ/mol	NIST Webbook
hfus	19.45	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.697		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1558.30		NIST Webbook
tb	587.69	K	Joback Method
tc	808.46	K	Joback Method
tf	377.74	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.36	J/mol×K	587.69	Joback Method
cpg	408.52	J/mol×K	624.48	Joback Method
cpg	423.84	J/mol×K	661.28	Joback Method
cpg	438.39	J/mol×K	698.07	Joback Method
cpg	452.28	J/mol×K	734.87	Joback Method
cpg	465.58	J/mol×K	771.66	Joback Method

cpg	478.37	J/mol×K	808.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4436811&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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