5,5-DIMETHYL-4-(3-OXOBUTYL)DIHYDRO-2(3H)-F

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]: 184.24

Physical Properties

Property code	Value	Unit	Source
chs	-5451.30	kJ/mol	NIST Webbook
hfs	-773.20	kJ/mol	NIST Webbook
hfus	19.45	kJ/mol	Joback Method
logp	1.697		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
rinpol	1558.30		NIST Webbook

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
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices