1,3-Cyclohexanedione, 5,5-dimethyl-2-(4'-carbomethoxybutyro)-

Inchi: InChI=1S/C14H20O5/c1-14(2)7-10(16)13(11(17)8-14)9(15)5-4-6-12(18)19-3/h13H,4-8H2

InchiKey: HPNGSLHMOVJDNL-UHFFFAOYSA-N

Formula: C14H20O5

SMILES: COC(=O)CCCC(=O)C1C(=O)CC(C)(C)CC1=O

Mol. weight [g/mol]: 268.31

Physical Properties

Property code	Value	Unit	Source
gf	-529.77	kJ/mol	Joback Method
hf	-915.85	kJ/mol	Joback Method
hfus	22.03	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.473		Crippen Method
mcvol	209.410	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	800.64	K	Joback Method
tc	1029.36	K	Joback Method
tf	533.11	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.78	J/mol×K	800.64	Joback Method
cpg	671.25	J/mol×K	838.76	Joback Method
cpg	687.79	J/mol×K	876.88	Joback Method
cpg	703.46	J/mol×K	915.00	Joback Method
cpg	718.30	J/mol×K	953.12	Joback Method
cpg	732.34	J/mol×K	991.24	Joback Method
cpg	745.65	J/mol×K	1029.36	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=B6008224&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume