Cyclohexane-1,3-dione, 5,5-dimethyl-2-(3'-carbethoxypropyl)-

Inchi: InChI=1S/C14H22O4/c1-4-18-13(17)7-5-6-10-11(15)8-14(2,3)9-12(10)16/h10H,4-9H2,1-3

InchiKey: PHXXPPSDDGEKGC-UHFFFAOYSA-N

Formula: C14H22O4

SMILES: CCOC(=O)CCCC1C(=O)CC(C)(C)CC1=O

Mol. weight [g/mol]: 254.32

Physical Properties

Property code	Value	Unit	Source
gf	-400.85	kJ/mol	Joback Method
hf	-803.27	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	63.38	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.294		Crippen Method
mcvol	207.840	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
tb	746.77	K	Joback Method
tc	969.97	K	Joback Method
tf	483.18	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.32	J/mol×K	746.77	Joback Method
cpg	653.29	J/mol×K	783.97	Joback Method
cpg	671.33	J/mol×K	821.17	Joback Method
cpg	688.49	J/mol×K	858.37	Joback Method
cpg	704.79	J/mol×K	895.57	Joback Method
cpg	720.30	J/mol×K	932.77	Joback Method
cpg	735.05	J/mol×K	969.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008317&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume