Cyclohexane-1,3-dione, 2-acetyl-5,5-dimethyl-

Inchi: InChI=1S/C10H14O3/c1-6(11)9-7(12)4-10(2,3)5-8(9)13/h9H,4-5H2,1-3H3
InchiKey: ITSKWKZDPHAQNK-UHFFFAOYSA-N
Formula: C10H14O3
SMILES: CC(=O)C1C(=O)CC(C)(C)CC1=O
Mol. weight [g/mol]: 182.22
CAS: 1755-15-3

Physical Properties

Property code	Value	Unit	Source
gf	-329.53	kJ/mol	Joback Method
hf	-588.49	kJ/mol	Joback Method
hfus	8.88	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.150		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	632.83	K	Joback Method
tc	877.32	K	Joback Method
tf	415.87	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.09	J/mol×K	632.83	Joback Method
cpg	409.40	J/mol×K	673.58	Joback Method
cpg	425.83	J/mol×K	714.33	Joback Method
cpg	441.44	J/mol×K	755.07	Joback Method
cpg	456.30	J/mol×K	795.82	Joback Method
cpg	470.47	J/mol×K	836.57	Joback Method
cpg	484.01	J/mol×K	877.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1755153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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