Cyclobutanone, 3-acetoxy-2,2,4,4-tetramethyl-

Inchi: InChI=1S/C10H16O3/c1-6(11)13-8-9(2,3)7(12)10(8,4)5/h8H,1-5H3
InchiKey: JHCNFXVBXFAVSO-UHFFFAOYSA-N
Formula: C10H16O3
SMILES: CC(=O)OC1C(C)(C)C(=O)C1(C)C
Mol. weight [g/mol]: 184.23
CAS: 13487-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-300.94	kJ/mol	Joback Method
hf	-575.79	kJ/mol	Joback Method
hfus	9.53	kJ/mol	Joback Method
hvap	48.42	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.553		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	574.46	K	Joback Method
tc	795.85	K	Joback Method
tf	396.58	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.33	J/mol×K	574.46	Joback Method
cpg	401.99	J/mol×K	611.36	Joback Method
cpg	416.88	J/mol×K	648.26	Joback Method
cpg	431.16	J/mol×K	685.16	Joback Method
cpg	445.00	J/mol×K	722.05	Joback Method
cpg	458.54	J/mol×K	758.95	Joback Method
cpg	471.96	J/mol×K	795.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13487995&Units=SI

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