1,2-Cyclopentanedione, 3,3,5,5-tetramethyl-

Other names: 3,3,5,5-Tetramethyl-1,2-cyclopentanedione
Inchi: InChI=1S/C9H14O2/c1-8(2)5-9(3,4)7(11)6(8)10/h5H2,1-4H3
InchiKey: PSTFMALKVLSKOP-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CC1(C)CC(C)(C)C(=O)C1=O
Mol. weight [g/mol]: 154.21
CAS: 20633-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-202.42	kJ/mol	Joback Method
hf	-433.87	kJ/mol	Joback Method
hfus	0.50	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Joback Method
ie	8.76 ± 0.05	eV	NIST Webbook
log10ws	-1.56		Crippen Method
logp	1.581		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	552.05	K	Joback Method
tc	795.83	K	Joback Method
tf	382.09	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.21	J/mol×K	552.05	Joback Method
cpg	338.62	J/mol×K	592.68	Joback Method
cpg	354.16	J/mol×K	633.31	Joback Method
cpg	369.01	J/mol×K	673.94	Joback Method
cpg	383.37	J/mol×K	714.57	Joback Method
cpg	397.42	J/mol×K	755.20	Joback Method
cpg	411.36	J/mol×K	795.83	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=C20633061&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
ie:	Ionization energy
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