1,3-Cyclopentanedione, 2,2-dimethyl-

Other names: 2,2-Dimethyl-1,3-cyclopentanedione
Inchi: InChI=1S/C7H10O2/c1-7(2)5(8)3-4-6(7)9/h3-4H2,1-2H3
InchiKey: VXVZVJNSRQRUTI-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1(C)C(=O)CCC1=O
Mol. weight [g/mol]: 126.15
CAS: 3883-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-206.06	kJ/mol	Joback Method
hf	-387.49	kJ/mol	Joback Method
hfus	0.54	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
ie	9.08 ± 0.05	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
ie	9.22	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	0.945		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
tb	510.72	K	Joback Method
tc	753.88	K	Joback Method
tf	339.89	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.41	J/mol×K	510.72	Joback Method
cpg	245.57	J/mol×K	551.25	Joback Method
cpg	258.99	J/mol×K	591.77	Joback Method
cpg	271.75	J/mol×K	632.30	Joback Method
cpg	283.91	J/mol×K	672.83	Joback Method

cpg	295.55	J/mol×K	713.36	Joback Method
cpg	306.74	J/mol×K	753.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3883587&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
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