3,4-Dimethyl-1,2-cyclopentanedione

Other names:	1,2-Cyclopentanedione, 3,4-dimethyl- 3,4-dimethylcyclopentane-1,2-dione
Inchi:	InChI=1S/C7H10O2/c1-4-3-6(8)7(9)5(4)2/h4-5H,3H2,1-2H3
InchiKey:	WGAVDEVFJDQIMZ-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	CC1CC(=O)C(=O)C1C
Mol. weight [g/mol]:	126.15
CAS:	13494-06-9

Physical Properties

Property code	Value	Unit	Source
gf	-208.28	kJ/mol	Joback Method
hf	-423.07	kJ/mol	Joback Method
hfus	7.91	kJ/mol	Joback Method
hvap	39.62	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.801		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	1064.00		NIST Webbook
tb	505.81	K	Joback Method
tc	738.45	K	Joback Method
tf	311.75	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.74	J/mol×K	505.81	Joback Method
cpg	247.53	J/mol×K	544.58	Joback Method
cpg	261.79	J/mol×K	583.36	Joback Method
cpg	275.48	J/mol×K	622.13	Joback Method
cpg	288.55	J/mol×K	660.90	Joback Method
cpg	300.94	J/mol×K	699.67	Joback Method

cpg	312.62	J/mol×K	738.45	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=C13494069&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume