1,3-Cyclopentanedione, 2,4-dimethyl-

Other names: 2,4-Dimethyl-1,3-cyclopentanedione
Inchi: InChI=1S/C7H10O2/c1-4-3-6(8)5(2)7(4)9/h4-5H,3H2,1-2H3
InchiKey: FCELWXAACZZLJY-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1CC(=O)C(C)C1=O
Mol. weight [g/mol]: 126.15
CAS: 34598-80-6

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
ripol	1796.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1796.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34598806&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume