1,2-Cyclohexanedione, 3,3,6,6-tetramethyl-

Inchi: InChI=1S/C10H16O2/c1-9(2)5-6-10(3,4)8(12)7(9)11/h5-6H2,1-4H3
InchiKey: DTLUXZSCFRVBER-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CC1(C)CCC(C)(C)C(=O)C1=O
Mol. weight [g/mol]: 168.23
CAS: 20651-89-2

Physical Properties

Property code	Value	Unit	Source
gf	-206.10	kJ/mol	Joback Method
hf	-460.67	kJ/mol	Joback Method
hfus	0.99	kJ/mol	Joback Method
hvap	44.17	kJ/mol	Joback Method
ie	8.70 ± 0.05	eV	NIST Webbook
log10ws	-1.98		Crippen Method
logp	1.971		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
tb	579.20	K	Joback Method
tc	826.73	K	Joback Method
tf	389.84	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.54	J/mol×K	579.20	Joback Method
cpg	388.91	J/mol×K	620.45	Joback Method
cpg	406.37	J/mol×K	661.71	Joback Method
cpg	423.10	J/mol×K	702.96	Joback Method
cpg	439.32	J/mol×K	744.22	Joback Method
cpg	455.20	J/mol×K	785.47	Joback Method
cpg	470.94	J/mol×K	826.73	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=C20651892&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
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