1,3-Cyclohexanedione, 2-methyl-

Other names: 1-Methyl-2,6-cyclohexanedione
2-Methyl-1,3-cyclohexanedione
2-Methylcyclohexane-1,3-dione
Inchi: InChI=1S/C7H10O2/c1-5-6(8)3-2-4-7(5)9/h5H,2-4H2,1H3
InchiKey: VSGJHHIAMHUZKF-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1C(=O)CCCC1=O
Mol. weight [g/mol]: 126.15
CAS: 1193-55-1

Physical Properties

Property code	Value	Unit	Source
gf	-212.67	kJ/mol	Joback Method
hf	-408.89	kJ/mol	Joback Method
hfus	4.74	kJ/mol	Joback Method
hvap	40.10	kJ/mol	Joback Method
ie	9.37 ± 0.05	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	0.945		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	1006.00		NIST Webbook
rinpol	1006.00		NIST Webbook
tb	514.75	K	Joback Method
tc	756.60	K	Joback Method
tf	482.00 ± 3.00	K	NIST Webbook
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.21	J/mol×K	514.75	Joback Method
cpg	246.68	J/mol×K	555.06	Joback Method
cpg	261.54	J/mol×K	595.37	Joback Method

cpg	275.72	J/mol×K	635.67	Joback Method
cpg	289.17	J/mol×K	675.98	Joback Method
cpg	301.83	J/mol×K	716.29	Joback Method
cpg	313.64	J/mol×K	756.60	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=C1193551&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
ie:	Ionization energy
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