1,3-Cyclopentanedione

Other names: 1,3-Cyclopentadione
cyclopentane-1,3-dione
Inchi: InChI=1S/C5H6O2/c6-4-1-2-5(7)3-4/h1-3H2
InchiKey: LOGSONSNCYTHPS-UHFFFAOYSA-N
Formula: C5H6O2
SMILES: O=C1CCC(=O)C1
Mol. weight [g/mol]: 98.10
CAS: 3859-41-4

Physical Properties

Property code	Value	Unit	Source
gf	-209.70	kJ/mol	Joback Method
hf	-341.11	kJ/mol	Joback Method
hfus	0.59	kJ/mol	Joback Method
hvap	35.78	kJ/mol	Joback Method
ie	9.46 ± 0.05	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
log10ws	-0.37		Crippen Method
logp	0.308		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
tb	469.39	K	Joback Method
tc	710.95	K	Joback Method
tf	423.00 ± 3.00	K	NIST Webbook
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.97	J/mol×K	469.39	Joback Method
cpg	158.12	J/mol×K	509.65	Joback Method
cpg	168.92	J/mol×K	549.91	Joback Method
cpg	179.31	J/mol×K	590.17	Joback Method
cpg	189.25	J/mol×K	630.43	Joback Method

cpg	198.71	J/mol×K	670.69	Joback Method
cpg	207.63	J/mol×K	710.95	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=C3859414&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