1,3-Cyclopentanedione, 2-ethyl-

Other names: 2-Ethyl-1,3-cyclopentanedione
2-ethylcyclopentane-1,3-dione
Inchi: InChI=1S/C7H10O2/c1-2-5-6(8)3-4-7(5)9/h5H,2-4H2,1H3
InchiKey: YDFBIBUYOUFJMR-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CCC1C(=O)CCC1=O
Mol. weight [g/mol]: 126.15
CAS: 823-36-9

Physical Properties

Property code	Value	Unit	Source
gf	-200.57	kJ/mol	Joback Method
hf	-402.73	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	39.93	kJ/mol	Joback Method
ie	9.40 ± 0.10	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	0.945		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	510.48	K	Joback Method
tc	743.22	K	Joback Method
tf	315.99	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.44	J/mol×K	510.48	Joback Method
cpg	245.85	J/mol×K	549.27	Joback Method
cpg	259.69	J/mol×K	588.06	Joback Method
cpg	272.95	J/mol×K	626.85	Joback Method
cpg	285.56	J/mol×K	665.64	Joback Method
cpg	297.50	J/mol×K	704.43	Joback Method

cpg	308.72	J/mol×K	743.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C823369&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
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