5,5-Dimethyl-1,3-cyclohexanedione

Other names: 5,5-Dimethyl-cyclohex-2-enone-3-ol
Inchi: InChI=1S/C8H12O2/c1-8(2)4-6(9)3-7(10)5-8/h3,9H,4-5H2,1-2H3
InchiKey: PQZVNKWTNLBLHJ-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CC1(C)CC(=O)C=C(O)C1
Mol. weight [g/mol]: 140.18
CAS: 3471-13-4

Physical Properties

Property code	Value	Unit	Source
gf	-203.64	kJ/mol	Joback Method
hf	-382.51	kJ/mol	Joback Method
hfus	6.44	kJ/mol	Joback Method
hvap	54.56	kJ/mol	Joback Method
ie	9.45	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.817		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	566.37	K	Joback Method
tc	782.58	K	Joback Method
tf	353.52	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.38	J/mol×K	566.37	Joback Method
cpg	295.89	J/mol×K	602.41	Joback Method
cpg	307.76	J/mol×K	638.44	Joback Method
cpg	319.06	J/mol×K	674.48	Joback Method
cpg	329.87	J/mol×K	710.51	Joback Method
cpg	340.26	J/mol×K	746.55	Joback Method
cpg	350.31	J/mol×K	782.58	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=C3471134&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