2-Cyclopenten-1-one, 2-hydroxy-3,4-dimethyl-

Other names:	3,4-Dimethyl-2-hydroxycyclopent-2-en-1-one
	2-Hydroxy-3,4-dimethyl-2-cyclopenten-1-one
	3,4-Dimethyl-2-hydroxy-2-cyclopentenone
	2-hydroxy-3,4-dimethylcyclopent-2-en-1-one
Inchi:	InChI=1S/C7H10O2/c1-4-3-6(8)7(9)5(4)2/h4,9H,3H2,1-2H3
InchiKey:	GXUQPCUHTNAVRJ-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	CC1=C(O)C(=O)CC1C
Mol. weight [g/mol]:	126.15
CAS:	21835-00-7

Physical Properties

Property code	Value	Unit	Source
gf	-204.10	kJ/mol	Joback Method
hf	-382.42	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.427		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	1075.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1075.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1839.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1840.00		NIST Webbook
tb	543.96	K	Joback Method
tc	749.04	K	Joback Method
tf	334.39	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.68	J/mol×K	543.96	Joback Method
cpg	249.51	J/mol×K	578.14	Joback Method
cpg	259.90	J/mol×K	612.32	Joback Method
cpg	269.85	J/mol×K	646.50	Joback Method
cpg	279.33	J/mol×K	680.68	Joback Method
cpg	288.35	J/mol×K	714.86	Joback Method
cpg	296.89	J/mol×K	749.04	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=C21835007&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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume