2-Hydroxy-4,4-dimethyl-2-cyclopenten-1-one

Other names: 2-Cyclopenten-1-one, 2-hydroxy-4,4-dimethyl
Inchi: InChI=1S/C7H10O2/c1-7(2)3-5(8)6(9)4-7/h3,8H,4H2,1-2H3
InchiKey: VMJQWHBQSDAUBG-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1(C)C=C(O)C(=O)C1
Mol. weight [g/mol]: 126.15

Physical Properties

Property code	Value	Unit	Source
gf	-199.96	kJ/mol	Joback Method
hf	-355.71	kJ/mol	Joback Method
hfus	5.95	kJ/mol	Joback Method
hvap	52.16	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.427		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
rinpol	973.00		NIST Webbook
rinpol	973.00		NIST Webbook
ripol	1660.00		NIST Webbook
tb	539.22	K	Joback Method
tc	751.51	K	Joback Method
tf	345.77	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.61	J/mol×K	539.22	Joback Method
cpg	249.31	J/mol×K	574.60	Joback Method
cpg	259.44	J/mol×K	609.98	Joback Method
cpg	269.06	J/mol×K	645.36	Joback Method
cpg	278.26	J/mol×K	680.74	Joback Method
cpg	287.10	J/mol×K	716.13	Joback Method

cpg	295.67	J/mol×K	751.51	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=R53276&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

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