2-Hydroxy-4-methyl-2-cyclopenten-1-one

Other names: 2-Cyclopenten-1-one, 2-hydroxy-4-methyl
Inchi: InChI=1S/C6H8O2/c1-4-2-5(7)6(8)3-4/h2,4,7H,3H2,1H3
InchiKey: SFSXQNIOJABGSJ-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1C=C(O)C(=O)C1
Mol. weight [g/mol]: 112.13
CAS: 15899-72-6

Physical Properties

Property code	Value	Unit	Source
gf	-202.89	kJ/mol	Joback Method
hf	-350.31	kJ/mol	Joback Method
hfus	9.66	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	1.037		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	948.00		NIST Webbook
rinpol	948.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1688.00		NIST Webbook
tb	516.10	K	Joback Method
tc	723.20	K	Joback Method
tf	310.60	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.23	J/mol×K	516.10	Joback Method
cpg	206.21	J/mol×K	550.62	Joback Method
cpg	215.78	J/mol×K	585.13	Joback Method
cpg	224.91	J/mol×K	619.65	Joback Method

cpg	233.62	J/mol×K	654.16	Joback Method
cpg	241.89	J/mol×K	688.68	Joback Method
cpg	249.71	J/mol×K	723.20	Joback Method

Sources

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=C15899726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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