2-Cyclopenten-1-one, 2-hydroxy-4-ethyl-3-methyl

Other names: 4-Ethyl-3-methyl-2-hydroxycyclopent-2-en-1-one
4-Ethyl-3-methyl-2-hydroxy-2-cyclopenten-1-one
2-Cyclopenten-1-one, 4-ethyl-2-hydroxy-3-methyl
Inchi: InChI=1S/C8H12O2/c1-3-6-4-7(9)8(10)5(6)2/h6,10H,3-4H2,1-2H3
InchiKey: FFJYTCCZZSZBGQ-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CCC1CC(=O)C(O)=C1C
Mol. weight [g/mol]: 140.18
CAS: 71387-71-8

Physical Properties

Property code	Value	Unit	Source
gf	-195.68	kJ/mol	Joback Method
hf	-403.06	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.817		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	1154.00		NIST Webbook
rinpol	1154.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1845.00		NIST Webbook
tb	566.84	K	Joback Method
tc	768.88	K	Joback Method
tf	345.66	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.61	J/mol×K	566.84	Joback Method

cpg	295.46	J/mol×K	600.51	Joback Method
cpg	306.81	J/mol×K	634.19	Joback Method
cpg	317.65	J/mol×K	667.86	Joback Method
cpg	327.96	J/mol×K	701.53	Joback Method
cpg	337.75	J/mol×K	735.21	Joback Method
cpg	347.01	J/mol×K	768.88	Joback Method

Sources

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=C71387718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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