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

Other names:	3-Ethyl-2-hydroxy-2-cyclopenten-1-one
	2-Cyclopenten-1-one, 2-hydroxy-3-ethyl
	2-Hydroxy-3-ethyl-2-cyclopenten-1-one
	3-Ethyl-2-hydroxy-2-cyclopentenone
	3-ethyl-2-hydroxycyclopent-2-en-1-one
Inchi:	InChI=1S/C7H10O2/c1-2-5-3-4-6(8)7(5)9/h9H,2-4H2,1H3
InchiKey:	JHWFWLUAUPZUCP-UHFFFAOYSA-N
Formula:	C7H10O2
SMILES:	CCC1=C(O)C(=O)CC1
Mol. weight [g/mol]:	126.15
CAS:	21835-01-8

Physical Properties

Property code	Value	Unit	Source
gf	-196.39	kJ/mol	Joback Method
hf	-362.08	kJ/mol	Joback Method
hfus	10.79	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.571		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1891.00		NIST Webbook
ripol	1845.00		NIST Webbook
ripol	1924.00		NIST Webbook

ripol	1892.00		NIST Webbook
ripol	1893.00		NIST Webbook
tb	548.63	K	Joback Method
tc	753.86	K	Joback Method
tf	338.63	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.75	J/mol×K	548.63	Joback Method
cpg	247.22	J/mol×K	582.83	Joback Method
cpg	257.24	J/mol×K	617.04	Joback Method
cpg	266.79	J/mol×K	651.24	Joback Method
cpg	275.88	J/mol×K	685.45	Joback Method
cpg	284.51	J/mol×K	719.65	Joback Method
cpg	292.68	J/mol×K	753.86	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=C21835018&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