2-Cyclopenten-1-one, 2-hydroxy-5-ethyl-3-methyl

Other names: 5-Ethyl-2-hydroxy-3-methyl-2-cyclopenten-1-one
2-Cyclopenten-1-one, 5-ethyl-2-hydroxy-3-methyl
5-ethyl-2-hydroxy-3-methylcyclopent-2-en-1-one

Inchi: InChI=1S/C8H12O2/c1-3-6-4-5(2)7(9)8(6)10/h6,9H,3-4H2,1-2H3

InchiKey: ARHWUYVUNJLMRR-UHFFFAOYSA-N

Formula: C8H12O2

SMILES: CCC1CC(C)=C(O)C1=O

Mol. weight [g/mol]: 140.18

CAS: 53263-58-4

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	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1799.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53263584&Units=SI
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

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