4-Ethyl-3-methyl-2-hydroxycyclopent-2-en-1-one

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

Physical Properties

Property code	Value	Unit	Source
hfus	14.45	kJ/mol	Joback Method
logp	1.817		Crippen Method
mcvol	115.860	ml/mol	McGowan 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

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71387718&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices