5-Ethylcyclopent-2-en-1-one

Inchi: InChI=1S/C7H10O/c1-2-6-4-3-5-7(6)8/h3,5-6H,2,4H2,1H3
InchiKey: ZUWLMAOLTHLUHS-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CCC1CC=CC1=O
Mol. weight [g/mol]: 110.15

Physical Properties

Property code	Value	Unit	Source
gf	-48.02	kJ/mol	Joback Method
hf	-207.25	kJ/mol	Joback Method
hfus	8.55	kJ/mol	Joback Method
hvap	35.97	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.542		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	966.00		NIST Webbook
tb	441.82	K	Joback Method
tc	658.94	K	Joback Method
tf	248.53	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.63	J/mol×K	441.82	Joback Method
cpg	203.97	J/mol×K	478.01	Joback Method
cpg	216.72	J/mol×K	514.19	Joback Method
cpg	228.89	J/mol×K	550.38	Joback Method
cpg	240.47	J/mol×K	586.57	Joback Method
cpg	251.47	J/mol×K	622.75	Joback Method
cpg	261.89	J/mol×K	658.94	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=R522799&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume