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

Other names: 3-Ethyl-2-cyclopenten-1-one
Inchi: InChI=1S/C7H10O/c1-2-6-3-4-7(8)5-6/h5H,2-4H2,1H3
InchiKey: XHAHAEVXYYITIQ-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CCC1=CC(=O)CC1
Mol. weight [g/mol]: 110.15
CAS: 5682-69-9

Physical Properties

Property code	Value	Unit	Source
gf	-49.94	kJ/mol	Joback Method
hf	-198.38	kJ/mol	Joback Method
hfus	7.09	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.686		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1029.00		NIST Webbook
rinpol	1029.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1611.00		NIST Webbook
tb	451.47	K	Joback Method
tc	670.37	K	Joback Method
tf	265.29	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.39	J/mol×K	451.47	Joback Method
cpg	202.95	J/mol×K	487.95	Joback Method

cpg	214.96	J/mol×K	524.44	Joback Method
cpg	226.42	J/mol×K	560.92	Joback Method
cpg	237.33	J/mol×K	597.40	Joback Method
cpg	247.70	J/mol×K	633.88	Joback Method
cpg	257.52	J/mol×K	670.37	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5682699&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