3-Ethylcyclopentanone

Inchi: InChI=1S/C7H12O/c1-2-6-3-4-7(8)5-6/h6H,2-5H2,1H3
InchiKey: XERALSLWOPMNRJ-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CCC1CCC(=O)C1
Mol. weight [g/mol]: 112.17
CAS: 10264-55-8

Physical Properties

Property code	Value	Unit	Source
gf	-77.98	kJ/mol	Joback Method
hf	-265.03	kJ/mol	Joback Method
hfus	7.33	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
rinpol	965.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	959.00		NIST Webbook
tb	442.66	K	Joback Method
tc	657.51	K	Joback Method
tf	247.77	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.10	J/mol×K	442.66	Joback Method

cpg	219.78	J/mol×K	478.47	Joback Method
cpg	233.83	J/mol×K	514.28	Joback Method
cpg	247.27	J/mol×K	550.08	Joback Method
cpg	260.08	J/mol×K	585.89	Joback Method
cpg	272.27	J/mol×K	621.70	Joback Method
cpg	283.83	J/mol×K	657.51	Joback Method

Sources

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=C10264558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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