2-Ethylidenecyclohexanone

Other names: 2-Ethylidenecyclohexanone (c,t)
Inchi: InChI=1S/C8H12O/c1-2-7-5-3-4-6-8(7)9/h2H,3-6H2,1H3/b7-2-
InchiKey: YPRIHWWNQRSAQL-UQCOIBPSSA-N
Formula: C8H12O
SMILES: CC=C1CCCCC1=O
Mol. weight [g/mol]: 124.18
CAS: 1122-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-28.49	kJ/mol	Joback Method
hf	-195.46	kJ/mol	Joback Method
hfus	7.07	kJ/mol	Joback Method
hvap	39.17	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.076		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
tb	481.12	K	Joback Method
tc	709.80	K	Joback Method
tf	270.12	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.37	J/mol×K	481.12	Joback Method
cpg	245.68	J/mol×K	519.23	Joback Method
cpg	260.23	J/mol×K	557.35	Joback Method
cpg	274.04	J/mol×K	595.46	Joback Method
cpg	287.11	J/mol×K	633.57	Joback Method
cpg	299.45	J/mol×K	671.69	Joback Method
cpg	311.05	J/mol×K	709.80	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=C1122243&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume