Cyclohexanone, 3-ethyl-

Other names: 3-Ethylcyclohexanone
Inchi: InChI=1S/C8H14O/c1-2-7-4-3-5-8(9)6-7/h7H,2-6H2,1H3
InchiKey: IEVRHAUJJJBXFH-UHFFFAOYSA-N
Formula: C8H14O
SMILES: CCC1CCCC(=O)C1
Mol. weight [g/mol]: 126.20
CAS: 22461-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-81.66	kJ/mol	Joback Method
hf	-291.83	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	38.08	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	467.08 ± 0.50	K	NIST Webbook
tc	690.17	K	Joback Method
tf	210.88 ± 0.20	K	NIST Webbook
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.75	J/mol×K	469.81	Joback Method
cpg	263.69	J/mol×K	506.54	Joback Method
cpg	279.88	J/mol×K	543.26	Joback Method
cpg	295.31	J/mol×K	579.99	Joback Method
cpg	309.98	J/mol×K	616.71	Joback Method
cpg	323.89	J/mol×K	653.44	Joback Method
cpg	337.02	J/mol×K	690.17	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=C22461898&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