cis-2-Methyl-3-ethylcyclohexanone

Inchi: InChI=1S/C9H16O/c1-3-8-5-4-6-9(10)7(8)2/h7-8H,3-6H2,1-2H3/t7-,8-/m0/s1
InchiKey: CZXZZEIHDIVIEH-YUMQZZPRSA-N
Formula: C9H16O
SMILES: CCC1CCCC(=O)C1C
Mol. weight [g/mol]: 140.22
CAS: 78707-79-6

Physical Properties

Property code	Value	Unit	Source
gf	-80.95	kJ/mol	Joback Method
hf	-332.81	kJ/mol	Joback Method
hfus	11.48	kJ/mol	Joback Method
hvap	40.00	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	488.02	K	Joback Method
tc	704.74	K	Joback Method
tf	262.55	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.05	J/mol×K	488.02	Joback Method
cpg	310.41	J/mol×K	524.14	Joback Method
cpg	327.98	J/mol×K	560.26	Joback Method
cpg	344.74	J/mol×K	596.38	Joback Method
cpg	360.70	J/mol×K	632.50	Joback Method
cpg	375.83	J/mol×K	668.62	Joback Method
cpg	390.13	J/mol×K	704.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78707796&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume