Cyclohexanone, 5-methyl-2-propyl, cis

Inchi: InChI=1S/C10H18O/c1-3-4-9-6-5-8(2)7-10(9)11/h8-9H,3-7H2,1-2H3/t8-,9+/m0/s1
InchiKey: NTUYHILVAVUKKB-DTWKUNHWSA-N
Formula: C10H18O
SMILES: CCCC1CCC(C)CC1=O
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-72.53	kJ/mol	Joback Method
hf	-353.45	kJ/mol	Joback Method
hfus	14.07	kJ/mol	Joback Method
hvap	42.22	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1186.00		NIST Webbook
tb	510.90	K	Joback Method
tc	724.22	K	Joback Method
tf	273.82	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.79	J/mol×K	510.90	Joback Method
cpg	358.06	J/mol×K	546.45	Joback Method
cpg	376.47	J/mol×K	582.01	Joback Method
cpg	394.01	J/mol×K	617.56	Joback Method
cpg	410.68	J/mol×K	653.11	Joback Method
cpg	426.47	J/mol×K	688.67	Joback Method
cpg	441.37	J/mol×K	724.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R578673&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume