3,5-Di-tert-butylcyclohexanone

Inchi: InChI=1S/C14H26O/c1-13(2,3)10-7-11(14(4,5)6)9-12(15)8-10/h10-11H,7-9H2,1-6H3
InchiKey: VTGCARYDRSRJMW-UHFFFAOYSA-N
Formula: C14H26O
SMILES: CC(C)(C)C1CC(=O)CC(C(C)(C)C)C1
Mol. weight [g/mol]: 210.36
CAS: 92319-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-33.17	kJ/mol	Joback Method
hf	-453.51	kJ/mol	Joback Method
hfus	9.60	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	4.064		Crippen Method
mcvol	198.830	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
tb	595.96	K	Joback Method
tc	821.13	K	Joback Method
tf	323.74	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.53	J/mol×K	595.96	Joback Method
cpg	572.61	J/mol×K	633.49	Joback Method
cpg	595.17	J/mol×K	671.02	Joback Method
cpg	616.24	J/mol×K	708.54	Joback Method
cpg	635.89	J/mol×K	746.07	Joback Method
cpg	654.16	J/mol×K	783.60	Joback Method
cpg	671.11	J/mol×K	821.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92319147&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