2,2,6,6,-Tetramethylcyclohexanone

Inchi: InChI=1S/C10H18O/c1-9(2)6-5-7-10(3,4)8(9)11/h5-7H2,1-4H3
InchiKey: PLWBUOOIBTVSNN-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1(C)CCCC(C)(C)C1=O
Mol. weight [g/mol]: 154.25
CAS: 1195-93-3

Physical Properties

Property code	Value	Unit	Source
gf	-83.51	kJ/mol	Joback Method
hf	-322.97	kJ/mol	Joback Method
hfus	1.48	kJ/mol	Joback Method
hvap	39.92	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.792		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	511.38	K	Joback Method
tc	743.60	K	Joback Method
tf	321.62	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.78	J/mol×K	511.38	Joback Method
cpg	358.04	J/mol×K	550.08	Joback Method
cpg	376.04	J/mol×K	588.79	Joback Method
cpg	392.97	J/mol×K	627.49	Joback Method
cpg	409.03	J/mol×K	666.19	Joback Method
cpg	424.42	J/mol×K	704.90	Joback Method
cpg	439.34	J/mol×K	743.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1195933&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