3,3,4,5-tetramethylcyclohexan-1-one

Inchi: InChI=1S/C10H18O/c1-7-5-9(11)6-10(3,4)8(7)2/h7-8H,5-6H2,1-4H3
InchiKey: RIAQBNSPOHNARJ-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CC1CC(=O)CC(C)(C)C1C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-85.73	kJ/mol	Joback Method
hf	-358.55	kJ/mol	Joback Method
hfus	8.84	kJ/mol	Joback Method
hvap	40.76	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.648		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook
tb	506.47	K	Joback Method
tc	728.80	K	Joback Method
tf	293.48	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.35	J/mol×K	506.47	Joback Method
cpg	359.07	J/mol×K	543.53	Joback Method
cpg	377.75	J/mol×K	580.58	Joback Method
cpg	395.47	J/mol×K	617.64	Joback Method
cpg	412.30	J/mol×K	654.69	Joback Method
cpg	428.32	J/mol×K	691.75	Joback Method
cpg	443.60	J/mol×K	728.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R407046&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

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