Cyclopentanone, 2,2,5,5-tetramethyl-

Other names: 2,2,5,5-Tetramethylcyclopentanone
Inchi: InChI=1S/C9H16O/c1-8(2)5-6-9(3,4)7(8)10/h5-6H2,1-4H3
InchiKey: BXYUQRQZHXARGL-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CC1(C)CCC(C)(C)C1=O
Mol. weight [g/mol]: 140.22
CAS: 4541-35-9

Physical Properties

Property code	Value	Unit	Source
gf	-79.83	kJ/mol	Joback Method
hf	-296.17	kJ/mol	Joback Method
hfus	0.99	kJ/mol	Joback Method
hvap	37.52	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.402		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	484.23	K	Joback Method
tc	711.66	K	Joback Method
tf	313.87	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.00	J/mol×K	484.23	Joback Method
cpg	310.45	J/mol×K	522.13	Joback Method
cpg	326.66	J/mol×K	560.04	Joback Method
cpg	341.81	J/mol×K	597.94	Joback Method
cpg	356.09	J/mol×K	635.85	Joback Method
cpg	369.71	J/mol×K	673.75	Joback Method
cpg	382.85	J/mol×K	711.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4541359&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume