Cyclopentanone, 2,2-dimethyl-

Other names: 2,2-Dimethylcyclopentanone
Inchi: InChI=1S/C7H12O/c1-7(2)5-3-4-6(7)8/h3-5H2,1-2H3
InchiKey: FTGZMZBYOHMEPS-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CC1(C)CCCC1=O
Mol. weight [g/mol]: 112.17
CAS: 4541-32-6

Physical Properties

Property code	Value	Unit	Source
gf	-83.47	kJ/mol	Joback Method
hf	-249.79	kJ/mol	Joback Method
hfus	1.03	kJ/mol	Joback Method
hvap	34.53	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	442.90	K	Joback Method
tc	667.64	K	Joback Method
tf	271.67	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.92	J/mol×K	442.90	Joback Method
cpg	220.91	J/mol×K	480.36	Joback Method
cpg	234.93	J/mol×K	517.81	Joback Method
cpg	248.07	J/mol×K	555.27	Joback Method
cpg	260.43	J/mol×K	592.73	Joback Method
cpg	272.11	J/mol×K	630.19	Joback Method
cpg	283.18	J/mol×K	667.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4541326&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