3-Pentanone, 4-chloro-2-methyl

Inchi: InChI=1S/C6H11ClO/c1-4(2)6(8)5(3)7/h4-5H,1-3H3
InchiKey: YZZGXNYEUGNGFC-UHFFFAOYSA-N
Formula: C6H11ClO
SMILES: CC(C)C(=O)C(C)Cl
Mol. weight [g/mol]: 134.60

Physical Properties

Property code	Value	Unit	Source
gf	-146.09	kJ/mol	Joback Method
hf	-306.05	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	39.31	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.839		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
tb	427.10	K	Joback Method
tc	620.79	K	Joback Method
tf	207.23	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.33	J/mol×K	427.10	Joback Method
cpg	250.96	J/mol×K	588.51	Joback Method
cpg	242.34	J/mol×K	556.23	Joback Method
cpg	233.28	J/mol×K	523.94	Joback Method
cpg	223.77	J/mol×K	491.66	Joback Method
cpg	213.79	J/mol×K	459.38	Joback Method
cpg	259.15	J/mol×K	620.79	Joback Method
dvisc	0.0003215	Pa×s	427.10	Joback Method

dvisc	0.0004344	Pa×s	390.46	Joback Method
dvisc	0.0006245	Pa×s	353.81	Joback Method
dvisc	0.0009763	Pa×s	317.17	Joback Method
dvisc	0.0017155	Pa×s	280.52	Joback Method
dvisc	0.0035708	Pa×s	243.88	Joback Method
dvisc	0.0096323	Pa×s	207.23	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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