3-Pentanone, 2-chloro-2-methyl

Inchi: InChI=1S/C6H11ClO/c1-4-5(8)6(2,3)7/h4H2,1-3H3
InchiKey: AZCURUYAXYRZKN-UHFFFAOYSA-N
Formula: C6H11ClO
SMILES: CCC(=O)C(C)(C)Cl
Mol. weight [g/mol]: 134.60

Physical Properties

Property code	Value	Unit	Source
gf	-138.37	kJ/mol	Joback Method
hf	-304.24	kJ/mol	Joback Method
hfus	9.68	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.983		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	828.00		NIST Webbook
rinpol	828.00		NIST Webbook
tb	424.75	K	Joback Method
tc	622.09	K	Joback Method
tf	239.65	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.61	J/mol×K	424.75	Joback Method
cpg	216.65	J/mol×K	457.64	Joback Method
cpg	227.04	J/mol×K	490.53	Joback Method
cpg	236.83	J/mol×K	523.42	Joback Method
cpg	246.04	J/mol×K	556.31	Joback Method
cpg	254.69	J/mol×K	589.20	Joback Method
cpg	262.82	J/mol×K	622.09	Joback Method
dvisc	0.0060123	Pa×s	239.65	Joback Method

dvisc	0.0028981	Pa×s	270.50	Joback Method
dvisc	0.0016221	Pa×s	301.35	Joback Method
dvisc	0.0010112	Pa×s	332.20	Joback Method
dvisc	0.0006831	Pa×s	363.05	Joback Method
dvisc	0.0004907	Pa×s	393.90	Joback Method
dvisc	0.0003699	Pa×s	424.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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