2-Butanone, 3-chloro-3-methyl-

Inchi: InChI=1S/C5H9ClO/c1-4(7)5(2,3)6/h1-3H3
InchiKey: FTJRNNIDCLELRD-UHFFFAOYSA-N
Formula: C5H9ClO
SMILES: CC(=O)C(C)(C)Cl
Mol. weight [g/mol]: 120.58
CAS: 5950-19-6

Physical Properties

Property code	Value	Unit	Source
gf	-146.79	kJ/mol	Joback Method
hf	-283.60	kJ/mol	Joback Method
hfus	7.09	kJ/mol	Joback Method
hvap	36.56	kJ/mol	Joback Method
ie	9.70	eV	NIST Webbook
log10ws	-1.46		Crippen Method
logp	1.593		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	763.00		NIST Webbook
rinpol	763.00		NIST Webbook
tb	401.87	K	Joback Method
tc	601.08	K	Joback Method
tf	228.38	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.29	J/mol×K	401.87	Joback Method
cpg	211.47	J/mol×K	567.88	Joback Method
cpg	203.89	J/mol×K	534.68	Joback Method
cpg	195.82	J/mol×K	501.47	Joback Method
cpg	187.21	J/mol×K	468.27	Joback Method
cpg	178.04	J/mol×K	435.07	Joback Method

cpg	218.56	J/mol×K	601.08	Joback Method
dvisc	0.0003928	Pa×s	401.87	Joback Method
dvisc	0.0005185	Pa×s	372.96	Joback Method
dvisc	0.0007172	Pa×s	344.04	Joback Method
dvisc	0.0010528	Pa×s	315.12	Joback Method
dvisc	0.0016700	Pa×s	286.21	Joback Method
dvisc	0.0029388	Pa×s	257.30	Joback Method
dvisc	0.0059669	Pa×s	228.38	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5950196&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ie: Ionization energy
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