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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

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

Latest version available from:
https://www.chemeo.com/cid/88-046-4/2-Butanone-3-chloro-3-methyl.pdf

Generated by Cheméo on 2024-10-12 02:22:41.521497325 +0000 UTC m=+3280624.158466573.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.