

2-Butanone, 3-chloro-3-methyl

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

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
log10ws	-1.46		Crippen Method
logp	1.593		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	725.00		NIST Webbook
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tb	401.87	K	Joback Method
tc	601.08	K	Joback Method
tf	228.38	K	Joback Method
vc	0.359	m ³ /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	Paxs	401.87	Joback Method

dvisc	0.0005185	Paxs	372.96	Joback Method
dvisc	0.0007172	Paxs	344.04	Joback Method
dvisc	0.0010528	Paxs	315.12	Joback Method
dvisc	0.0016700	Paxs	286.21	Joback Method
dvisc	0.0029388	Paxs	257.30	Joback Method
dvisc	0.0059669	Paxs	228.38	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=R629533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

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