2-Butanone, 3-chloro-

Other names:	1-Chloroethyl methyl ketone
	2-Chloro-3-butanone
	3-Chloro-2-butanone
	3-Chlorobutanone
	3-chlorobutan-2-one
Inchi:	InChI=1S/C4H7ClO/c1-3(5)4(2)6/h3H,1-2H3
InchiKey:	OIMRLHCSLQUXLL-UHFFFAOYSA-N
Formula:	C4H7ClO
SMILES:	CC(=O)C(C)Cl
Mol. weight [g/mol]:	106.55
CAS:	4091-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-160.49	kJ/mol	Joback Method
hf	-259.49	kJ/mol	Joback Method
hfus	8.39	kJ/mol	Joback Method
hvap	35.24	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.203		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	748.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	704.00		NIST Webbook
tb	388.20	K	NIST Webbook
tc	573.96	K	Joback Method
tf	199.69	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.55	J/mol×K	381.78	Joback Method
cpg	138.84	J/mol×K	413.81	Joback Method
cpg	145.81	J/mol×K	445.84	Joback Method
cpg	152.47	J/mol×K	477.87	Joback Method
cpg	158.83	J/mol×K	509.90	Joback Method
cpg	164.89	J/mol×K	541.93	Joback Method
cpg	170.67	J/mol×K	573.96	Joback Method
dvisc	0.0053672	Pa×s	199.69	Joback Method
dvisc	0.0025233	Pa×s	230.04	Joback Method
dvisc	0.0014145	Pa×s	260.39	Joback Method
dvisc	0.0008947	Pa×s	290.74	Joback Method
dvisc	0.0006172	Pa×s	321.08	Joback Method
dvisc	0.0004539	Pa×s	351.43	Joback Method
dvisc	0.0003505	Pa×s	381.78	Joback Method
hvapt	38.80	kJ/mol	351.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61158e+01
Coeff. B	-4.50148e+03
Temperature range (K), min.	284.40
Temperature range (K), max.	416.63

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4091398&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume