2-Butanone, 1-chloro-

Other names: 1-Chloro-2-butanone
1-chlorobutan-2-one
Inchi: InChI=1S/C4H7ClO/c1-2-4(6)3-5/h2-3H2,1H3
InchiKey: AALRHBLMAVGWRR-UHFFFAOYSA-N
Formula: C4H7ClO
SMILES: CCC(=O)CCl
Mol. weight [g/mol]: 106.55
CAS: 616-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-158.05	kJ/mol	Joback Method
hf	-254.21	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.204		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	756.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	757.00		NIST Webbook
rinpol	753.00		NIST Webbook
tb	382.22	K	Joback Method
tc	569.79	K	Joback Method
tf	214.69	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.37	J/mol×K	569.79	Joback Method
cpg	131.57	J/mol×K	382.22	Joback Method
cpg	138.59	J/mol×K	413.48	Joback Method

cpg	145.30	J/mol×K	444.74	Joback Method
cpg	151.74	J/mol×K	476.01	Joback Method
cpg	157.89	J/mol×K	507.27	Joback Method
cpg	163.76	J/mol×K	538.53	Joback Method
dvisc	0.0003618	Pa×s	382.22	Joback Method
dvisc	0.0034502	Pa×s	214.69	Joback Method
dvisc	0.0019085	Pa×s	242.61	Joback Method
dvisc	0.0011929	Pa×s	270.53	Joback Method
dvisc	0.0008142	Pa×s	298.46	Joback Method
dvisc	0.0005932	Pa×s	326.38	Joback Method
dvisc	0.0004543	Pa×s	354.30	Joback Method
hvapt	49.20	kJ/mol	359.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40701e+01
Coeff. B	-2.51367e+03
Coeff. C	-1.25570e+02
Temperature range (K), min.	307.00
Temperature range (K), max.	412.56

Sources

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

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=C616273&Units=SI

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