2-Propanone, 1-chloro-

Other names:	1-Chloro-2-propanone
	1-Chloropropanone
	3-Chloro-2-propanone
	A-Stoff
	Acetone, chloro-
	Acetonyl chloride
	CH3COCH2Cl
	Chloracetone
	Chloro-2-propanone
	Chloroacetone
	Chloromethyl methyl ketone
	Chloropropanone
	Monochloracetone
	Monochloroacetone
	NSC 30673
	Tonite
	UN 1695
	«alpha»-Chloroacetone
	Â«alphaÂ»-Chloroacetone
Inchi:	InChI=1S/C3H5ClO/c1-3(5)2-4/h2H2,1H3
InchiKey:	BULLHNJGPPOUOX-UHFFFAOYSA-N
Formula:	C3H5ClO
SMILES:	CC(=O)CCl
Mol. weight [g/mol]:	92.52
CAS:	78-95-5

Physical Properties

Property code	Value	Unit	Source
gf	-166.47	kJ/mol	Joback Method
hf	-233.57	kJ/mol	Joback Method
hfus	9.32	kJ/mol	Joback Method
hvap	33.40	kJ/mol	Joback Method
ie	10.00 ± 0.01	eV	NIST Webbook
ie	9.92 ± 0.03	eV	NIST Webbook
ie	9.98 ± 0.01	eV	NIST Webbook
ie	9.93 ± 0.02	eV	NIST Webbook
ie	9.98 ± 0.13	eV	NIST Webbook

ie	9.91 ± 0.03	eV	NIST Webbook
ie	9.88	eV	NIST Webbook
log10ws	-0.51		Crippen Method
logp	0.814		Crippen Method
mcvol	66.940	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
rinpol	627.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	677.00		NIST Webbook
rinpol	675.00		NIST Webbook
rinpol	653.00		NIST Webbook
rinpol	675.00		NIST Webbook
tb	393.20	K	NIST Webbook
tc	547.77	K	Joback Method
tf	203.42	K	Joback Method
vc	0.259	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.49	J/mol×K	359.34	Joback Method
cpg	104.90	J/mol×K	390.75	Joback Method
cpg	110.08	J/mol×K	422.15	Joback Method
cpg	115.05	J/mol×K	453.56	Joback Method
cpg	119.80	J/mol×K	484.96	Joback Method
cpg	124.35	J/mol×K	516.37	Joback Method
cpg	128.69	J/mol×K	547.77	Joback Method
dvisc	0.0030601	Pa×s	203.42	Joback Method
dvisc	0.0017433	Pa×s	229.41	Joback Method
dvisc	0.0011136	Pa×s	255.39	Joback Method
dvisc	0.0007728	Pa×s	281.38	Joback Method
dvisc	0.0005704	Pa×s	307.37	Joback Method
dvisc	0.0004415	Pa×s	333.35	Joback Method
dvisc	0.0003546	Pa×s	359.34	Joback Method
hvapt	40.10	kJ/mol	354.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73466e+01
Coeff. B	-5.18459e+03
Coeff. C	1.41300e+01
Temperature range (K), min.	289.79
Temperature range (K), max.	416.66

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=C78955&Units=SI
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

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
ie:	Ionization energy
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