2-Propanone, 1,1-dichloro-

Other names:	1,1-Dichloro-2-propanone
	1,1-Dichloroacetone
	1,1-Dichloropropanone
	DCP
	Dichloromethyl methyl ketone
	«alpha»,«alpha»-Dichloroacetone
	Â«alphaÂ»,Â«alphaÂ»-Dichloroacetone
Inchi:	InChI=1S/C3H4Cl2O/c1-2(6)3(4)5/h3H,1H3
InchiKey:	CSVFWMMPUJDVKH-UHFFFAOYSA-N
Formula:	C3H4Cl2O
SMILES:	CC(=O)C(Cl)Cl
Mol. weight [g/mol]:	126.97
CAS:	513-88-2

Physical Properties

Property code	Value	Unit	Source
gf	-180.84	kJ/mol	Joback Method
hf	-254.59	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	37.40	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.379		Crippen Method
mcvol	79.180	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
rinpol	714.00		NIST Webbook
rinpol	707.20		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	707.00		NIST Webbook
tb	393.20	K	NIST Webbook
tb	390.70	K	NIST Webbook
tc	598.36	K	Joback Method
tf	218.34	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.45	J/mol×K	598.36	Joback Method
cpg	118.90	J/mol×K	396.33	Joback Method
cpg	124.33	J/mol×K	430.00	Joback Method
cpg	129.47	J/mol×K	463.67	Joback Method
cpg	134.35	J/mol×K	497.35	Joback Method
cpg	138.97	J/mol×K	531.02	Joback Method
cpg	143.33	J/mol×K	564.69	Joback Method
dvisc	0.0004135	Pa×s	396.33	Joback Method
dvisc	0.0050802	Pa×s	218.34	Joback Method
dvisc	0.0026045	Pa×s	248.01	Joback Method
dvisc	0.0015401	Pa×s	277.67	Joback Method
dvisc	0.0010079	Pa×s	307.34	Joback Method
dvisc	0.0007108	Pa×s	337.00	Joback Method
dvisc	0.0005304	Pa×s	366.66	Joback Method
hvapt	35.80	kJ/mol	337.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32647e+01
Coeff. B	-2.95648e+03
Coeff. C	-5.12670e+01
Temperature range (K), min.	274.15
Temperature range (K), max.	423.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Henry s Law Constants of Organic Compounds in Water and n-Octane at T = 298.2 K: https://www.doi.org/10.1021/je900711h

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=C513882&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