2-Propanone, 1,3-dichloro-

Other names:	1,3-Dichloro-2-propanone
	1,3-Dichloroacetone
	Bis(chloromethyl) ketone
	NSC 8745
	UN 2649
	s-Dichloroacetone
	sym-Dichloroacetone
	«alpha»,«alpha»'-Dichloroacetone
	«alpha»,«gamma»-Dichloroacetone
	Â«alphaÂ»,Â«alphaÂ»'-Dichloroacetone
	Â«alphaÂ»,Â«gammaÂ»-Dichloroacetone
Inchi:	InChI=1S/C3H4Cl2O/c4-1-3(6)2-5/h1-2H2
InchiKey:	SUNMBRGCANLOEG-UHFFFAOYSA-N
Formula:	C3H4Cl2O
SMILES:	O=C(CCl)CCl
Mol. weight [g/mol]:	126.97
CAS:	534-07-6

Physical Properties

Property code	Value	Unit	Source
gf	-178.40	kJ/mol	Joback Method
hf	-249.31	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	37.79	kJ/mol	Joback Method
ie	10.03 ± 0.02	eV	NIST Webbook
log10ws	-0.66		Crippen Method
logp	1.033		Crippen Method
mcvol	79.180	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
rinpol	866.00		NIST Webbook
rinpol	866.00		NIST Webbook
rinpol	870.00		NIST Webbook
tb	446.60	K	NIST Webbook
tc	593.93	K	Joback Method
tf	233.34	K	Joback Method
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.32	J/mol×K	593.93	Joback Method
cpg	118.84	J/mol×K	396.77	Joback Method
cpg	124.04	J/mol×K	429.63	Joback Method
cpg	128.97	J/mol×K	462.49	Joback Method
cpg	133.67	J/mol×K	495.35	Joback Method
cpg	138.11	J/mol×K	528.21	Joback Method
cpg	142.33	J/mol×K	561.07	Joback Method
dvisc	0.0004283	Pa×s	396.77	Joback Method
dvisc	0.0034494	Pa×s	233.34	Joback Method
dvisc	0.0020316	Pa×s	260.58	Joback Method
dvisc	0.0013226	Pa×s	287.82	Joback Method
dvisc	0.0009274	Pa×s	315.06	Joback Method
dvisc	0.0006881	Pa×s	342.29	Joback Method
dvisc	0.0005335	Pa×s	369.53	Joback Method
hvapt	49.60	kJ/mol	396.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58368e+01
Coeff. B	-4.45933e+03
Coeff. C	-4.91000e+01
Temperature range (K), min.	335.89
Temperature range (K), max.	472.78

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=C534076&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
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