Acetophenone, 2-chloro-

Other names:	(2-Chloro-1-oxoethyl)benzene
	1-Chloroacetophenone
	1-Phenyl-2-chloro-1-ethanone
	2-Chloro-1-phenylethanone
	2-Chloroacetophenone
	Benzoylmethyl chloride
	CAF
	CAP
	CN
	CN (lacrimator)
	Chemical mace
	Chloracetophenone
	Chloroacetophenone
	Chloromethyl phenyl ketone
	Ethanone, 2-chloro-1-phenyl-
	Mace
	Mace (lacrimator)
	NCI-C55107
	NSC 41666
	Phenacyl chloride
	Phenyl chloromethyl ketone
	Tear Gas
	UN 1697
	a-Chloroacetophenone
	«alpha»-Chloroacetophenone
	«alpha»-Phenacyl chloride
	«omega»-Chloroacetophenone
	Â«alphaÂ»-Chloroacetophenone
	Â«alphaÂ»-Phenacyl chloride
	Â«omegaÂ»-Chloroacetophenone
Inchi:	InChI=1S/C8H7ClO/c9-6-8(10)7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	IMACFCSSMIZSPP-UHFFFAOYSA-N
Formula:	C8H7ClO
SMILES:	O=C(CCl)c1ccccc1
Mol. weight [g/mol]:	154.59
CAS:	532-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-11.96	kJ/mol	Joback Method
hf	-100.24	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	46.81	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
ie	9.65 ± 0.01	eV	NIST Webbook
ie	9.44 ± 0.05	eV	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.108		Crippen Method
mcvol	113.630	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1283.00		NIST Webbook
rinpol	1230.20		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1283.00		NIST Webbook
ripol	2101.00		NIST Webbook
ripol	2083.40		NIST Webbook
ripol	2114.40		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2114.00		NIST Webbook
ripol	2113.00		NIST Webbook
ripol	2101.00		NIST Webbook
tb	517.70	K	NIST Webbook
tb	520.20	K	NIST Webbook
tc	728.04	K	Joback Method
tf	286.19	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.55	J/mol×K	500.42	Joback Method

cpg	227.58	J/mol×K	538.36	Joback Method
cpg	237.84	J/mol×K	576.29	Joback Method
cpg	247.37	J/mol×K	614.23	Joback Method
cpg	256.20	J/mol×K	652.17	Joback Method
cpg	264.36	J/mol×K	690.11	Joback Method
cpg	271.90	J/mol×K	728.04	Joback Method
dvisc	0.0016339	Pa×s	321.89	Joback Method
dvisc	0.0029389	Pa×s	286.19	Joback Method
dvisc	0.0010214	Pa×s	357.60	Joback Method
dvisc	0.0006953	Pa×s	393.30	Joback Method
dvisc	0.0005047	Pa×s	429.01	Joback Method
dvisc	0.0003848	Pa×s	464.71	Joback Method
dvisc	0.0003049	Pa×s	500.42	Joback Method
hsubt	90.70	kJ/mol	300.50	NIST Webbook
hvapt	87.70	kJ/mol	298.15	Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	1.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C532274&Units=SI

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

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

Experimental thermochemical study of 2-chloroacetophenone and 2,4'-dichloroacetophenone: https://www.doi.org/10.1016/j.jct.2013.07.026

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume