Ethanone, 1-(4-chlorophenyl)-

Other names:	1-(4-Chlorophenyl)ethanone
	1-acetyl-4-chlorobenzene
	4'-Chloroacetophenone
	4-Chloroacetophenone
	Acetophenone, 4'-chloro-
	USAF do-1
	p-Chloroacetophenone
Inchi:	InChI=1S/C8H7ClO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,1H3
InchiKey:	BUZYGTVTZYSBCU-UHFFFAOYSA-N
Formula:	C8H7ClO
SMILES:	CC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	154.59
CAS:	99-91-2

Physical Properties

Property code	Value	Unit	Source
affp	856.60	kJ/mol	NIST Webbook
basg	824.80	kJ/mol	NIST Webbook
ea	0.57 ± 0.01	eV	NIST Webbook
ea	0.55 ± 0.09	eV	NIST Webbook
ea	0.58 ± 0.09	eV	NIST Webbook
gf	-21.59	kJ/mol	Joback Method
hf	-111.71	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
ie	9.64 ± 0.15	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.60 ± 0.05	eV	NIST Webbook
ie	9.47 ± 0.05	eV	NIST Webbook
ie	9.60 ± 0.10	eV	NIST Webbook
ie	9.63	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.543		Crippen Method
mcvol	113.630	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
rinpol	1204.00		NIST Webbook

rinpol	1204.00		NIST Webbook
tb	505.20	K	NIST Webbook
tc	734.29	K	Joback Method
tf	291.55 ± 0.05	K	NIST Webbook
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.97	J/mol×K	619.84	Joback Method
cpg	270.00	J/mol×K	734.29	Joback Method
cpg	262.58	J/mol×K	696.14	Joback Method
cpg	254.59	J/mol×K	657.99	Joback Method
cpg	216.19	J/mol×K	505.40	Joback Method
cpg	226.80	J/mol×K	543.55	Joback Method
cpg	236.72	J/mol×K	581.70	Joback Method
dvisc	0.0002938	Pa×s	505.40	Joback Method
dvisc	0.0006184	Pa×s	402.06	Joback Method
dvisc	0.0004640	Pa×s	436.50	Joback Method
dvisc	0.0003631	Pa×s	470.95	Joback Method
dvisc	0.0021784	Pa×s	298.71	Joback Method
dvisc	0.0013126	Pa×s	333.16	Joback Method
dvisc	0.0008697	Pa×s	367.61	Joback Method
hvapt	50.70	kJ/mol	440.00	NIST Webbook
hvapt	54.00	kJ/mol	513.50	NIST Webbook
rhol	1188.90	kg/m3	298.15	Ultrasonic Studies of Binary Mixtures of Some Aromatic Ketones with N-Methyl-acetamide at 308.15 K
speedsl	1390.00	m/s	308.15	Ultrasonic studies on binary mixtures of some aromatic ketones with acetonitrile at T = 308.15 K

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67680e+01
Coeff. B	-4.95985e+03
Coeff. C	-7.91500e+01
Temperature range (K), min.	380.10
Temperature range (K), max.	512.08

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
308.15	101.30	0.0022930

Reference *https://www.doi.org/10.1016/j.jct.2005.05.006*

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Ultrasonic studies on binary mixtures of some aromatic ketones with acetonitrile at T = 308.15 K:	https://www.doi.org/10.1016/j.jct.2006.01.009
THERMODYNAMIC PROPERTIES OF DONOR ACCEPTOR COMPLEXES OF TERTIARY AMINE WITH ARYL KETONES IN HEXANE MEDIUM:	https://www.doi.org/10.1016/j.tca.2012.02.018
The Yaws Handbook of Vapor Pressures	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Density and viscosity of binary liquid systems of N-methylacetamide with aromatic ketones at T = 308.15 K:	https://www.doi.org/10.1016/j.jct.2005.05.006
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99912&Units=SI
Ultrasonic Studies of Binary Mixtures of Some Aromatic Ketones with N-Methyl-acetamide at 308.15 K:	https://www.doi.org/10.1021/je040008e

Legend

affp:	Proton affinity
basg:	Gas basicity

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume