Ethanone, 1-(2-chlorophenyl)-

Other names:	Acetophenone, 2'-chloro- o-Chloroacetophenone 2'-Chloroacetophenone o-Chloroacetophonone 1-(2-Chlorophenyl)ethanone 2-Chlorophenyl methyl ketone Methyl 2-chlorophenyl ketone o-Chlorophenyl methyl ketone 2-Chloro-1-acetylbenzene NSC 405474
Inchi:	InChI=1S/C8H7ClO/c1-6(10)7-4-2-3-5-8(7)9/h2-5H,1H3
InchiKey:	ZDOYHCIRUPHUHN-UHFFFAOYSA-N
Formula:	C8H7ClO
SMILES:	CC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	154.59
CAS:	2142-68-9

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-2.82		Crippen Method
logp	2.543		Crippen Method
mcvol	113.630	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
rinpol	1193.80		NIST Webbook
rinpol	1251.10		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1183.50		NIST Webbook
rinpol	1236.60		NIST Webbook
rinpol	1240.70		NIST Webbook
rinpol	1245.40		NIST Webbook
tb	505.40	K	Joback Method
tc	734.29	K	Joback Method
tf	298.71	K	Joback Method

vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	245.97	J/mol×K	619.84	Joback Method
cpg	254.59	J/mol×K	657.99	Joback Method
cpg	262.58	J/mol×K	696.14	Joback Method
cpg	270.00	J/mol×K	734.29	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
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	0.0002938	Pa×s	505.40	Joback Method

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=C2142689&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume