Acetophenone, 3'-chloro-

Other names: Ethanone, 1-(3-chlorophenyl)-
m-Chloroacetophenone
3'-Chloroacetophenone
3'-Chloroacetylphenone
1-(3-Chlorophenyl)ethanone
Inchi: InChI=1S/C8H7ClO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3
InchiKey: UUWJBXKHMMQDED-UHFFFAOYSA-N
Formula: C8H7ClO
SMILES: CC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 154.59
CAS: 99-02-5

Physical Properties

Property code	Value	Unit	Source
affp	846.90	kJ/mol	NIST Webbook
basg	815.10	kJ/mol	NIST Webbook
ea	0.62 ± 0.09	eV	NIST Webbook
ea	0.58 ± 0.09	eV	NIST Webbook
ea	0.58 ± 0.01	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	9.50 ± 0.10	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
tb	501.20	K	NIST Webbook
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

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=C99025&Units=SI

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume