Ethanone, 1-(3,4-dichlorophenyl)-

Other names:	1-(3,4-dichlorophenyl)ethan-1-one
	3',4'-dichloroacetophenone
	3,4-Dichloroacetophenone
	Acetophenone, 3',4'-dichloro-
Inchi:	InChI=1S/C8H6Cl2O/c1-5(11)6-2-3-7(9)8(10)4-6/h2-4H,1H3
InchiKey:	WBPAOUHWPONFEQ-UHFFFAOYSA-N
Formula:	C8H6Cl2O
SMILES:	CC(=O)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	189.04
CAS:	2642-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-43.15	kJ/mol	Joback Method
hf	-138.92	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	52.52	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.196		Crippen Method
mcvol	125.870	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	547.81	K	Joback Method
tc	782.69	K	Joback Method
tf	341.15	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.65	J/mol×K	547.81	Joback Method
cpg	247.15	J/mol×K	586.96	Joback Method
cpg	256.00	J/mol×K	626.10	Joback Method
cpg	264.24	J/mol×K	665.25	Joback Method
cpg	271.89	J/mol×K	704.39	Joback Method

cpg	278.97	J/mol×K	743.54	Joback Method
cpg	285.50	J/mol×K	782.69	Joback Method
dvisc	0.0016858	Pa×s	341.15	Joback Method
dvisc	0.0011014	Pa×s	375.59	Joback Method
dvisc	0.0007729	Pa×s	410.04	Joback Method
dvisc	0.0005730	Pa×s	444.48	Joback Method
dvisc	0.0004435	Pa×s	478.92	Joback Method
dvisc	0.0003553	Pa×s	513.37	Joback Method
dvisc	0.0002927	Pa×s	547.81	Joback Method
hvapt	90.80	kJ/mol	298.15	Thermochemical study of some dichloroacetophenone isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	1.60	NIST Webbook

Sources

Thermochemical study of some dichloroacetophenone isomers:	https://www.doi.org/10.1016/j.jct.2010.09.005
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=C2642639&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

hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume