3-Chloro-4-fluoroacetophenone

Other names: Ethanone, 1-(3-chloro-4-fluorophenyl)-
3'-chloro-4'-fluoroacetophenone
Inchi: InChI=1S/C8H6ClFO/c1-5(11)6-2-3-8(10)7(9)4-6/h2-4H,1H3
InchiKey: PCJPESKRPOTNGU-UHFFFAOYSA-N
Formula: C8H6ClFO
SMILES: CC(=O)c1ccc(F)c(Cl)c1
Mol. weight [g/mol]: 172.58
CAS: 2923-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-226.03	kJ/mol	Joback Method
hf	-319.29	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	47.32	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.682		Crippen Method
mcvol	115.400	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	509.65	K	Joback Method
tc	727.74	K	Joback Method
tf	311.82	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.08	J/mol×K	509.65	Joback Method
cpg	233.76	J/mol×K	546.00	Joback Method
cpg	242.86	J/mol×K	582.35	Joback Method
cpg	251.40	J/mol×K	618.69	Joback Method
cpg	259.39	J/mol×K	655.04	Joback Method
cpg	266.86	J/mol×K	691.39	Joback Method
cpg	273.82	J/mol×K	727.74	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=C2923662&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume