«alpha»-Chloro-4'-fluoropropiophenone

Inchi: InChI=1S/C9H8ClFO/c1-6(10)9(12)7-2-4-8(11)5-3-7/h2-6H,1H3
InchiKey: AGQLOTJUTCKLOE-UHFFFAOYSA-N
Formula: C9H8ClFO
SMILES: CC(Cl)C(=O)c1ccc(F)cc1
Mol. weight [g/mol]: 186.61
CAS: 81112-09-6

Physical Properties

Property code	Value	Unit	Source
gf	-210.42	kJ/mol	Joback Method
hf	-333.74	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	48.49	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.636		Crippen Method
mcvol	129.490	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	527.11	K	Joback Method
tc	745.30	K	Joback Method
tf	295.57	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.15	J/mol×K	527.11	Joback Method
cpg	278.62	J/mol×K	563.48	Joback Method
cpg	289.35	J/mol×K	599.84	Joback Method
cpg	299.37	J/mol×K	636.21	Joback Method
cpg	308.71	J/mol×K	672.57	Joback Method
cpg	317.40	J/mol×K	708.94	Joback Method
cpg	325.46	J/mol×K	745.30	Joback Method

Sources

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=C81112096&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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