2-Chloro-6-fluorophenol, methyl ether

Inchi: InChI=1S/C7H6ClFO/c1-10-7-5(8)3-2-4-6(7)9/h2-4H,1H3
InchiKey: QASFEHCRPLPGES-UHFFFAOYSA-N
Formula: C7H6ClFO
SMILES: COc1c(F)cccc1Cl
Mol. weight [g/mol]: 160.57

Physical Properties

Property code	Value	Unit	Source
gf	-210.53	kJ/mol	Joback Method
hf	-318.29	kJ/mol	Joback Method
hfus	15.61	kJ/mol	Joback Method
hvap	40.75	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.488		Crippen Method
mcvol	105.610	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1054.20		NIST Webbook
tb	455.32	K	Joback Method
tc	664.31	K	Joback Method
tf	272.85	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.23	J/mol×K	455.32	Joback Method
cpg	202.33	J/mol×K	490.15	Joback Method
cpg	211.02	J/mol×K	524.98	Joback Method
cpg	219.31	J/mol×K	559.82	Joback Method
cpg	227.19	J/mol×K	594.65	Joback Method
cpg	234.66	J/mol×K	629.48	Joback Method
cpg	241.74	J/mol×K	664.31	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=U352539&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume