2-Chloro-6-fluorophenol

Other names: Phenol, 2-chloro-6-fluoro-
Inchi: InChI=1S/C6H4ClFO/c7-4-2-1-3-5(8)6(4)9/h1-3,9H
InchiKey: QIAQIYQASAWZPP-UHFFFAOYSA-N
Formula: C6H4ClFO
SMILES: Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 146.55
CAS: 2040-90-6

Physical Properties

Property code	Value	Unit	Source
gf	-258.94	kJ/mol	Joback Method
hf	-331.27	kJ/mol	Joback Method
hfus	18.01	kJ/mol	Joback Method
hvap	48.47	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.185		Crippen Method
mcvol	91.520	ml/mol	McGowan Method
pc	5022.80	kPa	Joback Method
rinpol	1061.70		NIST Webbook
tb	485.66	K	Joback Method
tc	713.84	K	Joback Method
tf	338.55	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.28	J/mol×K	485.66	Joback Method
cpg	182.99	J/mol×K	523.69	Joback Method
cpg	190.04	J/mol×K	561.72	Joback Method
cpg	196.47	J/mol×K	599.75	Joback Method
cpg	202.38	J/mol×K	637.78	Joback Method
cpg	207.82	J/mol×K	675.81	Joback Method
cpg	212.86	J/mol×K	713.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040906&Units=SI
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

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