2-Chloro-4-fluorothiophenol

Inchi: InChI=1S/C6H4ClFS/c7-5-3-4(8)1-2-6(5)9/h1-3,9H
InchiKey: KUAPPJSILOMQPC-UHFFFAOYSA-N
Formula: C6H4ClFS
SMILES: Fc1ccc(S)c(Cl)c1
Mol. weight [g/mol]: 162.61
CAS: 175277-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-84.56	kJ/mol	Joback Method
hf	-126.95	kJ/mol	Joback Method
hfus	15.88	kJ/mol	Joback Method
hvap	42.86	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.768		Crippen Method
mcvol	102.000	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	472.88	K	Joback Method
tc	711.66	K	Joback Method
tf	275.81	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.49	J/mol×K	472.88	Joback Method
cpg	181.75	J/mol×K	512.68	Joback Method
cpg	189.46	J/mol×K	552.47	Joback Method
cpg	196.65	J/mol×K	592.27	Joback Method
cpg	203.33	J/mol×K	632.07	Joback Method
cpg	209.53	J/mol×K	671.87	Joback Method
cpg	215.27	J/mol×K	711.66	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=C175277993&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