2-Chloro-4-fluorobenzonitrile

Other names: Benzonitrile, 2-chloro-4-fluoro-
Inchi: InChI=1S/C7H3ClFN/c8-7-3-6(9)2-1-5(7)4-10/h1-3H
InchiKey: PGKPNNMOFHNZJX-UHFFFAOYSA-N
Formula: C7H3ClFN
SMILES: N#Cc1ccc(F)cc1Cl
Mol. weight [g/mol]: 155.56
CAS: 60702-69-4

Physical Properties

Property code	Value	Unit	Source
gf	27.65	kJ/mol	Joback Method
hf	-21.19	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	48.82	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.351		Crippen Method
mcvol	101.120	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	534.98	K	Joback Method
tc	765.78	K	Joback Method
tf	315.61	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.39	J/mol×K	534.98	Joback Method
cpg	195.62	J/mol×K	573.45	Joback Method
cpg	202.36	J/mol×K	611.91	Joback Method
cpg	208.65	J/mol×K	650.38	Joback Method
cpg	214.48	J/mol×K	688.85	Joback Method
cpg	219.89	J/mol×K	727.31	Joback Method
cpg	224.89	J/mol×K	765.78	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=C60702694&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