3-Chloro-2-fluorobenzonitrile

Other names: 3-Chloro-2-fluorobenzonitrile
Inchi: InChI=1S/C7H3ClFN/c8-6-3-1-2-5(4-10)7(6)9/h1-3H
InchiKey: CHKLNKWJIDQKFV-UHFFFAOYSA-N
Formula: C7H3ClFN
SMILES: N#Cc1cccc(Cl)c1F
Mol. weight [g/mol]: 155.56

Physical Properties

Property code	Value	Unit	Source
hf	21.63	kJ/mol	Cheméo Relay (1.0)
hfus	15.93	kJ/mol	Joback Method
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-2.80		Cheméo Relay (1.0)
logp	2.351		Crippen Method
mcvol	101.120	ml/mol	McGowan Method
tb	485.18	K	Cheméo Relay (1.0)
tf	335.29	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94087408&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point