3-Chloro-2-fluorobenzamide

Inchi: InChI=1S/C7H5ClFNO/c8-5-3-1-2-4(6(5)9)7(10)11/h1-3H,(H2,10,11)
InchiKey: KGTCFPJGIYHDRZ-UHFFFAOYSA-N
Formula: C7H5ClFNO
SMILES: NC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 173.57
CAS: 104326-94-5

Physical Properties

Property code	Value	Unit	Source
gf	-168.00	kJ/mol	Joback Method
hf	-264.86	kJ/mol	Joback Method
hfus	21.22	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.578		Crippen Method
mcvol	111.290	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	559.30	K	Joback Method
tc	790.89	K	Joback Method
tf	383.81	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.32	J/mol×K	559.30	Joback Method
cpg	237.92	J/mol×K	597.90	Joback Method
cpg	245.92	J/mol×K	636.50	Joback Method
cpg	253.35	J/mol×K	675.09	Joback Method
cpg	260.23	J/mol×K	713.69	Joback Method
cpg	266.58	J/mol×K	752.29	Joback Method
cpg	272.42	J/mol×K	790.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104326945&Units=SI

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