2-Chloro-4-fluorobenzaldehyde

Other names: Benzaldehyde, 2-chloro-4-fluoro-
Inchi: InChI=1S/C7H4ClFO/c8-7-3-6(9)2-1-5(7)4-10/h1-4H
InchiKey: KMQWNQKESAHDKD-UHFFFAOYSA-N
Formula: C7H4ClFO
SMILES: O=Cc1ccc(F)cc1Cl
Mol. weight [g/mol]: 158.56
CAS: 84194-36-5

Physical Properties

Property code	Value	Unit	Source
gf	-205.05	kJ/mol	Joback Method
hf	-271.65	kJ/mol	Joback Method
hfus	16.71	kJ/mol	Joback Method
hvap	45.06	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.292		Crippen Method
mcvol	101.310	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	481.56	K	Joback Method
tc	697.48	K	Joback Method
tf	292.62	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.94	J/mol×K	481.56	Joback Method
cpg	194.05	J/mol×K	517.55	Joback Method
cpg	201.67	J/mol×K	553.53	Joback Method
cpg	208.82	J/mol×K	589.52	Joback Method
cpg	215.51	J/mol×K	625.51	Joback Method
cpg	221.75	J/mol×K	661.50	Joback Method
cpg	227.57	J/mol×K	697.48	Joback Method

Sources

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=C84194365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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