3-Chloro-2-fluorobenzoic acid, ethyl ester

Inchi: InChI=1S/C9H8ClFO2/c1-2-13-9(12)6-4-3-5-7(10)8(6)11/h3-5H,2H2,1H3
InchiKey: MCNAALBXEILIIB-UHFFFAOYSA-N
Formula: C9H8ClFO2
SMILES: CCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 202.61

Physical Properties

Property code	Value	Unit	Source
gf	-322.61	kJ/mol	Joback Method
hf	-472.15	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.656		Crippen Method
mcvol	135.360	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	1363.00		NIST Webbook
rinpol	1363.00		NIST Webbook
tb	554.95	K	Joback Method
tc	767.13	K	Joback Method
tf	345.32	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.39	J/mol×K	554.95	Joback Method
cpg	299.04	J/mol×K	590.31	Joback Method
cpg	309.11	J/mol×K	625.68	Joback Method
cpg	318.61	J/mol×K	661.04	Joback Method
cpg	327.55	J/mol×K	696.40	Joback Method
cpg	335.92	J/mol×K	731.76	Joback Method
cpg	343.75	J/mol×K	767.13	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=U338877&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume