3-Chloro-2-fluorobenzoic acid, methyl ester

Inchi: InChI=1S/C8H6ClFO2/c1-12-8(11)5-3-2-4-6(9)7(5)10/h2-4H,1H3
InchiKey: WBTHSEQMJLZATD-UHFFFAOYSA-N
Formula: C8H6ClFO2
SMILES: COC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 188.58

Physical Properties

Property code	Value	Unit	Source
gf	-331.03	kJ/mol	Joback Method
hf	-451.51	kJ/mol	Joback Method
hfus	19.80	kJ/mol	Joback Method
hvap	49.73	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.266		Crippen Method
mcvol	121.270	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
tb	532.07	K	Joback Method
tc	747.81	K	Joback Method
tf	334.05	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.16	J/mol×K	532.07	Joback Method
cpg	254.72	J/mol×K	568.03	Joback Method
cpg	263.75	J/mol×K	603.98	Joback Method
cpg	272.28	J/mol×K	639.94	Joback Method
cpg	280.31	J/mol×K	675.90	Joback Method
cpg	287.83	J/mol×K	711.85	Joback Method
cpg	294.85	J/mol×K	747.81	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=U357736&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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