3-Chloro-2-fluorobenzoic acid, 2-methoxyethyl ester

Inchi: InChI=1S/C10H10ClFO3/c1-14-5-6-15-10(13)7-3-2-4-8(11)9(7)12/h2-4H,5-6H2,1H3
InchiKey: RNNNNESXXKWNTO-UHFFFAOYSA-N
Formula: C10H10ClFO3
SMILES: COCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 232.64

Physical Properties

Property code	Value	Unit	Source
gf	-419.19	kJ/mol	Joback Method
hf	-625.01	kJ/mol	Joback Method
hfus	26.17	kJ/mol	Joback Method
hvap	56.59	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.282		Crippen Method
mcvol	155.320	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1599.00		NIST Webbook
tb	600.25	K	Joback Method
tc	806.83	K	Joback Method
tf	378.82	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.72	J/mol×K	600.25	Joback Method
cpg	368.19	J/mol×K	634.68	Joback Method
cpg	379.06	J/mol×K	669.11	Joback Method
cpg	389.32	J/mol×K	703.54	Joback Method
cpg	398.98	J/mol×K	737.97	Joback Method
cpg	408.02	J/mol×K	772.40	Joback Method
cpg	416.44	J/mol×K	806.83	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=U357326&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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