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

Inchi: InChI=1S/C11H12ClFO3/c1-2-15-6-7-16-11(14)8-4-3-5-9(12)10(8)13/h3-5H,2,6-7H2,1H3

InchiKey: MJIQDRXIQVTIFN-UHFFFAOYSA-N

Formula: C11H12ClFO3

SMILES: CCOCCOC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 246.66

Physical Properties

Property code	Value	Unit	Source
gf	-410.77	kJ/mol	Joback Method
hf	-645.65	kJ/mol	Joback Method
hfus	28.76	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.672		Crippen Method
mcvol	169.410	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	623.13	K	Joback Method
tc	826.65	K	Joback Method
tf	390.09	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.45	J/mol×K	623.13	Joback Method
cpg	416.72	J/mol×K	657.05	Joback Method
cpg	428.33	J/mol×K	690.97	Joback Method
cpg	439.28	J/mol×K	724.89	Joback Method
cpg	449.58	J/mol×K	758.81	Joback Method
cpg	459.21	J/mol×K	792.73	Joback Method
cpg	468.18	J/mol×K	826.65	Joback Method

Sources

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=U357329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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