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

Inchi: InChI=1S/C15H12ClFO2/c1-2-10-5-3-6-11(9-10)19-15(18)12-7-4-8-13(16)14(12)17/h3-9H

InchiKey: QVKNACNKMFVVOS-UHFFFAOYSA-N

Formula: C15H12ClFO2

SMILES: CCc1cccc(OC(=O)c2cccc(Cl)c2F)c1

Mol. weight [g/mol]: 278.71

Physical Properties

Property code	Value	Unit	Source
gf	-169.31	kJ/mol	Joback Method
hf	-370.93	kJ/mol	Joback Method
hfus	31.59	kJ/mol	Joback Method
hvap	68.25	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.261		Crippen Method
mcvol	196.140	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	723.89	K	Joback Method
tc	956.04	K	Joback Method
tf	451.88	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.53	J/mol×K	723.89	Joback Method
cpg	509.80	J/mol×K	762.58	Joback Method
cpg	522.05	J/mol×K	801.27	Joback Method
cpg	533.29	J/mol×K	839.97	Joback Method
cpg	543.56	J/mol×K	878.66	Joback Method
cpg	552.90	J/mol×K	917.35	Joback Method
cpg	561.34	J/mol×K	956.04	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=U360586&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