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

Inchi: InChI=1S/C15H20ClFO2/c1-3-5-7-11(4-2)10-19-15(18)12-8-6-9-13(16)14(12)17/h6,8-9,1

InchiKey: SKMMTQPNCQYOFR-UHFFFAOYSA-N

Formula: C15H20ClFO2

SMILES: CCCCC(CC)COC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 286.77

Physical Properties

Property code	Value	Unit	Source
gf	-274.53	kJ/mol	Joback Method
hf	-601.27	kJ/mol	Joback Method
hfus	34.41	kJ/mol	Joback Method
hvap	64.92	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.852		Crippen Method
mcvol	219.900	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	1912.00		NIST Webbook
tb	691.79	K	Joback Method
tc	890.33	K	Joback Method
tf	397.94	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.43	J/mol×K	691.79	Joback Method
cpg	598.49	J/mol×K	724.88	Joback Method
cpg	612.68	J/mol×K	757.97	Joback Method
cpg	626.03	J/mol×K	791.06	Joback Method
cpg	638.54	J/mol×K	824.15	Joback Method
cpg	650.25	J/mol×K	857.24	Joback Method
cpg	661.17	J/mol×K	890.33	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=U357725&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