3-Chloro-2-fluorobenzoic acid, octyl ester

Inchi: InChI=1S/C15H20ClFO2/c1-2-3-4-5-6-7-11-19-15(18)12-9-8-10-13(16)14(12)17/h8-10H,
InchiKey: FYYLECUEXKEEKF-UHFFFAOYSA-N
Formula: C15H20ClFO2
SMILES: CCCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 286.77

Physical Properties

Property code	Value	Unit	Source
gf	-272.09	kJ/mol	Joback Method
hf	-595.99	kJ/mol	Joback Method
hfus	37.93	kJ/mol	Joback Method
hvap	65.31	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.996		Crippen Method
mcvol	219.900	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	692.23	K	Joback Method
tc	887.63	K	Joback Method
tf	412.94	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.92	J/mol×K	692.23	Joback Method
cpg	597.72	J/mol×K	724.80	Joback Method
cpg	611.68	J/mol×K	757.36	Joback Method
cpg	624.83	J/mol×K	789.93	Joback Method
cpg	637.19	J/mol×K	822.50	Joback Method
cpg	648.78	J/mol×K	855.06	Joback Method
cpg	659.61	J/mol×K	887.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338885&Units=SI
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

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