3-Chloro-2-fluorobenzoic acid, nonyl ester

Inchi: InChI=1S/C16H22ClFO2/c1-2-3-4-5-6-7-8-12-20-16(19)13-10-9-11-14(17)15(13)18/h9-11
InchiKey: YEPDZSCGKHKQML-UHFFFAOYSA-N
Formula: C16H22ClFO2
SMILES: CCCCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 300.80

Physical Properties

Property code	Value	Unit	Source
gf	-263.67	kJ/mol	Joback Method
hf	-616.63	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	67.53	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.387		Crippen Method
mcvol	233.990	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	715.11	K	Joback Method
tc	908.91	K	Joback Method
tf	424.21	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.96	J/mol×K	715.11	Joback Method
cpg	652.18	J/mol×K	747.41	Joback Method
cpg	666.53	J/mol×K	779.71	Joback Method
cpg	680.03	J/mol×K	812.01	Joback Method
cpg	692.72	J/mol×K	844.31	Joback Method
cpg	704.61	J/mol×K	876.61	Joback Method
cpg	715.72	J/mol×K	908.91	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=U338886&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