3-Chloro-2-fluorobenzoic acid, undecyl ester

Inchi: InChI=1S/C18H26ClFO2/c1-2-3-4-5-6-7-8-9-10-14-22-18(21)15-12-11-13-16(19)17(15)20
InchiKey: NVFSTLBFRMMBBJ-UHFFFAOYSA-N
Formula: C18H26ClFO2
SMILES: CCCCCCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 328.85

Physical Properties

Property code	Value	Unit	Source
gf	-246.83	kJ/mol	Joback Method
hf	-657.91	kJ/mol	Joback Method
hfus	45.70	kJ/mol	Joback Method
hvap	71.99	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.167		Crippen Method
mcvol	262.170	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	2312.00		NIST Webbook
rinpol	2312.00		NIST Webbook
tb	760.87	K	Joback Method
tc	952.94	K	Joback Method
tf	446.75	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.50	J/mol×K	760.87	Joback Method
cpg	764.43	J/mol×K	792.88	Joback Method
cpg	779.43	J/mol×K	824.89	Joback Method
cpg	793.53	J/mol×K	856.90	Joback Method
cpg	806.75	J/mol×K	888.92	Joback Method
cpg	819.13	J/mol×K	920.93	Joback Method
cpg	830.68	J/mol×K	952.94	Joback Method

Sources

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=U338888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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