3-Chloro-2-fluorobenzoic acid, decyl ester

Inchi: InChI=1S/C17H24ClFO2/c1-2-3-4-5-6-7-8-9-13-21-17(20)14-11-10-12-15(18)16(14)19/h1
InchiKey: LAXTXOAECWTBSP-UHFFFAOYSA-N
Formula: C17H24ClFO2
SMILES: CCCCCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 314.82

Physical Properties

Property code	Value	Unit	Source
gf	-255.25	kJ/mol	Joback Method
hf	-637.27	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	69.76	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.777		Crippen Method
mcvol	248.080	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	737.99	K	Joback Method
tc	930.67	K	Joback Method
tf	435.48	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.18	J/mol×K	737.99	Joback Method
cpg	707.77	J/mol×K	770.10	Joback Method
cpg	722.46	J/mol×K	802.22	Joback Method
cpg	736.28	J/mol×K	834.33	Joback Method
cpg	749.25	J/mol×K	866.44	Joback Method
cpg	761.40	J/mol×K	898.56	Joback Method
cpg	772.75	J/mol×K	930.67	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=U338887&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