3-Chloro2-fluorobenzoic acid, 3-dodecyl ester

Inchi: InChI=1S/C19H28ClFO2/c1-3-5-6-7-8-9-10-12-15(4-2)23-19(22)16-13-11-14-17(20)18(1
InchiKey: XFIDLLHSWWZOJA-UHFFFAOYSA-N
Formula: C19H28ClFO2
SMILES: CCCCCCCCCC(CC)OC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 342.88

Physical Properties

Property code	Value	Unit	Source
gf	-240.85	kJ/mol	Joback Method
hf	-683.83	kJ/mol	Joback Method
hfus	44.77	kJ/mol	Joback Method
hvap	73.82	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.555		Crippen Method
mcvol	276.260	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	783.31	K	Joback Method
tc	977.36	K	Joback Method
tf	443.02	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.36	J/mol×K	783.31	Joback Method
cpg	822.78	J/mol×K	815.65	Joback Method
cpg	838.21	J/mol×K	847.99	Joback Method
cpg	852.68	J/mol×K	880.33	Joback Method
cpg	866.22	J/mol×K	912.68	Joback Method
cpg	878.86	J/mol×K	945.02	Joback Method
cpg	890.62	J/mol×K	977.36	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=U338638&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