3-Chloro2-fluorobenzoic acid, 2-tetradecyl ester

Inchi: InChI=1S/C21H32ClFO2/c1-3-4-5-6-7-8-9-10-11-12-14-17(2)25-21(24)18-15-13-16-19(22

InchiKey: SJIDFYGXVIUOFZ-UHFFFAOYSA-N

Formula: C21H32ClFO2

SMILES: CCCCCCCCCCCCC(C)OC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 370.93

Physical Properties

Property code	Value	Unit	Source
gf	-224.01	kJ/mol	Joback Method
hf	-725.11	kJ/mol	Joback Method
hfus	49.95	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.335		Crippen Method
mcvol	304.440	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook
tb	829.07	K	Joback Method
tc	1024.31	K	Joback Method
tf	465.56	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.79	J/mol×K	829.07	Joback Method
cpg	940.76	J/mol×K	861.61	Joback Method
cpg	956.68	J/mol×K	894.15	Joback Method
cpg	971.57	J/mol×K	926.69	Joback Method
cpg	985.47	J/mol×K	959.23	Joback Method
cpg	998.41	J/mol×K	991.77	Joback Method
cpg	1010.42	J/mol×K	1024.31	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=U338645&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