3-Chloro2-fluorobenzoic acid, 3-pentadecyl ester

Inchi: InChI=1S/C22H34ClFO2/c1-3-5-6-7-8-9-10-11-12-13-15-18(4-2)26-22(25)19-16-14-17-20

InchiKey: NCKVIIVNUUTDCG-UHFFFAOYSA-N

Formula: C22H34ClFO2

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

Mol. weight [g/mol]: 384.96

Physical Properties

Property code	Value	Unit	Source
gf	-215.59	kJ/mol	Joback Method
hf	-745.75	kJ/mol	Joback Method
hfus	52.54	kJ/mol	Joback Method
hvap	80.50	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.726		Crippen Method
mcvol	318.530	ml/mol	McGowan Method
pc	1070.06	kPa	Joback Method
rinpol	2602.00		NIST Webbook
rinpol	2602.00		NIST Webbook
tb	851.95	K	Joback Method
tc	1048.82	K	Joback Method
tf	476.83	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.73	J/mol×K	851.95	Joback Method
cpg	1000.99	J/mol×K	884.76	Joback Method
cpg	1017.15	J/mol×K	917.57	Joback Method
cpg	1032.24	J/mol×K	950.39	Joback Method
cpg	1046.31	J/mol×K	983.20	Joback Method
cpg	1059.38	J/mol×K	1016.01	Joback Method
cpg	1071.50	J/mol×K	1048.82	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=U338650&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