3-Chloro2-fluorobenzoic acid, 4-tridecyl ester

Inchi: InChI=1S/C20H30ClFO2/c1-3-5-6-7-8-9-10-13-16(12-4-2)24-20(23)17-14-11-15-18(21)19

InchiKey: ZFVRGZWETCIWAG-UHFFFAOYSA-N

Formula: C20H30ClFO2

SMILES: CCCCCCCCCC(CCC)OC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 356.90

Physical Properties

Property code	Value	Unit	Source
gf	-232.43	kJ/mol	Joback Method
hf	-704.47	kJ/mol	Joback Method
hfus	47.36	kJ/mol	Joback Method
hvap	76.05	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.945		Crippen Method
mcvol	290.350	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	806.19	K	Joback Method
tc	1000.51	K	Joback Method
tf	454.29	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.64	J/mol×K	806.19	Joback Method
cpg	881.34	J/mol×K	838.58	Joback Method
cpg	897.01	J/mol×K	870.96	Joback Method
cpg	911.70	J/mol×K	903.35	Joback Method
cpg	925.42	J/mol×K	935.73	Joback Method
cpg	938.22	J/mol×K	968.12	Joback Method
cpg	950.12	J/mol×K	1000.51	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=U338644&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