3-Chloro-2-fluorobenzoic acid, tridecyl ester

Inchi: InChI=1S/C20H30ClFO2/c1-2-3-4-5-6-7-8-9-10-11-12-16-24-20(23)17-14-13-15-18(21)19
InchiKey: LPBHSXJAFYJXGC-UHFFFAOYSA-N
Formula: C20H30ClFO2
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 356.90

Physical Properties

Property code	Value	Unit	Source
gf	-229.99	kJ/mol	Joback Method
hf	-699.19	kJ/mol	Joback Method
hfus	50.88	kJ/mol	Joback Method
hvap	76.44	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.947		Crippen Method
mcvol	290.350	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	806.63	K	Joback Method
tc	999.22	K	Joback Method
tf	469.29	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	864.12	J/mol×K	806.63	Joback Method
cpg	880.68	J/mol×K	838.73	Joback Method
cpg	896.23	J/mol×K	870.83	Joback Method
cpg	910.83	J/mol×K	902.92	Joback Method
cpg	924.49	J/mol×K	935.02	Joback Method
cpg	937.24	J/mol×K	967.12	Joback Method
cpg	949.12	J/mol×K	999.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338890&Units=SI
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

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