3-Chloro-2-fluorobenzoic acid, neopentyl ester

Inchi: InChI=1S/C12H14ClFO2/c1-12(2,3)7-16-11(15)8-5-4-6-9(13)10(8)14/h4-6H,7H2,1-3H3
InchiKey: RNIWQEWNUXFRAW-UHFFFAOYSA-N
Formula: C12H14ClFO2
SMILES: CC(C)(C)COC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 244.69

Physical Properties

Property code	Value	Unit	Source
gf	-294.51	kJ/mol	Joback Method
hf	-542.82	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	57.33	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.682		Crippen Method
mcvol	177.630	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
tb	620.36	K	Joback Method
tc	834.35	K	Joback Method
tf	381.55	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.07	J/mol×K	620.36	Joback Method
cpg	445.82	J/mol×K	656.02	Joback Method
cpg	458.69	J/mol×K	691.69	Joback Method
cpg	470.71	J/mol×K	727.35	Joback Method
cpg	481.91	J/mol×K	763.02	Joback Method
cpg	492.33	J/mol×K	798.68	Joback Method
cpg	501.99	J/mol×K	834.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357720&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