3-Chloro-2-fluorobenzoic acid, 3-methylbutyl-2 ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-302.23	kJ/mol	Joback Method
hf	-544.63	kJ/mol	Joback Method
hfus	23.12	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.680		Crippen Method
mcvol	177.630	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1589.00		NIST Webbook
rinpol	1589.00		NIST Webbook
tb	622.71	K	Joback Method
tc	833.20	K	Joback Method
tf	349.13	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.66	J/mol×K	622.71	Joback Method
cpg	443.42	J/mol×K	657.79	Joback Method
cpg	456.38	J/mol×K	692.87	Joback Method
cpg	468.55	J/mol×K	727.95	Joback Method
cpg	479.95	J/mol×K	763.03	Joback Method
cpg	490.59	J/mol×K	798.12	Joback Method
cpg	500.48	J/mol×K	833.20	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=U360579&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

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