2-Chlorobenzoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C12H13ClO2/c1-9(2)7-8-15-12(14)10-5-3-4-6-11(10)13/h3-7H,8H2,1-2H3
InchiKey: ATGFDZGHHGODGL-UHFFFAOYSA-N
Formula: C12H13ClO2
SMILES: CC(C)=CCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 224.68

Physical Properties

Property code	Value	Unit	Source
gf	-21.24	kJ/mol	Joback Method
hf	-219.06	kJ/mol	Joback Method
hfus	26.36	kJ/mol	Joback Method
hvap	58.82	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.463		Crippen Method
mcvol	171.560	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
tb	623.38	K	Joback Method
tc	846.88	K	Joback Method
tf	346.98	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.99	J/mol×K	623.38	Joback Method
cpg	413.60	J/mol×K	660.63	Joback Method
cpg	426.34	J/mol×K	697.88	Joback Method
cpg	438.23	J/mol×K	735.13	Joback Method
cpg	449.31	J/mol×K	772.38	Joback Method
cpg	459.62	J/mol×K	809.63	Joback Method
cpg	469.21	J/mol×K	846.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299298&Units=SI

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