3-Methylbut-3-enyl 3-chlorobenzoate

Inchi: InChI=1S/C12H13ClO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-5,8H,1,6-7H2,2H3
InchiKey: YUDOYCVLABYOMK-UHFFFAOYSA-N
Formula: C12H13ClO2
SMILES: C=C(C)CCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 224.68

Physical Properties

Property code	Value	Unit	Source
gf	-13.62	kJ/mol	Joback Method
hf	-210.85	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	58.20	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.463		Crippen Method
mcvol	171.560	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	615.90	K	Joback Method
tc	834.66	K	Joback Method
tf	350.30	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.77	J/mol×K	615.90	Joback Method
cpg	413.33	J/mol×K	652.36	Joback Method
cpg	426.04	J/mol×K	688.82	Joback Method
cpg	437.92	J/mol×K	725.28	Joback Method
cpg	449.01	J/mol×K	761.74	Joback Method
cpg	459.33	J/mol×K	798.20	Joback Method
cpg	468.91	J/mol×K	834.66	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=U373555&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