3,7-Dimethyloct-6-enyl 3-chlorobenzoate

Inchi: InChI=1S/C17H23ClO2/c1-13(2)6-4-7-14(3)10-11-20-17(19)15-8-5-9-16(18)12-15/h5-6,8
InchiKey: WEZDEOWFQYRKRF-UHFFFAOYSA-N
Formula: C17H23ClO2
SMILES: CC(C)=CCCC(C)CCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 294.82

Physical Properties

Property code	Value	Unit	Source
gf	18.42	kJ/mol	Joback Method
hf	-327.54	kJ/mol	Joback Method
hfus	35.79	kJ/mol	Joback Method
hvap	69.57	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.269		Crippen Method
mcvol	242.010	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2109.00		NIST Webbook
rinpol	2109.00		NIST Webbook
tb	737.34	K	Joback Method
tc	947.69	K	Joback Method
tf	388.33	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.32	J/mol×K	737.34	Joback Method
cpg	677.55	J/mol×K	772.40	Joback Method
cpg	692.77	J/mol×K	807.46	Joback Method
cpg	707.01	J/mol×K	842.52	Joback Method
cpg	720.33	J/mol×K	877.58	Joback Method
cpg	732.78	J/mol×K	912.63	Joback Method
cpg	744.39	J/mol×K	947.69	Joback Method

Sources

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=U373556&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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