(Z)-Dec-4-enyl 3-chlorobenzoate

Inchi: InChI=1S/C17H23ClO2/c1-2-3-4-5-6-7-8-9-13-20-17(19)15-11-10-12-16(18)14-15/h6-7,1
InchiKey: VOLMYSSMSCCCBL-SREVYHEPSA-N
Formula: C17H23ClO2
SMILES: CCCCCC=CCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 294.82

Physical Properties

Property code	Value	Unit	Source
gf	29.41	kJ/mol	Joback Method
hf	-312.47	kJ/mol	Joback Method
hfus	40.62	kJ/mol	Joback Method
hvap	69.87	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.413		Crippen Method
mcvol	242.010	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	737.90	K	Joback Method
tc	942.28	K	Joback Method
tf	417.29	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.12	J/mol×K	737.90	Joback Method
cpg	676.90	J/mol×K	771.96	Joback Method
cpg	691.73	J/mol×K	806.03	Joback Method
cpg	705.64	J/mol×K	840.09	Joback Method
cpg	718.68	J/mol×K	874.16	Joback Method
cpg	730.89	J/mol×K	908.22	Joback Method
cpg	742.32	J/mol×K	942.28	Joback Method
dvisc	0.0010361	Pa×s	417.29	Joback Method

dvisc	0.0005380	Pa×s	470.73	Joback Method
dvisc	0.0003193	Pa×s	524.16	Joback Method
dvisc	0.0002087	Pa×s	577.60	Joback Method
dvisc	0.0001466	Pa×s	631.03	Joback Method
dvisc	0.0001088	Pa×s	684.46	Joback Method
dvisc	0.0000843	Pa×s	737.90	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=U373567&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
dvisc:	Dynamic viscosity
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