2,4-Dimethylpentan-3-yl 3-chlorobenzoate

Inchi: InChI=1S/C14H19ClO2/c1-9(2)13(10(3)4)17-14(16)11-6-5-7-12(15)8-11/h5-10,13H,1-4H
InchiKey: NVRCYPVMPDPSNP-UHFFFAOYSA-N
Formula: C14H19ClO2
SMILES: CC(C)C(OC(=O)c1cccc(Cl)c1)C(C)C
Mol. weight [g/mol]: 254.75

Physical Properties

Property code	Value	Unit	Source
gf	-83.39	kJ/mol	Joback Method
hf	-383.61	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.177		Crippen Method
mcvol	204.040	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1677.00		NIST Webbook
tb	663.78	K	Joback Method
tc	880.10	K	Joback Method
tf	343.56	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.31	J/mol×K	663.78	Joback Method
cpg	594.87	J/mol×K	844.05	Joback Method
cpg	582.69	J/mol×K	808.00	Joback Method
cpg	569.57	J/mol×K	771.94	Joback Method
cpg	555.49	J/mol×K	735.89	Joback Method
cpg	540.41	J/mol×K	699.83	Joback Method
cpg	606.14	J/mol×K	880.10	Joback Method
dvisc	0.0001117	Pa×s	663.78	Joback Method
dvisc	0.0001505	Pa×s	610.41	Joback Method

dvisc	0.0002146	Pa×s	557.04	Joback Method
dvisc	0.0003302	Pa×s	503.67	Joback Method
dvisc	0.0005625	Pa×s	450.30	Joback Method
dvisc	0.0011058	Pa×s	396.93	Joback Method
dvisc	0.0026821	Pa×s	343.56	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=U373572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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