1-tert-Butoxypropan-2-yl 4-chlorobenzoate

Inchi: InChI=1S/C14H19ClO3/c1-10(9-17-14(2,3)4)18-13(16)11-5-7-12(15)8-6-11/h5-8,10H,9H
InchiKey: PPCPJLRXEOEWQF-UHFFFAOYSA-N
Formula: C14H19ClO3
SMILES: CC(COC(C)(C)C)OC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 270.75

Physical Properties

Property code	Value	Unit	Source
gf	-180.67	kJ/mol	Joback Method
hf	-514.02	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Joback Method
hvap	63.96	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.700		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1736.00		NIST Webbook
tb	683.85	K	Joback Method
tc	901.09	K	Joback Method
tf	398.21	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.88	J/mol×K	683.85	Joback Method
cpg	620.84	J/mol×K	864.88	Joback Method
cpg	609.22	J/mol×K	828.67	Joback Method
cpg	596.65	J/mol×K	792.47	Joback Method
cpg	583.09	J/mol×K	756.26	Joback Method
cpg	568.51	J/mol×K	720.06	Joback Method
cpg	631.53	J/mol×K	901.09	Joback Method
dvisc	0.0000851	Pa×s	683.85	Joback Method
dvisc	0.0001125	Pa×s	636.24	Joback Method

dvisc	0.0001556	Pa×s	588.64	Joback Method
dvisc	0.0002278	Pa×s	541.03	Joback Method
dvisc	0.0003591	Pa×s	493.42	Joback Method
dvisc	0.0006236	Pa×s	445.82	Joback Method
dvisc	0.0012360	Pa×s	398.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378317&Units=SI
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

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