

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

Inchi:	InChI=1S/C14H19ClO3/c1-10(9-17-14(2,3)4)18-13(16)11-7-5-6-8-12(11)15/h5-8,10H,9H
InchiKey:	MCQGMGYMJDUQAH-UHFFFAOYSA-N
Formula:	C14H19ClO3
SMILES:	CC(COC(C)(C)C)OC(=O)c1ccccc1Cl
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
rinsol	1742.00		NIST Webbook
rinsol	1742.00		NIST Webbook
tb	683.85	K	Joback Method
tc	901.09	K	Joback Method
tf	398.21	K	Joback Method
vc	0.785	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.88	J/molxK	683.85	Joback Method
cpg	620.84	J/molxK	864.88	Joback Method
cpg	609.22	J/molxK	828.67	Joback Method
cpg	596.65	J/molxK	792.47	Joback Method
cpg	583.09	J/molxK	756.26	Joback Method
cpg	568.51	J/molxK	720.06	Joback Method
cpg	631.53	J/molxK	901.09	Joback Method
dvisc	0.0000851	Paxs	683.85	Joback Method

dvisc	0.0001125	Paxs	636.24	Joback Method
dvisc	0.0001556	Paxs	588.64	Joback Method
dvisc	0.0002278	Paxs	541.03	Joback Method
dvisc	0.0003591	Paxs	493.42	Joback Method
dvisc	0.0006236	Paxs	445.82	Joback Method
dvisc	0.0012360	Paxs	398.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U378316&Units=SI

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

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