

# 1-Butoxypropan-2-yl 2-chlorobenzoate

<b>Inchi:</b>	InChI=1S/C14H19ClO3/c1-3-4-9-17-10-11(2)18-14(16)12-7-5-6-8-13(12)15/h5-8,11H,3-4
<b>InchiKey:</b>	QUTXSDYNUBWDOH-UHFFFAOYSA-N
<b>Formula:</b>	C14H19ClO3
<b>SMILES:</b>	CCCCOCC(C)OC(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	270.75

## Physical Properties

Property code	Value	Unit	Source
gf	-183.51	kJ/mol	Joback Method
hf	-505.27	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	65.26	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.702		Crippen Method
mvol	209.910	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	687.08	K	Joback Method
tc	893.55	K	Joback Method
tf	395.79	K	Joback Method
vc	0.796	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.11	J/molxK	687.08	Joback Method
cpg	616.63	J/molxK	859.14	Joback Method
cpg	605.11	J/molxK	824.73	Joback Method
cpg	592.71	J/molxK	790.32	Joback Method
cpg	579.41	J/molxK	755.90	Joback Method
cpg	565.22	J/molxK	721.49	Joback Method
cpg	627.28	J/molxK	893.55	Joback Method
dvisc	0.0001005	Paxs	687.08	Joback Method

dvisc	0.0001298	Paxs	638.53	Joback Method
dvisc	0.0001748	Paxs	589.98	Joback Method
dvisc	0.0002483	Paxs	541.43	Joback Method
dvisc	0.0003781	Paxs	492.89	Joback Method
dvisc	0.0006310	Paxs	444.34	Joback Method
dvisc	0.0011940	Paxs	395.79	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U378264&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U378264&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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