

# 3-Chlorobenzoic acid, 3-methylphenyl ester

<b>Inchi:</b>	InChI=1S/C14H11ClO2/c1-10-4-2-7-13(8-10)17-14(16)11-5-3-6-12(15)9-11/h2-9H,1H3
<b>InchiKey:</b>	XJYMREBPKIWXCH-UHFFFAOYSA-N
<b>Formula:</b>	C14H11ClO2
<b>SMILES:</b>	Cc1cccc(OC(=O)c2cccc(Cl)c2)c1
<b>Mol. weight [g/mol]:</b>	246.69

## Physical Properties

Property code	Value	Unit	Source
gf	26.71	kJ/mol	Joback Method
hf	-142.71	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.868		Crippen Method
mcvol	180.280	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpola	1989.00		NIST Webbook
rinpola	1989.00		NIST Webbook
tb	696.76	K	Joback Method
tc	943.81	K	Joback Method
tf	427.50	K	Joback Method
vc	0.676	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.48	J/molxK	696.76	Joback Method
cpg	495.79	J/molxK	902.64	Joback Method
cpg	486.41	J/molxK	861.46	Joback Method
cpg	476.03	J/molxK	820.29	Joback Method
cpg	464.61	J/molxK	779.11	Joback Method
cpg	452.11	J/molxK	737.94	Joback Method
cpg	504.22	J/molxK	943.81	Joback Method
dvisc	0.0001405	Paxs	696.76	Joback Method

dvisc	0.0001735	Paxs	651.88	Joback Method
dvisc	0.0002210	Paxs	607.01	Joback Method
dvisc	0.0002925	Paxs	562.13	Joback Method
dvisc	0.0004065	Paxs	517.25	Joback Method
dvisc	0.0006014	Paxs	472.38	Joback Method
dvisc	0.0009660	Paxs	427.50	Joback Method

## Sources

<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>
<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=U357785&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357785&amp;Units=SI</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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