

# 3-Chlorobenzoic acid, 4-chlorophenyl ester

<b>Inchi:</b>	InChI=1S/C13H8Cl2O2/c14-10-4-6-12(7-5-10)17-13(16)9-2-1-3-11(15)8-9/h1-8H
<b>InchiKey:</b>	FORQJPGZPJPPMV-UHFFFAOYSA-N
<b>Formula:</b>	C13H8Cl2O2
<b>SMILES:</b>	O=C(Oc1ccc(Cl)cc1)c1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	267.11

## Physical Properties

Property code	Value	Unit	Source
gf	6.36	kJ/mol	Joback Method
hf	-137.81	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.213		Crippen Method
mcvol	178.430	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpola	2090.00		NIST Webbook
tb	711.31	K	Joback Method
tc	966.18	K	Joback Method
tf	446.15	K	Joback Method
vc	0.669	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.63	J/molxK	711.31	Joback Method
cpg	422.43	J/molxK	753.79	Joback Method
cpg	433.14	J/molxK	796.27	Joback Method
cpg	442.82	J/molxK	838.75	Joback Method
cpg	451.51	J/molxK	881.22	Joback Method
cpg	459.25	J/molxK	923.70	Joback Method
cpg	466.10	J/molxK	966.18	Joback Method
dvisc	0.0009179	Paxs	446.15	Joback Method
dvisc	0.0005874	Paxs	490.34	Joback Method

dvisc	0.0004047	Paxs	534.54	Joback Method
dvisc	0.0002951	Paxs	578.73	Joback Method
dvisc	0.0002251	Paxs	622.92	Joback Method
dvisc	0.0001780	Paxs	667.12	Joback Method
dvisc	0.0001449	Paxs	711.31	Joback Method

## Sources

<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=U357786&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357786&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>

## 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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