

# 3-Chlorobenzoic acid, 2-biphenyl ester

<b>Inchi:</b>	InChI=1S/C19H13ClO2/c20-16-10-6-9-15(13-16)19(21)22-18-12-5-4-11-17(18)14-7-2-1-3
<b>InchiKey:</b>	PLCHZGCESRFODF-UHFFFAOYSA-N
<b>Formula:</b>	C19H13ClO2
<b>SMILES:</b>	O=C(Oc1ccccc1-c1ccccc1)c1ccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	308.76

## Physical Properties

Property code	Value	Unit	Source
gf	181.22	kJ/mol	Joback Method
hf	-9.38	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	79.58	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.226		Crippen Method
mcvol	226.970	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpola	2429.00		NIST Webbook
tb	837.84	K	Joback Method
tc	1102.95	K	Joback Method
tf	510.27	K	Joback Method
vc	0.849	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.13	J/molxK	837.84	Joback Method
cpg	664.97	J/molxK	1058.76	Joback Method
cpg	656.67	J/molxK	1014.58	Joback Method
cpg	647.24	J/molxK	970.39	Joback Method
cpg	636.56	J/molxK	926.21	Joback Method
cpg	624.56	J/molxK	882.02	Joback Method
cpg	672.23	J/molxK	1102.95	Joback Method
dvisc	0.0000796	Paxs	837.84	Joback Method
dvisc	0.0000991	Paxs	783.25	Joback Method

dvisc	0.0001276	Paxs	728.65	Joback Method
dvisc	0.0001711	Paxs	674.06	Joback Method
dvisc	0.0002415	Paxs	619.46	Joback Method
dvisc	0.0003644	Paxs	564.87	Joback Method
dvisc	0.0006004	Paxs	510.27	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357402&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357402&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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