

# 4-Chlorobenzoic acid, 2,4,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C13H6Cl4O2/c14-8-3-1-7(2-4-8)13(18)19-12-6-10(16)9(15)5-11(12)17/h1-6H
<b>InchiKey:</b>	FJPROMXTNPFWDV-UHFFFAOYSA-N
<b>Formula:</b>	C13H6Cl4O2
<b>SMILES:</b>	O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	336.00

## Physical Properties

Property code	Value	Unit	Source
gf	-36.76	kJ/mol	Joback Method
hf	-192.23	kJ/mol	Joback Method
hfus	35.53	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.519		Crippen Method
mcvol	202.910	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	2418.00		NIST Webbook
tb	796.13	K	Joback Method
tc	1055.94	K	Joback Method
tf	531.03	K	Joback Method
vc	0.767	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.65	J/molxK	796.13	Joback Method
cpg	482.89	J/molxK	1012.64	Joback Method
cpg	477.47	J/molxK	969.33	Joback Method
cpg	471.17	J/molxK	926.03	Joback Method
cpg	463.95	J/molxK	882.73	Joback Method
cpg	455.79	J/molxK	839.43	Joback Method
cpg	487.47	J/molxK	1055.94	Joback Method
dvisc	0.0001186	Paxs	796.13	Joback Method
dvisc	0.0001421	Paxs	751.95	Joback Method

dvisc	0.0001742	Paxs	707.76	Joback Method
dvisc	0.0002193	Paxs	663.58	Joback Method
dvisc	0.0002854	Paxs	619.40	Joback Method
dvisc	0.0003867	Paxs	575.21	Joback Method
dvisc	0.0005512	Paxs	531.03	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=U354630&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354630&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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