

# 3,4,5-trichlorodiphenyl ether

<b>Inchi:</b>	InChI=1S/C12H7Cl3O/c13-10-6-9(7-11(14)12(10)15)16-8-4-2-1-3-5-8/h1-7H
<b>InchiKey:</b>	ZQCCHNBMSHOJAT-UHFFFAOYSA-N
<b>Formula:</b>	C12H7Cl3O
<b>SMILES:</b>	Clc1cc(Oc2ccccc2)cc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	273.55

## Physical Properties

Property code	Value	Unit	Source
gf	105.30	kJ/mol	Joback Method
hf	-31.80	kJ/mol	Joback Method
hfus	27.53	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-6.77		Aqueous Solubility Prediction Method
logp	5.439		Crippen Method
mcvol	175.010	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	676.97	K	Joback Method
tc	935.56	K	Joback Method
tf	427.39	K	Joback Method
vc	0.656	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.90	J/molxK	676.97	Joback Method
cpg	383.39	J/molxK	720.07	Joback Method
cpg	393.89	J/molxK	763.17	Joback Method
cpg	403.43	J/molxK	806.27	Joback Method
cpg	412.06	J/molxK	849.36	Joback Method
cpg	419.81	J/molxK	892.46	Joback Method
cpg	426.71	J/molxK	935.56	Joback Method
dvisc	0.0008107	Paxs	427.39	Joback Method
dvisc	0.0005365	Paxs	468.99	Joback Method

dvisc	0.0003797	Paxs	510.58	Joback Method
dvisc	0.0002831	Paxs	552.18	Joback Method
dvisc	0.0002200	Paxs	593.78	Joback Method
dvisc	0.0001766	Paxs	635.37	Joback Method
dvisc	0.0001457	Paxs	676.97	Joback Method

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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>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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