

# 2,2',4,4',5,6'-Hexachlorodiphenyl ether

<b>Inchi:</b>	InChI=1S/C12H4Cl6O/c13-5-1-9(17)12(10(18)2-5)19-11-4-7(15)6(14)3-8(11)16/h1-4H
<b>InchiKey:</b>	XKQUAQGQLZDDBV-UHFFFAOYSA-N
<b>Formula:</b>	C12H4Cl6O
<b>SMILES:</b>	Clc1cc(Cl)c(Oc2cc(Cl)c(Cl)cc2Cl)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	376.88

## Physical Properties

Property code	Value	Unit	Source
gf	40.62	kJ/mol	Joback Method
hf	-113.43	kJ/mol	Joback Method
hfus	38.95	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-8.04		Aqueous Solubility Prediction Method
logp	7.399		Crippen Method
mcvol	211.730	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	804.20	K	Joback Method
tc	1070.09	K	Joback Method
tf	554.71	K	Joback Method
vc	0.803	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.11	J/molxK	804.20	Joback Method
cpg	430.92	J/molxK	848.51	Joback Method
cpg	437.87	J/molxK	892.83	Joback Method
cpg	443.98	J/molxK	937.14	Joback Method
cpg	449.28	J/molxK	981.46	Joback Method
cpg	453.76	J/molxK	1025.77	Joback Method
cpg	457.46	J/molxK	1070.09	Joback Method
dvisc	0.0004031	Paxs	554.71	Joback Method
dvisc	0.0003000	Paxs	596.29	Joback Method

dvisc	0.0002321	Paxs	637.87	Joback Method
dvisc	0.0001852	Paxs	679.46	Joback Method
dvisc	0.0001517	Paxs	721.04	Joback Method
dvisc	0.0001270	Paxs	762.62	Joback Method
dvisc	0.0001083	Paxs	804.20	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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