# 2,3,3',4,4'-pentachlorodiphenyl ether

**Inchi:** InChI=1S/C12H5Cl5O/c13-7-2-1-6(5-9(7)15)18-10-4-3-8(14)11(16)12(10)17/h1-5H
**InchiKey:** PKEGIXYNAGGYPN-UHFFFAOYSA-N
**Formula:** C12H5Cl5O
**SMILES:** Clc1ccc(Oc2ccc(Cl)c(Cl)c2Cl)cc1Cl
**Mol. weight [g/mol]:** 342.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 62.18 | kJ/mol | Joback Method |
| hf | -86.22 | kJ/mol | Joback Method |
| hfus | 35.15 | kJ/mol | Joback Method |
| hvap | 74.50 | kJ/mol | Joback Method |
| log10ws | -7.67 | | Aqueous Solubility Prediction Method |
| logp | 6.746 | | Crippen Method |
| mcvol | 199.490 | ml/mol | McGowan Method |
| pc | 2537.93 | kPa | Joback Method |
| tb | 761.79 | K | Joback Method |
| tc | 1025.61 | K | Joback Method |
| tf | 512.27 | K | Joback Method |
| vc | 0.754 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 407.73 | J/mol×K | 761.79 | Joback Method |
| cpg | 416.71 | J/mol×K | 805.76 | Joback Method |
| cpg | 424.79 | J/mol×K | 849.73 | Joback Method |
| cpg | 432.00 | J/mol×K | 893.70 | Joback Method |
| cpg | 438.38 | J/mol×K | 937.67 | Joback Method |
| cpg | 443.94 | J/mol×K | 981.64 | Joback Method |
| cpg | 448.70 | J/mol×K | 1025.61 | Joback Method |
| dvisc | 0.0005027 | Pa×s | 512.27 | Joback Method |
| dvisc | 0.0003626 | Pa×s | 553.86 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002737 | Pa×s | 595.44 | Joback Method |
| dvisc | 0.0002143 | Pa×s | 637.03 | Joback Method |
| dvisc | 0.0001730 | Pa×s | 678.62 | Joback Method |
| dvisc | 0.0001431 | Pa×s | 720.20 | Joback Method |
| dvisc | 0.0001208 | Pa×s | 761.79 | Joback Method |

# Sources

**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/ci990307l

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**gf:** Standard Gibbs free energy of formation
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**log10ws:** Log10 of Water solubility in mol/l
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pc:** Critical Pressure
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume