

3,3',4,4'-tetrachlorodiphenyl ether

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H6Cl4O/c13-9-3-1-7(5-11(9)15)17-8-2-4-10(14)12(16)6-8/h1-6H |
| InchiKey: | DHLVZXZRIZBPKG-UHFFFAOYSA-N |
| Formula: | C12H6Cl4O |
| SMILES: | Clc1ccc(Oc2ccc(Cl)c(Cl)c2)cc1Cl |
| Mol. weight [g/mol]: | 307.99 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|--------------------------------------|
| gf | 83.74 | kJ/mol | Joback Method |
| hf | -59.01 | kJ/mol | Joback Method |
| hfus | 31.34 | kJ/mol | Joback Method |
| hvap | 69.46 | kJ/mol | Joback Method |
| log10ws | -6.98 | | Aqueous Solubility Prediction Method |
| logp | 6.092 | | Crippen Method |
| mcvol | 187.250 | ml/mol | McGowan Method |
| pc | 2676.31 | kPa | Joback Method |
| tb | 719.38 | K | Joback Method |
| tc | 980.81 | K | Joback Method |
| tf | 469.83 | K | Joback Method |
| vc | 0.706 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 390.71 | J/mol×K | 719.38 | Joback Method |
| cpg | 400.91 | J/mol×K | 762.95 | Joback Method |
| cpg | 410.17 | J/mol×K | 806.52 | Joback Method |
| cpg | 418.52 | J/mol×K | 850.09 | Joback Method |
| cpg | 426.00 | J/mol×K | 893.66 | Joback Method |
| cpg | 432.64 | J/mol×K | 937.23 | Joback Method |
| cpg | 438.47 | J/mol×K | 980.81 | Joback Method |
| dvisc | 0.0006337 | Paxs | 469.83 | Joback Method |
| dvisc | 0.0004398 | Paxs | 511.42 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003225 | Paxs | 553.01 | Joback Method |
| dvisc | 0.0002470 | Paxs | 594.61 | Joback Method |
| dvisc | 0.0001959 | Paxs | 636.20 | Joback Method |
| dvisc | 0.0001598 | Paxs | 677.79 | Joback Method |
| dvisc | 0.0001335 | Paxs | 719.38 | Joback Method |

Sources

Crippen Method:

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

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>

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 |

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