

Bis(4-fluorophenyl)ether

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| Other names: | 4-Fluorophenyl ether Bis(p-fluorophenyl) ether Benzene, 1,1'-oxybis[4-fluoro-1,1'-oxybis(4-fluorobenzene) |
| Inchi: | InChI=1S/C12H8F2O/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H |
| InchiKey: | UUKHFGSOCZLVJO-UHFFFAOYSA-N |
| Formula: | C12H8F2O |
| SMILES: | Fc1ccc(Oc2ccc(F)cc2)cc1 |
| Mol. weight [g/mol]: | 206.19 |
| CAS: | 330-93-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -238.90 | kJ/mol | Joback Method |
| hf | -365.33 | kJ/mol | Joback Method |
| hfus | 21.49 | kJ/mol | Joback Method |
| hvap | 48.96 | kJ/mol | Joback Method |
| log10ws | -3.77 | | Crippen Method |
| logp | 3.757 | | Crippen Method |
| mcvol | 141.830 | ml/mol | McGowan Method |
| pc | 2937.70 | kPa | Joback Method |
| tb | 558.24 | K | Joback Method |
| tc | 781.89 | K | Joback Method |
| tf | 326.29 | K | Joback Method |
| vc | 0.545 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 318.55 | J/molxK | 558.24 | Joback Method |
| cpg | 332.10 | J/molxK | 595.52 | Joback Method |
| cpg | 344.77 | J/molxK | 632.79 | Joback Method |
| cpg | 356.58 | J/molxK | 670.07 | Joback Method |
| cpg | 367.55 | J/molxK | 707.34 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 377.72 | J/mol×K | 744.62 | Joback Method |
| cpg | 387.11 | J/mol×K | 781.89 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C330938&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvac: | 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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