# 4,4'-Bis[2-hydroxyhexafluoroisopropyl]diphenyl ether

**InChI:** InChI=1S/C18H10F12O3/c19-15(20,21)13(31,16(22,23)24)9-1-5-11(6-2-9)33-12-7-3-10(4
**InchiKey:** PRBPSTYDUVSNOK-UHFFFAOYSA-N
**Formula:** C18H10F12O3
**SMILES:** OC(c1ccc(Oc2ccc(C(O)(C(F)(F)F)C(F)(F)F)cc2)cc1)(C(F)(F)F)C(F)(F)F
**Mol. weight [g/mol]:** 502.25
**CAS:** 2093-04-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2393.08 | kJ/mol | Joback Method |
| hf | -2807.23 | kJ/mol | Joback Method |
| hfus | 31.52 | kJ/mol | Joback Method |
| hvap | 79.73 | kJ/mol | Joback Method |
| log10ws | -7.06 | | Crippen Method |
| logp | 6.103 | | Crippen Method |
| mcvol | 255.810 | ml/mol | McGowan Method |
| pc | 1510.50 | kPa | Joback Method |
| tb | 853.20 | K | Joback Method |
| tc | 1045.14 | K | Joback Method |
| tf | 535.97 | K | Joback Method |
| vc | 1.034 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 818.85 | J/mol×K | 853.20 | Joback Method |
| cpg | 827.43 | J/mol×K | 885.19 | Joback Method |
| cpg | 835.43 | J/mol×K | 917.18 | Joback Method |
| cpg | 842.97 | J/mol×K | 949.17 | Joback Method |
| cpg | 850.18 | J/mol×K | 981.16 | Joback Method |
| cpg | 857.20 | J/mol×K | 1013.15 | Joback Method |
| cpg | 864.15 | J/mol×K | 1045.14 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2093041&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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

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|---|---|
| **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 |
| **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 |