# 2,2',4,4'-Tetramethyldiphenylsulphone

**Other names:** Benzene, 1,1'-sulfonylbis[2,4-dimethyl-
di-2,4-xylyl sulphone
**Inchi:** InChI=1S/C16H18O2S/c1-11-5-7-15(13(3)9-11)19(17,18)16-8-6-12(2)10-14(16)4/h5-10H
**InchiKey:** CWZZFEROKOHBGT-UHFFFAOYSA-N
**Formula:** C16H18O2S
**SMILES:** Cc1ccc(S(=O)(=O)c2ccc(C)cc2C)c(C)c1
**Mol. weight [g/mol]:** 274.38
**CAS:** 5184-75-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -198.40 | kJ/mol | Joback Method |
| hf | -399.74 | kJ/mol | Joback Method |
| hfus | 35.10 | kJ/mol | Joback Method |
| hvap | 77.05 | kJ/mol | Joback Method |
| log10ws | -4.74 | | Crippen Method |
| logp | 3.753 | | Crippen Method |
| mcvol | 216.870 | ml/mol | McGowan Method |
| pc | 2507.52 | kPa | Joback Method |
| tb | 686.54 | K | Joback Method |
| tc | 910.52 | K | Joback Method |
| tf | 393.00 ± 2.00 | K | NIST Webbook |
| vc | 0.842 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 559.18 | J/mol×K | 686.54 | Joback Method |
| cpg | 576.01 | J/mol×K | 723.87 | Joback Method |
| cpg | 591.65 | J/mol×K | 761.20 | Joback Method |
| cpg | 606.12 | J/mol×K | 798.53 | Joback Method |
| cpg | 619.43 | J/mol×K | 835.86 | Joback Method |
| cpg | 631.60 | J/mol×K | 873.19 | Joback Method |
| cpg | 642.67 | J/mol×K | 910.52 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5184758&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |