# 4-[3-(4-hydroxyphenyl)-1,1-dioxobenzo[c]oxathiol

**Inchi:** InChI=1S/C19H14O5S/c20-15-9-5-13(6-10-15)19(14-7-11-16(21)12-8-14)17-3-1-2-4-18(
**InchiKey:** BELBBZDIHDAJOR-UHFFFAOYSA-N
**Formula:** C19H14O5S
**SMILES:** O=S1(=O)OC(c2ccc(O)cc2)(c2ccc(O)cc2)c2ccccc21
**Mol. weight [g/mol]:** 354.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -365.20 | kJ/mol | Joback Method |
| hf | -585.91 | kJ/mol | Joback Method |
| hfus | 48.99 | kJ/mol | Joback Method |
| hvap | 112.31 | kJ/mol | Joback Method |
| log10ws | -3.07 | | Aqueous Solubility Prediction Method |
| logp | 3.109 | | Crippen Method |
| mcvol | 242.130 | ml/mol | McGowan Method |
| pc | 4640.32 | kPa | Joback Method |
| tb | 941.14 | K | Joback Method |
| tc | 1215.23 | K | Joback Method |
| tf | 775.13 | K | Joback Method |
| vc | 0.801 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 736.88 | J/mol×K | 941.14 | Joback Method |
| cpg | 755.66 | J/mol×K | 986.82 | Joback Method |
| cpg | 775.97 | J/mol×K | 1032.50 | Joback Method |
| cpg | 798.33 | J/mol×K | 1078.19 | Joback Method |
| cpg | 823.24 | J/mol×K | 1123.87 | Joback Method |
| cpg | 851.21 | J/mol×K | 1169.55 | Joback Method |
| cpg | 882.77 | J/mol×K | 1215.23 | Joback Method |

# Sources

| | |
|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |
| **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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