# Phenol, 2,2'-thiobis[4-(1,1,3,3-tetramethylbutyl)-

**Other names:** 2,2'-Thiobis[4-(1,1,3,3-tetramethylbutyl)phenol]

**Inchi:** InChI=1S/C28H42O2S/c1-25(2,3)17-27(7,8)19-11-13-21(29)23(15-19)31-24-16-20(12-14

**InchiKey:** WQYFETFRIRDUPJ-UHFFFAOYSA-N

**Formula:** C28H42O2S

**SMILES:** CC(C)(C)CC(C)(C)c1ccc(O)c(Sc2cc(C(C)(C)CC(C)(C)C)ccc2O)c1

**Mol. weight [g/mol]:** 442.70

**CAS:** 3294-03-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 125.68 | kJ/mol | Joback Method |
| hf | -518.88 | kJ/mol | Joback Method |
| hfus | 41.62 | kJ/mol | Joback Method |
| hvap | 111.46 | kJ/mol | Joback Method |
| log10ws | -8.48 | | Crippen Method |
| logp | 8.677 | | Crippen Method |
| mcvol | 385.950 | ml/mol | McGowan Method |
| pc | 1203.12 | kPa | Joback Method |
| tb | 1120.46 | K | Joback Method |
| tc | 1383.14 | K | Joback Method |
| tf | 750.72 | K | Joback Method |
| vc | 1.329 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1367.30 | J/mol×K | 1120.46 | Joback Method |
| cpg | 1393.92 | J/mol×K | 1164.24 | Joback Method |
| cpg | 1422.00 | J/mol×K | 1208.02 | Joback Method |
| cpg | 1451.96 | J/mol×K | 1251.80 | Joback Method |
| cpg | 1484.24 | J/mol×K | 1295.58 | Joback Method |
| cpg | 1519.24 | J/mol×K | 1339.36 | Joback Method |
| cpg | 1557.42 | J/mol×K | 1383.14 | Joback Method |

# Sources

| | |
|---|---|
| **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=C3294039&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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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