# Bithiopyranylidene, 2,2',6,6'-tetramethyl-

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|---|---|
| **Other names:** | 4H-Thiopyran, 4-(2,6-dimethyl-4H-thiopyran-4-ylidene)-2,6-dimethyl-<br>4H-Thiine, 2,6-dimethyl-4-(2,6-dimethyl-4H-thiin-4-ylideno)- |
| **Inchi:** | InChI=1S/C14H16S2/c1-9-5-13(6-10(2)15-9)14-7-11(3)16-12(4)8-14/h5-8H,1-4H3 |
| **InchiKey:** | KIVKMHQZJLNIOQ-UHFFFAOYSA-N |
| **Formula:** | C14H16S2 |
| **SMILES:** | CC1=CC(=C2C=C(C)SC(C)=C2)C=C(C)S1 |
| **Mol. weight [g/mol]:** | 248.41 |
| **CAS:** | 42506-61-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 303.06 | kJ/mol | Joback Method |
| hf | 127.63 | kJ/mol | Joback Method |
| hfus | 24.63 | kJ/mol | Joback Method |
| hvap | 65.29 | kJ/mol | Joback Method |
| ie | 6.23 | eV | NIST Webbook |
| log10ws | -6.49 | | Crippen Method |
| logp | 5.392 | | Crippen Method |
| mcvol | 197.600 | ml/mol | McGowan Method |
| pc | 2480.12 | kPa | Joback Method |
| tb | 689.50 | K | Joback Method |
| tc | 951.60 | K | Joback Method |
| tf | 516.60 | K | Joback Method |
| vc | 0.710 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 483.34 | J/mol×K | 689.50 | Joback Method |
| cpg | 499.81 | J/mol×K | 733.18 | Joback Method |
| cpg | 515.08 | J/mol×K | 776.87 | Joback Method |
| cpg | 529.19 | J/mol×K | 820.55 | Joback Method |
| cpg | 542.21 | J/mol×K | 864.23 | Joback Method |
| cpg | 554.19 | J/mol×K | 907.91 | Joback Method |

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|---|---|---|---|---|
| cpg | 565.21 | J/mol×K | 951.60 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C42506616&Units=SI |

# 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 |
| **ie:** | Ionization energy |
| **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 |