# 2,6-Dimethylthiophenol

**Other names:** 2,6-Dimethylbenzenethiol
Benzenethiol, 2,6-dimethyl-
**Inchi:** InChI=1S/C8H10S/c1-6-4-3-5-7(2)8(6)9/h3-5,9H,1-2H3
**InchiKey:** QCLJODDRBGKIRW-UHFFFAOYSA-N
**Formula:** C8H10S
**SMILES:** Cc1cccc(C)c1S
**Mol. weight [g/mol]:** 138.23
**CAS:** 118-72-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 139.02 | kJ/mol | Joback Method |
| hf | 43.62 | kJ/mol | Joback Method |
| hfus | 13.78 | kJ/mol | Joback Method |
| hvap | 43.74 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 2.592 | | Crippen Method |
| mcvol | 116.170 | ml/mol | McGowan Method |
| pc | 3805.69 | kPa | Joback Method |
| rinpol | 1213.20 | | NIST Webbook |
| rinpol | 1226.00 | | NIST Webbook |
| rinpol | 1226.00 | | NIST Webbook |
| tb | 481.94 | K | Joback Method |
| tc | 719.76 | K | Joback Method |
| tf | 267.84 | K | Joback Method |
| vc | 0.429 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 221.55 | J/mol×K | 481.94 | Joback Method |
| cpg | 233.86 | J/mol×K | 521.58 | Joback Method |
| cpg | 245.45 | J/mol×K | 561.21 | Joback Method |
| cpg | 256.34 | J/mol×K | 600.85 | Joback Method |

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|---|---|---|---|---|
| cpg | 266.57 | J/mol×K | 640.49 | Joback Method |
| cpg | 276.15 | J/mol×K | 680.13 | Joback Method |
| cpg | 285.11 | J/mol×K | 719.76 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.47964e+01 |
| Coeff. B | -4.16901e+03 |
| Coeff. C | -7.72170e+01 |
| Temperature range (K), min. | 364.56 |
| Temperature range (K), max. | 516.76 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C118729&Units=SI

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**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

**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

| | |
|---|---|
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |