# Disulfide, methyl phenyl

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|---|---|
| **Other names:** | Methyl phenyl disulfide |
| | Methyldisulfanylbenzene |
| | methyl phenyl disulphide |
| **Inchi:** | InChI=1S/C7H8S2/c1-8-9-7-5-3-2-4-6-7/h2-6H,1H3 |
| **InchiKey:** | LMSQHVXHZCNJEP-UHFFFAOYSA-N |
| **Formula:** | C7H8S2 |
| **SMILES:** | CSSc1ccccc1 |
| **Mol. weight [g/mol]:** | 156.27 |
| **CAS:** | 14173-25-2 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 186.71 | kJ/mol | Joback Method |
| hf | 132.46 | kJ/mol | Joback Method |
| hfus | 16.19 | kJ/mol | Joback Method |
| hvap | 47.09 | kJ/mol | Joback Method |
| log10ws | -3.09 | | Crippen Method |
| logp | 3.057 | | Crippen Method |
| mcvol | 118.430 | ml/mol | McGowan Method |
| pc | 4299.92 | kPa | Joback Method |
| rinpol | 1303.00 | | NIST Webbook |
| tb | 523.80 | K | Joback Method |
| tc | 787.37 | K | Joback Method |
| tf | 263.87 | K | Joback Method |
| vc | 0.427 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 226.59 | J/mol×K | 523.80 | Joback Method |
| cpg | 238.91 | J/mol×K | 567.73 | Joback Method |
| cpg | 250.33 | J/mol×K | 611.66 | Joback Method |
| cpg | 260.86 | J/mol×K | 655.59 | Joback Method |
| cpg | 270.53 | J/mol×K | 699.51 | Joback Method |

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|---|---|---|---|---|
| cpg | 279.35 | J/mol×K | 743.44 | Joback Method |
| cpg | 287.35 | J/mol×K | 787.37 | Joback Method |

# Sources

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|---|---|
| **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=C14173252&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

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