# 2-Methylmercaptoaniline

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|---|---|
| **Other names:** | 2-(Methylthio)aniline |
| | o-Thioanisidine |
| | Benzenamine, 2-(methylthio)- |
| **Inchi:** | InChI=1S/C7H9NS/c1-9-7-5-3-2-4-6(7)8/h2-5H,8H2,1H3 |
| **InchiKey:** | WBRPQQSADOCKCH-UHFFFAOYSA-N |
| **Formula:** | C7H9NS |
| **SMILES:** | CSc1ccccc1N |
| **Mol. weight [g/mol]:** | 139.22 |
| **CAS:** | 2987-53-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 210.41 | kJ/mol | Joback Method |
| hf | 112.91 | kJ/mol | Joback Method |
| hfus | 16.86 | kJ/mol | Joback Method |
| hvap | 51.57 | kJ/mol | Joback Method |
| log10ws | -1.85 | | Crippen Method |
| logp | 1.991 | | Crippen Method |
| mcvol | 112.060 | ml/mol | McGowan Method |
| pc | 4444.44 | kPa | Joback Method |
| tb | 507.20 | K | NIST Webbook |
| tc | 783.92 | K | Joback Method |
| tf | 325.25 | K | Joback Method |
| vc | 0.403 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 231.94 | J/mol×K | 532.53 | Joback Method |
| cpg | 243.64 | J/mol×K | 574.43 | Joback Method |
| cpg | 254.54 | J/mol×K | 616.33 | Joback Method |
| cpg | 264.66 | J/mol×K | 658.23 | Joback Method |
| cpg | 274.04 | J/mol×K | 700.13 | Joback Method |
| cpg | 282.69 | J/mol×K | 742.02 | Joback Method |

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|---|---|---|---|---|
| cpg | 290.64 | J/mol×K | 783.92 | 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=C2987533&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |