

# 2-Aminothiophenol, N,N,S-trimethyl-

|                      |                                                         |
|----------------------|---------------------------------------------------------|
| Inchi:               | InChI=1S/C9H13NS/c1-10(2)8-6-4-5-7-9(8)11-3/h4-7H,1-3H3 |
| InchiKey:            | BMVUVEYWVYKKNB-UHFFFAOYSA-N                             |
| Formula:             | C9H13NS                                                 |
| SMILES:              | CSc1ccccc1N(C)C                                         |
| Mol. weight [g/mol]: | 167.27                                                  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 271.58  | kJ/mol  | Joback Method  |
| hf            | 105.37  | kJ/mol  | Joback Method  |
| hfus          | 19.87   | kJ/mol  | Joback Method  |
| hvap          | 47.43   | kJ/mol  | Joback Method  |
| log10ws       | -2.12   |         | Crippen Method |
| logp          | 2.475   |         | Crippen Method |
| mcvol         | 140.240 | ml/mol  | McGowan Method |
| pc            | 3261.58 | kPa     | Joback Method  |
| rinpol        | 1393.70 |         | NIST Webbook   |
| rinpol        | 1393.70 |         | NIST Webbook   |
| tb            | 518.20  | K       | Joback Method  |
| tc            | 746.36  | K       | Joback Method  |
| tf            | 297.00  | K       | Joback Method  |
| vc            | 0.503   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 298.54 | J/mol×K | 518.20          | Joback Method |
| cpg           | 313.41 | J/mol×K | 556.23          | Joback Method |
| cpg           | 327.35 | J/mol×K | 594.25          | Joback Method |
| cpg           | 340.37 | J/mol×K | 632.28          | Joback Method |
| cpg           | 352.53 | J/mol×K | 670.30          | Joback Method |
| cpg           | 363.85 | J/mol×K | 708.33          | Joback Method |
| cpg           | 374.37 | J/mol×K | 746.36          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U353085&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353085&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |

# Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpola:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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