

# Benzenesulfonamide, N,4-dimethyl-N-phenyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | N,4-dimethyl-n-phenylbenzenesulfonamide  |
| <b>Inchi:</b>               | InChI=1S/C14H15NO2S/c1-12-8-10-14(11-9-12)18(16,17)15(2)13-6-4-3-5-7-13/h3-11H,1 |
| <b>InchiKey:</b>            | HEFFCQILGLLHQC-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C14H15NO2S   |
| <b>SMILES:</b>              | <chem>Cc1ccc(S(=O)(=O)N(C)c2ccccc2)cc1</chem>                                    |
| <b>Mol. weight [g/mol]:</b> | 261.34   |
| <b>CAS:</b>                 | 599-62-2   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -75.57  | kJ/mol               | Joback Method  |
| hf            | -256.52 | kJ/mol               | Joback Method  |
| hfus          | 34.11   | kJ/mol               | Joback Method  |
| hvap          | 72.65   | kJ/mol               | Joback Method  |
| log10ws       | -3.35   |                      | Crippen Method |
| logp          | 2.820   |                      | Crippen Method |
| mcvol         | 198.670 | ml/mol               | McGowan Method |
| pc            | 3220.98 | kPa                  | Joback Method  |
| tb            | 638.28  | K                    | Joback Method  |
| tc            | 864.53  | K                    | Joback Method  |
| tf            | 383.93  | K                    | Joback Method  |
| vc            | 0.748   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 495.04 | J/molxK | 638.28          | Joback Method |
| cpg           | 512.02 | J/molxK | 675.99          | Joback Method |
| cpg           | 527.69 | J/molxK | 713.70          | Joback Method |
| cpg           | 542.08 | J/molxK | 751.41          | Joback Method |
| cpg           | 555.26 | J/molxK | 789.12          | Joback Method |
| cpg           | 567.26 | J/molxK | 826.82          | Joback Method |
| cpg           | 578.14 | J/molxK | 864.53          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C599622&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C599622&amp;Units=SI</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>h vap:</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>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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