

# Phenethylsulfamide

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C8H12N2O2S/c9-13(11,12)10-7-6-8-4-2-1-3-5-8/h1-5,10H,6-7H2,(H2,9,11,12) |
| <b>InchiKey:</b>            | PJPREWNCIPMGIS-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C8H12N2O2S   |
| <b>SMILES:</b>              | NS(=O)(=O)NCCc1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 200.26   |
| <b>CAS:</b>                 | 710-15-6   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -183.81 | kJ/mol  | Joback Method  |
| hf            | -338.01 | kJ/mol  | Joback Method  |
| hfus          | 32.19   | kJ/mol  | Joback Method  |
| hvap          | 71.39   | kJ/mol  | Joback Method  |
| log10ws       | -1.71   |         | Crippen Method |
| logp          | 0.022   |         | Crippen Method |
| mcvol         | 147.870 | ml/mol  | McGowan Method |
| pc            | 4890.21 | kPa     | Joback Method  |
| tb            | 579.60  | K       | Joback Method  |
| tc            | 794.27  | K       | Joback Method  |
| tf            | 380.82  | K       | Joback Method  |
| vc            | 0.566   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 352.36 | J/molxK | 579.60          | Joback Method |
| cpg           | 365.55 | J/molxK | 615.38          | Joback Method |
| cpg           | 377.87 | J/molxK | 651.16          | Joback Method |
| cpg           | 389.32 | J/molxK | 686.94          | Joback Method |
| cpg           | 399.93 | J/molxK | 722.72          | Joback Method |
| cpg           | 409.71 | J/molxK | 758.50          | Joback Method |
| cpg           | 418.69 | J/molxK | 794.27          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=C710156&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C710156&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <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>                                     |

# 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>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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