

# 4-vinyl-3-methoxyphenol

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C9H10O2/c1-3-7-4-5-8(10)6-9(7)11-2/h3-6,10H,1H2,2H3 |
| <b>InchiKey:</b>            | UMDJLUGAMDTLDI-UHFFFAOYSA-N                                  |
| <b>Formula:</b>             | C9H10O2  |
| <b>SMILES:</b>              | C=Cc1ccc(O)cc1OC   |
| <b>Mol. weight [g/mol]:</b> | 150.17   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -44.10  | kJ/mol               | Joback Method  |
| hf            | -188.13 | kJ/mol               | Joback Method  |
| hfus          | 18.41   | kJ/mol               | Joback Method  |
| hvap          | 53.32   | kJ/mol               | Joback Method  |
| log10ws       | -1.96   |                      | Crippen Method |
| logp          | 2.044   |                      | Crippen Method |
| mcvol         | 121.350 | ml/mol               | McGowan Method |
| pc            | 3945.61 | kPa                  | Joback Method  |
| rinpole       | 1322.00 |                      | NIST Webbook   |
| ripole        | 2177.00 |                      | NIST Webbook   |
| ripole        | 2177.00 |                      | NIST Webbook   |
| tb            | 536.70  | K                    | Joback Method  |
| tc            | 762.38  | K                    | Joback Method  |
| tf            | 362.32  | K                    | Joback Method  |
| vc            | 0.397   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 271.06 | J/molxK | 536.70          | Joback Method |
| cpg           | 321.51 | J/molxK | 724.77          | Joback Method |
| cpg           | 312.69 | J/molxK | 687.15          | Joback Method |
| cpg           | 303.29 | J/molxK | 649.54          | Joback Method |
| cpg           | 293.26 | J/molxK | 611.93          | Joback Method |
| cpg           | 282.54 | J/molxK | 574.31          | Joback Method |
| cpg           | 329.83 | J/molxK | 762.38          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000529 | Paxs | 536.70 | Joback Method |
| dvisc | 0.0000785 | Paxs | 507.64 | Joback Method |
| dvisc | 0.0001224 | Paxs | 478.57 | Joback Method |
| dvisc | 0.0002020 | Paxs | 449.51 | Joback Method |
| dvisc | 0.0003573 | Paxs | 420.45 | Joback Method |
| dvisc | 0.0006881 | Paxs | 391.38 | Joback Method |
| dvisc | 0.0014717 | Paxs | 362.32 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>                                     |
| <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=R239180&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R239180&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <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>rinpol:</b>  | Non-polar retention indices                     |
| <b>ripol:</b>   | 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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