

# p-Anisic acid, 4-methoxyphenyl ester

**Inchi:** InChI=1S/C15H14O4/c1-17-12-5-3-11(4-6-12)15(16)19-14-9-7-13(18-2)8-10-14/h3-10H,1  
**InchiKey:** KVFFCZXWUPJFFQ-UHFFFAOYSA-N  
**Formula:** C15H14O4  
**SMILES:** COc1ccc(OC(=O)c2ccc(OC)cc2)cc1  
**Mol. weight [g/mol]:** 258.27

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -162.94 | kJ/mol  | Joback Method  |
| hf            | -412.05 | kJ/mol  | Joback Method  |
| hfus          | 27.07   | kJ/mol  | Joback Method  |
| hvap          | 68.84   | kJ/mol  | Joback Method  |
| log10ws       | -3.80   |         | Crippen Method |
| logp          | 2.923   |         | Crippen Method |
| mcvol         | 193.870 | ml/mol  | McGowan Method |
| pc            | 2465.36 | kPa     | Joback Method  |
| rinpol        | 2199.00 |         | NIST Webbook   |
| tb            | 727.05  | K       | Joback Method  |
| tc            | 959.54  | K       | Joback Method  |
| tf            | 453.31  | K       | Joback Method  |
| vc            | 0.720   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 516.43    | J/mol×K | 727.05          | Joback Method |
| cpg           | 530.98    | J/mol×K | 765.80          | Joback Method |
| cpg           | 544.39    | J/mol×K | 804.55          | Joback Method |
| cpg           | 556.66    | J/mol×K | 843.29          | Joback Method |
| cpg           | 567.78    | J/mol×K | 882.04          | Joback Method |
| cpg           | 577.76    | J/mol×K | 920.79          | Joback Method |
| cpg           | 586.59    | J/mol×K | 959.54          | Joback Method |
| dvisc         | 0.0005592 | Pa×s    | 453.31          | Joback Method |
| dvisc         | 0.0003516 | Pa×s    | 498.93          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002390 | Pa×s | 544.56 | Joback Method |
| dvisc | 0.0001724 | Pa×s | 590.18 | Joback Method |
| dvisc | 0.0001304 | Pa×s | 635.80 | Joback Method |
| dvisc | 0.0001023 | Pa×s | 681.43 | Joback Method |
| dvisc | 0.0000828 | Pa×s | 727.05 | 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=U307636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U307636&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>                                 |
| <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>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>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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