

# 2-Fluoro-4-methylanisole

|                      |                                                     |
|----------------------|-----------------------------------------------------|
| Inchi:               | InChI=1S/C8H9FO/c1-6-3-4-8(10-2)7(9)5-6/h3-5H,1-2H3 |
| InchiKey:            | FOVXANGOLMXKES-UHFFFAOYSA-N                         |
| Formula:             | C8H9FO                                              |
| SMILES:              | COc1ccc(C)cc1F                                      |
| Mol. weight [g/mol]: | 140.15                                              |
| CAS:                 | 399-55-3                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -190.18 | kJ/mol  | Joback Method  |
| hf            | -323.19 | kJ/mol  | Joback Method  |
| hfus          | 14.01   | kJ/mol  | Joback Method  |
| hvap          | 38.59   | kJ/mol  | Joback Method  |
| log10ws       | -2.40   |         | Crippen Method |
| logp          | 2.143   |         | Crippen Method |
| mcvol         | 107.460 | ml/mol  | McGowan Method |
| pc            | 3276.53 | kPa     | Joback Method  |
| tb            | 440.77  | K       | Joback Method  |
| tc            | 640.66  | K       | Joback Method  |
| tf            | 254.20  | K       | Joback Method  |
| vc            | 0.411   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 208.03 | J/mol×K | 440.77          | Joback Method |
| cpg           | 218.87 | J/mol×K | 474.08          | Joback Method |
| cpg           | 229.27 | J/mol×K | 507.40          | Joback Method |
| cpg           | 239.23 | J/mol×K | 540.71          | Joback Method |
| cpg           | 248.76 | J/mol×K | 574.03          | Joback Method |
| cpg           | 257.85 | J/mol×K | 607.34          | Joback Method |
| cpg           | 266.50 | J/mol×K | 640.66          | 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=C399553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C399553&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>hvac:</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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