

# Fumaric acid, monoamide, N-(2,4-dimethoxyphenyl)-, 2-pentyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C17H23NO5/c1-5-6-12(2)23-17(20)10-9-16(19)18-14-8-7-13(21-3)11-15(14)22 |
| <b>InchiKey:</b>            | HNKYHNJFNMDCCHA-MDZDMXLPSA-N   |
| <b>Formula:</b>             | C17H23NO5  |
| <b>SMILES:</b>              | CCCC(C)OC(=O)C=CC(=O)Nc1ccc(OC)cc1OC   |
| <b>Mol. weight [g/mol]:</b> | 321.37   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -220.26 | kJ/mol               | Joback Method  |
| hf            | -637.03 | kJ/mol               | Joback Method  |
| hfus          | 41.59   | kJ/mol               | Joback Method  |
| hvap          | 83.76   | kJ/mol               | Joback Method  |
| log10ws       | -3.67   |                      | Crippen Method |
| logp          | 2.930   |                      | Crippen Method |
| mcvol         | 253.060 | ml/mol               | McGowan Method |
| pc            | 1734.67 | kPa                  | Joback Method  |
| rinpola       | 2745.00 |                      | NIST Webbook   |
| tb            | 853.89  | K                    | Joback Method  |
| tc            | 1065.03 | K                    | Joback Method  |
| tf            | 531.94  | K                    | Joback Method  |
| vc            | 0.955   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 762.34 | J/mol×K | 853.89          | Joback Method |
| cpg           | 776.09 | J/mol×K | 889.08          | Joback Method |
| cpg           | 788.72 | J/mol×K | 924.27          | Joback Method |
| cpg           | 800.24 | J/mol×K | 959.46          | Joback Method |
| cpg           | 810.66 | J/mol×K | 994.65          | Joback Method |
| cpg           | 820.00 | J/mol×K | 1029.84         | Joback Method |
| cpg           | 828.26 | J/mol×K | 1065.03         | 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=U357499&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357499&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>                                 |

# 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>mccol:</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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