

# Succinic acid, 4-fluorophenethyl propyl ester

**Inchi:** InChI=1S/C15H19FO4/c1-2-10-19-14(17)7-8-15(18)20-11-9-12-3-5-13(16)6-4-12/h3-6H,1-2H3  
**InchiKey:** ZFWUSCGAKOLVDP-UHFFFAOYSA-N  
**Formula:** C15H19FO4  
**SMILES:** CCCOC(=O)CCC(=O)OCCc1ccc(F)cc1  
**Mol. weight [g/mol]:** 282.31

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -484.45 | kJ/mol               | Joback Method  |
| hf            | -813.58 | kJ/mol               | Joback Method  |
| hfus          | 36.91   | kJ/mol               | Joback Method  |
| hvap          | 69.42   | kJ/mol               | Joback Method  |
| log10ws       | -3.26   |                      | Crippen Method |
| logp          | 2.645   |                      | Crippen Method |
| mvol          | 215.100 | ml/mol               | McGowan Method |
| pc            | 1898.60 | kPa                  | Joback Method  |
| rmpol         | 1946.00 |                      | NIST Webbook   |
| rmpol         | 1946.00 |                      | NIST Webbook   |
| tb            | 726.11  | K                    | Joback Method  |
| tc            | 922.73  | K                    | Joback Method  |
| tf            | 442.66  | K                    | Joback Method  |
| vc            | 0.834   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 601.45 | J/mol×K | 726.11          | Joback Method |
| cpg           | 615.65 | J/mol×K | 758.88          | Joback Method |
| cpg           | 628.97 | J/mol×K | 791.65          | Joback Method |
| cpg           | 641.42 | J/mol×K | 824.42          | Joback Method |
| cpg           | 653.01 | J/mol×K | 857.19          | Joback Method |
| cpg           | 663.75 | J/mol×K | 889.96          | Joback Method |
| cpg           | 673.66 | J/mol×K | 922.73          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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=U381295&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381295&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinpola:</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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