

# Succinic acid, 2-chloro-6-fluorophenyl 3-ethylphenyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C18H16ClFO4/c1-2-12-5-3-6-13(11-12)23-16(21)9-10-17(22)24-18-14(19)7-4- |
| <b>InchiKey:</b>            | ALFARBSZLRJBHX-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C18H16ClFO4  |
| <b>SMILES:</b>              | CCc1cccc(OC(=O)CCC(=O)Oc2c(F)cccc2Cl)c1  |
| <b>Mol. weight [g/mol]:</b> | 350.77   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -377.97 | kJ/mol               | Joback Method  |
| hf            | -677.65 | kJ/mol               | Joback Method  |
| hfus          | 42.14   | kJ/mol               | Joback Method  |
| hvap          | 84.08   | kJ/mol               | Joback Method  |
| log10ws       | -5.57   |                      | Crippen Method |
| logp          | 4.333   |                      | Crippen Method |
| mvol          | 245.850 | ml/mol               | McGowan Method |
| pc            | 1859.51 | kPa                  | Joback Method  |
| rinpol        | 2460.00 |                      | NIST Webbook   |
| rinpol        | 2460.00 |                      | NIST Webbook   |
| tb            | 868.82  | K                    | Joback Method  |
| tc            | 1094.47 | K                    | Joback Method  |
| tf            | 557.85  | K                    | Joback Method  |
| vc            | 0.943   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 695.81 | J/molxK | 868.82          | Joback Method |
| cpg           | 707.68 | J/molxK | 906.43          | Joback Method |
| cpg           | 718.38 | J/molxK | 944.04          | Joback Method |
| cpg           | 727.92 | J/molxK | 981.65          | Joback Method |
| cpg           | 736.34 | J/molxK | 1019.26         | Joback Method |
| cpg           | 743.66 | J/molxK | 1056.87         | Joback Method |
| cpg           | 749.88 | J/molxK | 1094.47         | 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=U390106&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390106&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>h vap:</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>r in pol:</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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