

# Succinic acid, 2,3-dichlorophenyl 2,3-dimethylphenyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C18H16Cl2O4/c1-11-5-3-7-14(12(11)2)23-16(21)9-10-17(22)24-15-8-4-6-13(19) |
| <b>InchiKey:</b>            | NZLVRHCKUVFTRU-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C18H16Cl2O4  |
| <b>SMILES:</b>              | <chem>Cc1cccc(OC(=O)CCC(=O)Oc2cccc(Cl)c2Cl)c1C</chem>                              |
| <b>Mol. weight [g/mol]:</b> | 367.22   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -204.72 | kJ/mol               | Joback Method  |
| hf            | -508.75 | kJ/mol               | Joback Method  |
| hfus          | 42.87   | kJ/mol               | Joback Method  |
| hvap          | 89.94   | kJ/mol               | Joback Method  |
| log10ws       | -6.07   |                      | Crippen Method |
| logp          | 4.901   |                      | Crippen Method |
| mcvol         | 256.320 | ml/mol               | McGowan Method |
| pc            | 1848.33 | kPa                  | Joback Method  |
| rinpol        | 2844.00 |                      | NIST Webbook   |
| rinpol        | 2844.00 |                      | NIST Webbook   |
| tb            | 911.96  | K                    | Joback Method  |
| tc            | 1148.51 | K                    | Joback Method  |
| tf            | 599.70  | K                    | Joback Method  |
| vc            | 0.974   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 707.74    | J/molxK | 911.96          | Joback Method |
| cpg           | 749.81    | J/molxK | 1109.09         | Joback Method |
| cpg           | 743.84    | J/molxK | 1069.66         | Joback Method |
| cpg           | 736.66    | J/molxK | 1030.24         | Joback Method |
| cpg           | 728.26    | J/molxK | 990.81          | Joback Method |
| cpg           | 718.63    | J/molxK | 951.39          | Joback Method |
| cpg           | 754.59    | J/molxK | 1148.51         | Joback Method |
| dvisc         | 0.0000588 | Paxs    | 911.96          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000715 | Paxs | 859.92 | Joback Method |
| dvisc | 0.0000892 | Paxs | 807.87 | Joback Method |
| dvisc | 0.0001146 | Paxs | 755.83 | Joback Method |
| dvisc | 0.0001529 | Paxs | 703.79 | Joback Method |
| dvisc | 0.0002136 | Paxs | 651.74 | Joback Method |
| dvisc | 0.0003162 | Paxs | 599.70 | 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=U390029&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390029&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>cp<sub>g</sub>:</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>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</b>    | Octanol/Water partition coefficient             |
| <b>m<sub>cvol</sub>:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>                 | Critical Pressure                               |
| <b>rin<sub>pol</sub>:</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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