

# Succinic acid, 2-(2-chlorophenoxy)ethyl ethyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C14H17ClO5/c1-2-18-13(16)7-8-14(17)20-10-9-19-12-6-4-3-5-11(12)15/h3-6H |
| InchiKey:            | CHSIRNHJPJDHLW-UHFFFAOYSA-N  |
| Formula:             | C14H17ClO5   |
| SMILES:              | CCOC(=O)CCC(=O)OCCOc1ccccc1Cl  |
| Mol. weight [g/mol]: | 300.74   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -414.99 | kJ/mol  | Joback Method  |
| hf            | -744.79 | kJ/mol  | Joback Method  |
| hfus          | 36.63   | kJ/mol  | Joback Method  |
| hvap          | 74.80   | kJ/mol  | Joback Method  |
| log10ws       | -2.93   |         | Crippen Method |
| logp          | 2.605   |         | Crippen Method |
| mcvol         | 217.350 | ml/mol  | McGowan Method |
| pc            | 2051.17 | kPa     | Joback Method  |
| rinpol        | 2156.00 |         | NIST Webbook   |
| rinpol        | 2156.00 |         | NIST Webbook   |
| tb            | 763.81  | K       | Joback Method  |
| tc            | 971.80  | K       | Joback Method  |
| tf            | 482.95  | K       | Joback Method  |
| vc            | 0.827   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 592.22    | J/molxK | 763.81          | Joback Method |
| cpg           | 605.21    | J/molxK | 798.48          | Joback Method |
| cpg           | 617.25    | J/molxK | 833.14          | Joback Method |
| cpg           | 628.35    | J/molxK | 867.81          | Joback Method |
| cpg           | 638.48    | J/molxK | 902.47          | Joback Method |
| cpg           | 647.66    | J/molxK | 937.14          | Joback Method |
| cpg           | 655.88    | J/molxK | 971.80          | Joback Method |
| dvisc         | 0.0006127 | Paxs    | 482.95          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003779 | Paxs | 529.76 | Joback Method |
| dvisc | 0.0002521 | Paxs | 576.57 | Joback Method |
| dvisc | 0.0001788 | Paxs | 623.38 | Joback Method |
| dvisc | 0.0001330 | Paxs | 670.19 | Joback Method |
| dvisc | 0.0001028 | Paxs | 717.00 | Joback Method |
| dvisc | 0.0000820 | Paxs | 763.81 | 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=U381531&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381531&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>cpg:</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>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>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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