

# Succinic acid, 3-chlorophenethyl heptyl ester

**Inchi:** InChI=1S/C19H27ClO4/c1-2-3-4-5-6-13-23-18(21)10-11-19(22)24-14-12-16-8-7-9-17(20)  
**InchiKey:** OXWKPMFQUFURNJ-UHFFFAOYSA-N  
**Formula:** C19H27ClO4  
**SMILES:** CCCCCCOC(=O)CCC(=O)OCCc1cccc(Cl)c1  
**Mol. weight [g/mol]:** 354.87

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -267.89 | kJ/mol               | Joback Method  |
| hf            | -715.77 | kJ/mol               | Joback Method  |
| hfus          | 48.39   | kJ/mol               | Joback Method  |
| hvap          | 83.52   | kJ/mol               | Joback Method  |
| log10ws       | -5.29   |                      | Crippen Method |
| logp          | 4.719   |                      | Crippen Method |
| mvol          | 281.930 | ml/mol               | McGowan Method |
| pc            | 1401.69 | kPa                  | Joback Method  |
| rinpol        | 2536.00 |                      | NIST Webbook   |
| rinpol        | 2536.00 |                      | NIST Webbook   |
| tb            | 855.79  | K                    | Joback Method  |
| tc            | 1060.17 | K                    | Joback Method  |
| tf            | 517.07  | K                    | Joback Method  |
| vc            | 1.089   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 846.29    | J/molxK | 855.79          | Joback Method |
| cpg           | 861.04    | J/molxK | 889.85          | Joback Method |
| cpg           | 874.69    | J/molxK | 923.92          | Joback Method |
| cpg           | 887.26    | J/molxK | 957.98          | Joback Method |
| cpg           | 898.76    | J/molxK | 992.04          | Joback Method |
| cpg           | 909.23    | J/molxK | 1026.10         | Joback Method |
| cpg           | 918.69    | J/molxK | 1060.17         | Joback Method |
| dvisc         | 0.0005380 | Paxs    | 517.07          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003045 | Paxs | 573.52 | Joback Method |
| dvisc | 0.0001909 | Paxs | 629.98 | Joback Method |
| dvisc | 0.0001292 | Paxs | 686.43 | Joback Method |
| dvisc | 0.0000928 | Paxs | 742.88 | Joback Method |
| dvisc | 0.0000698 | Paxs | 799.34 | Joback Method |
| dvisc | 0.0000546 | Paxs | 855.79 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381498&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381498&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>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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