

# Succinic acid, hept-2-yl 2-chloro-4-methylphenyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C18H25ClO4/c1-4-5-6-7-14(3)22-17(20)10-11-18(21)23-16-9-8-13(2)12-15(16) |
| <b>InchiKey:</b>            | QVFHMPJMYPCHEJ-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C18H25ClO4  |
| <b>SMILES:</b>              | CCCCC(C)OC(=O)CCC(=O)Oc1ccc(C)cc1Cl   |
| <b>Mol. weight [g/mol]:</b> | 340.84  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -288.38 | kJ/mol               | Joback Method  |
| hf            | -711.88 | kJ/mol               | Joback Method  |
| hfus          | 41.89   | kJ/mol               | Joback Method  |
| hvap          | 81.57   | kJ/mol               | Joback Method  |
| log10ws       | -5.69   |                      | Crippen Method |
| logp          | 4.846   |                      | Crippen Method |
| mvol          | 267.840 | ml/mol               | McGowan Method |
| pc            | 1499.99 | kPa                  | Joback Method  |
| rinpol        | 2336.00 |                      | NIST Webbook   |
| rinpol        | 2336.00 |                      | NIST Webbook   |
| tb            | 837.45  | K                    | Joback Method  |
| tc            | 1044.56 | K                    | Joback Method  |
| tf            | 503.32  | K                    | Joback Method  |
| vc            | 1.026   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 788.01    | J/molxK | 837.45          | Joback Method |
| cpg           | 802.59    | J/molxK | 871.97          | Joback Method |
| cpg           | 816.08    | J/molxK | 906.49          | Joback Method |
| cpg           | 828.48    | J/molxK | 941.00          | Joback Method |
| cpg           | 839.81    | J/molxK | 975.52          | Joback Method |
| cpg           | 850.09    | J/molxK | 1010.04         | Joback Method |
| cpg           | 859.32    | J/molxK | 1044.56         | Joback Method |
| dvisc         | 0.0005729 | Paxs    | 503.32          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003239 | Paxs | 559.01 | Joback Method |
| dvisc | 0.0002030 | Paxs | 614.70 | Joback Method |
| dvisc | 0.0001375 | Paxs | 670.38 | Joback Method |
| dvisc | 0.0000989 | Paxs | 726.07 | Joback Method |
| dvisc | 0.0000745 | Paxs | 781.76 | Joback Method |
| dvisc | 0.0000583 | Paxs | 837.45 | 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=U390217&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390217&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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