

# Succinic acid, di(8-chlorooctyl) ester

**Inchi:** InChI=1S/C20H36Cl2O4/c21-15-9-5-1-3-7-11-17-25-19(23)13-14-20(24)26-18-12-8-4-2-6  
**InchiKey:** WSNMNGSFYRGKBL-UHFFFAOYSA-N  
**Formula:** C20H36Cl2O4  
**SMILES:** O=C(CCC(=O)OCCCCCCCCCl)OCCCCCCCCCl  
**Mol. weight [g/mol]:** 411.40

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -374.18 | kJ/mol               | Joback Method  |
| hf            | -977.21 | kJ/mol               | Joback Method  |
| hfus          | 61.52   | kJ/mol               | Joback Method  |
| hvap          | 87.20   | kJ/mol               | Joback Method  |
| log10ws       | -6.23   |                      | Crippen Method |
| logp          | 6.012   |                      | Crippen Method |
| mvol          | 332.020 | ml/mol               | McGowan Method |
| pc            | 1027.28 | kPa                  | Joback Method  |
| rinpol        | 3011.00 |                      | NIST Webbook   |
| rinpol        | 3011.00 |                      | NIST Webbook   |
| tb            | 884.44  | K                    | Joback Method  |
| tc            | 1082.98 | K                    | Joback Method  |
| tf            | 519.32  | K                    | Joback Method  |
| vc            | 1.302   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1030.28   | J/molxK | 884.44          | Joback Method |
| cpg           | 1046.71   | J/molxK | 917.53          | Joback Method |
| cpg           | 1062.00   | J/molxK | 950.62          | Joback Method |
| cpg           | 1076.16   | J/molxK | 983.71          | Joback Method |
| cpg           | 1089.23   | J/molxK | 1016.80         | Joback Method |
| cpg           | 1101.23   | J/molxK | 1049.89         | Joback Method |
| cpg           | 1112.18   | J/molxK | 1082.98         | Joback Method |
| dvisc         | 0.0005197 | Paxs    | 519.32          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002683 | Paxs | 580.17 | Joback Method |
| dvisc | 0.0001571 | Paxs | 641.03 | Joback Method |
| dvisc | 0.0001009 | Paxs | 701.88 | Joback Method |
| dvisc | 0.0000695 | Paxs | 762.73 | Joback Method |
| dvisc | 0.0000507 | Paxs | 823.59 | Joback Method |
| dvisc | 0.0000385 | Paxs | 884.44 | 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=U349298&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349298&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>logp:</b>               | Octanol/Water partition coefficient             |
| <b>m<sub>cvol</sub>:</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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