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

**Inchi:** InChI=1S/C19H27ClO5/c1-2-3-4-5-8-13-24-18(21)11-12-19(22)25-15-14-23-17-10-7-6-9-

**InchiKey:** BWADBRVWFQORHU-UHFFFAOYSA-N

**Formula:** C19H27ClO5

**SMILES:** CCCCCCCOC(=O)CCC(=O)OCCOc1ccccc1Cl

**Mol. weight [g/mol]:** 370.87

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -372.89 | kJ/mol | Joback Method |
| hf | -847.99 | kJ/mol | Joback Method |
| hfus | 49.58 | kJ/mol | Joback Method |
| hvap | 85.93 | kJ/mol | Joback Method |
| log10ws | -5.02 | | Crippen Method |
| logp | 4.556 | | Crippen Method |
| mcvol | 287.800 | ml/mol | McGowan Method |
| pc | 1384.02 | kPa | Joback Method |
| rinpol | 2645.00 | | NIST Webbook |
| rinpol | 2645.00 | | NIST Webbook |
| tb | 878.21 | K | Joback Method |
| tc | 1083.90 | K | Joback Method |
| tf | 539.30 | K | Joback Method |
| vc | 1.107 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 874.61 | J/mol×K | 878.21 | Joback Method |
| cpg | 888.85 | J/mol×K | 912.49 | Joback Method |
| cpg | 901.90 | J/mol×K | 946.77 | Joback Method |
| cpg | 913.75 | J/mol×K | 981.06 | Joback Method |
| cpg | 924.43 | J/mol×K | 1015.34 | Joback Method |
| cpg | 933.95 | J/mol×K | 1049.62 | Joback Method |
| cpg | 942.31 | J/mol×K | 1083.90 | Joback Method |
| dvisc | 0.0003777 | Pa×s | 539.30 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002186 | Pa×s | 595.78 | Joback Method |
| dvisc | 0.0001390 | Pa×s | 652.27 | Joback Method |
| dvisc | 0.0000951 | Pa×s | 708.75 | Joback Method |
| dvisc | 0.0000688 | Pa×s | 765.24 | Joback Method |
| dvisc | 0.0000520 | Pa×s | 821.72 | Joback Method |
| dvisc | 0.0000408 | Pa×s | 878.21 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381538&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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