# Succinic acid, 2-chlorophenethyl pentadecyl ester

**Inchi:** InChI=1S/C27H43ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-22-31-26(29)19-20-27(30)32-

**InchiKey:** IYKOBYPJOLNLND-UHFFFAOYSA-N

**Formula:** C27H43ClO4

**SMILES:** CCCCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1ccccc1Cl

**Mol. weight [g/mol]:** 467.08

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -200.53 | kJ/mol | Joback Method |
| hf | -880.89 | kJ/mol | Joback Method |
| hfus | 69.11 | kJ/mol | Joback Method |
| hvap | 101.33 | kJ/mol | Joback Method |
| log10ws | -8.64 | | Crippen Method |
| logp | 7.840 | | Crippen Method |
| mcvol | 394.650 | ml/mol | McGowan Method |
| pc | 845.54 | kPa | Joback Method |
| rinpol | 3330.00 | | NIST Webbook |
| rinpol | 3330.00 | | NIST Webbook |
| tb | 1038.83 | K | Joback Method |
| tc | 1276.26 | K | Joback Method |
| tf | 607.23 | K | Joback Method |
| vc | 1.536 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1332.19 | J/mol×K | 1038.83 | Joback Method |
| cpg | 1399.40 | J/mol×K | 1236.69 | Joback Method |
| cpg | 1389.11 | J/mol×K | 1197.12 | Joback Method |
| cpg | 1377.32 | J/mol×K | 1157.54 | Joback Method |
| cpg | 1363.95 | J/mol×K | 1117.97 | Joback Method |
| cpg | 1348.93 | J/mol×K | 1078.40 | Joback Method |
| cpg | 1408.26 | J/mol×K | 1276.26 | Joback Method |
| dvisc | 0.0000163 | Pa×s | 1038.83 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000213 | Pa×s | 966.90 | Joback Method |
| dvisc | 0.0000291 | Pa×s | 894.96 | Joback Method |
| dvisc | 0.0000420 | Pa×s | 823.03 | Joback Method |
| dvisc | 0.0000649 | Pa×s | 751.10 | Joback Method |
| dvisc | 0.0001099 | Pa×s | 679.16 | Joback Method |
| dvisc | 0.0002112 | Pa×s | 607.23 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U381486&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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