# Succinic acid, 8-chlorooctyl 1-phenylpropyl ester

**Inchi:** InChI=1S/C21H31ClO4/c1-2-19(18-12-8-7-9-13-18)26-21(24)15-14-20(23)25-17-11-6-4-3

**InchiKey:** CWBQLMJCHKSCJE-UHFFFAOYSA-N

**Formula:** C21H31ClO4

**SMILES:** CCC(OC(=O)CCC(=O)OCCCCCCCCCCl)c1ccccc1

**Mol. weight [g/mol]:** 382.92

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -243.86 | kJ/mol | Joback Method |
| hf | -750.86 | kJ/mol | Joback Method |
| hfus | 50.44 | kJ/mol | Joback Method |
| hvap | 86.92 | kJ/mol | Joback Method |
| log10ws | -6.05 | | Crippen Method |
| logp | 5.584 | | Crippen Method |
| mcvol | 310.110 | ml/mol | McGowan Method |
| pc | 1239.83 | kPa | Joback Method |
| rinpol | 2707.00 | | NIST Webbook |
| rinpol | 2707.00 | | NIST Webbook |
| tb | 896.13 | K | Joback Method |
| tc | 1103.49 | K | Joback Method |
| tf | 512.09 | K | Joback Method |
| vc | 1.194 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 965.62 | J/mol×K | 896.13 | Joback Method |
| cpg | 980.95 | J/mol×K | 930.69 | Joback Method |
| cpg | 995.06 | J/mol×K | 965.25 | Joback Method |
| cpg | 1007.99 | J/mol×K | 999.81 | Joback Method |
| cpg | 1019.78 | J/mol×K | 1034.37 | Joback Method |
| cpg | 1030.46 | J/mol×K | 1068.93 | Joback Method |
| cpg | 1040.07 | J/mol×K | 1103.49 | Joback Method |
| dvisc | 0.0005645 | Pa×s | 512.09 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002779 | Pa×s | 576.10 | Joback Method |
| dvisc | 0.0001576 | Pa×s | 640.10 | Joback Method |
| dvisc | 0.0000991 | Pa×s | 704.11 | Joback Method |
| dvisc | 0.0000673 | Pa×s | 768.12 | Joback Method |
| dvisc | 0.0000485 | Pa×s | 832.12 | Joback Method |
| dvisc | 0.0000367 | Pa×s | 896.13 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U389935&Units=SI |

# 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 |