# Sebacic acid, 2,4-dichlorophenyl pentyl ester

**Inchi:** InChI=1S/C21H30Cl2O4/c1-2-3-10-15-26-20(24)11-8-6-4-5-7-9-12-21(25)27-19-14-13-17
**InchiKey:** ZRVFOEACLDUNIK-UHFFFAOYSA-N
**Formula:** C21H30Cl2O4
**SMILES:** CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)cc1Cl
**Mol. weight [g/mol]:** 417.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -272.61 | kJ/mol | Joback Method |
| hf | -784.26 | kJ/mol | Joback Method |
| hfus | 57.38 | kJ/mol | Joback Method |
| hvap | 93.02 | kJ/mol | Joback Method |
| log10ws | -7.46 | | Crippen Method |
| logp | 6.753 | | Crippen Method |
| mcvol | 322.350 | ml/mol | McGowan Method |
| pc | 1176.85 | kPa | Joback Method |
| rinpol | 2988.00 | | NIST Webbook |
| rinpol | 2988.00 | | NIST Webbook |
| tb | 943.96 | K | Joback Method |
| tc | 1158.36 | K | Joback Method |
| tf | 582.05 | K | Joback Method |
| vc | 1.250 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 988.45 | J/mol×K | 943.96 | Joback Method |
| cpg | 1045.81 | J/mol×K | 1122.62 | Joback Method |
| cpg | 1036.72 | J/mol×K | 1086.89 | Joback Method |
| cpg | 1026.47 | J/mol×K | 1051.16 | Joback Method |
| cpg | 1015.03 | J/mol×K | 1015.43 | Joback Method |
| cpg | 1002.36 | J/mol×K | 979.69 | Joback Method |
| cpg | 1053.76 | J/mol×K | 1158.36 | Joback Method |
| dvisc | 0.0000353 | Pa×s | 943.96 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000448 | Pa×s | 883.64 | Joback Method |
| dvisc | 0.0000589 | Pa×s | 823.32 | Joback Method |
| dvisc | 0.0000809 | Pa×s | 763.00 | Joback Method |
| dvisc | 0.0001172 | Pa×s | 702.69 | Joback Method |
| dvisc | 0.0001821 | Pa×s | 642.37 | Joback Method |
| dvisc | 0.0003100 | Pa×s | 582.05 | Joback Method |

# Sources

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|---|---|
| **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=U354569&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |