# Succinic acid, 2,3-dichlorophenyl neopentyl ester

**Inchi:** InChI=1S/C15H18Cl2O4/c1-15(2,3)9-20-12(18)7-8-13(19)21-11-6-4-5-10(16)14(11)17/h4

**InchiKey:** KIAUQVRRYIUIEZ-UHFFFAOYSA-N

**Formula:** C15H18Cl2O4

**SMILES:** CC(C)(C)COC(=O)CCC(=O)Oc1cccc(Cl)c1Cl

**Mol. weight [g/mol]:** 333.21

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -320.29 | kJ/mol | Joback Method |
| hf | -669.17 | kJ/mol | Joback Method |
| hfus | 34.42 | kJ/mol | Joback Method |
| hvap | 78.37 | kJ/mol | Joback Method |
| log10ws | -4.71 | | Crippen Method |
| logp | 4.268 | | Crippen Method |
| mcvol | 237.810 | ml/mol | McGowan Method |
| pc | 1857.91 | kPa | Joback Method |
| rinpol | 2207.00 | | NIST Webbook |
| rinpol | 2207.00 | | NIST Webbook |
| tb | 803.45 | K | Joback Method |
| tc | 1023.67 | K | Joback Method |
| tf | 516.85 | K | Joback Method |
| vc | 0.902 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 645.24 | J/mol×K | 803.45 | Joback Method |
| cpg | 698.73 | J/mol×K | 986.97 | Joback Method |
| cpg | 689.94 | J/mol×K | 950.26 | Joback Method |
| cpg | 680.23 | J/mol×K | 913.56 | Joback Method |
| cpg | 669.56 | J/mol×K | 876.86 | Joback Method |
| cpg | 657.91 | J/mol×K | 840.15 | Joback Method |
| cpg | 706.62 | J/mol×K | 1023.67 | Joback Method |
| dvisc | 0.0000671 | Pa×s | 803.45 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000848 | Pa×s | 755.68 | Joback Method |
| dvisc | 0.0001106 | Pa×s | 707.92 | Joback Method |
| dvisc | 0.0001498 | Pa×s | 660.15 | Joback Method |
| dvisc | 0.0002129 | Pa×s | 612.38 | Joback Method |
| dvisc | 0.0003211 | Pa×s | 564.62 | Joback Method |
| dvisc | 0.0005224 | Pa×s | 516.85 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U389589&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 |

# 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 |