# Succinic acid, 2-fluorophenyl 2-chlorophenyl ester

**Inchi:** InChI=1S/C16H12ClFO4/c17-11-5-1-3-7-13(11)21-15(19)9-10-16(20)22-14-8-4-2-6-12(14

**InchiKey:** OQWPZCHJHDUMPG-UHFFFAOYSA-N

**Formula:** C16H12ClFO4

**SMILES:** O=C(CCC(=O)Oc1ccccc1Cl)Oc1ccccc1F

**Mol. weight [g/mol]:** 322.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -385.18 | kJ/mol | Joback Method |
| hf | -624.90 | kJ/mol | Joback Method |
| hfus | 37.35 | kJ/mol | Joback Method |
| hvap | 78.97 | kJ/mol | Joback Method |
| log10ws | -4.76 | | Crippen Method |
| logp | 3.770 | | Crippen Method |
| mcvol | 217.670 | ml/mol | McGowan Method |
| pc | 2241.88 | kPa | Joback Method |
| rinpol | 2339.00 | | NIST Webbook |
| rinpol | 2339.00 | | NIST Webbook |
| tb | 818.08 | K | Joback Method |
| tc | 1048.23 | K | Joback Method |
| tf | 522.79 | K | Joback Method |
| vc | 0.831 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 587.19 | J/mol×K | 818.08 | Joback Method |
| cpg | 598.70 | J/mol×K | 856.44 | Joback Method |
| cpg | 609.08 | J/mol×K | 894.80 | Joback Method |
| cpg | 618.38 | J/mol×K | 933.15 | Joback Method |
| cpg | 626.60 | J/mol×K | 971.51 | Joback Method |
| cpg | 633.78 | J/mol×K | 1009.87 | Joback Method |
| cpg | 639.93 | J/mol×K | 1048.23 | Joback Method |

# Sources

| | |
|---|---|
| **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=U389800&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |