# Succinic acid, 2-methylphenyl 3-fluorophenyl ester

**Inchi:** InChI=1S/C17H15FO4/c1-12-5-2-3-8-15(12)22-17(20)10-9-16(19)21-14-7-4-6-13(18)11-1

**InchiKey:** QHJJPLFXTLKRDO-UHFFFAOYSA-N

**Formula:** C17H15FO4

**SMILES:** Cc1ccccc1OC(=O)CCC(=O)Oc1cccc(F)c1

**Mol. weight [g/mol]:** 302.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -364.83 | kJ/mol | Joback Method |
| hf | -629.80 | kJ/mol | Joback Method |
| hfus | 35.74 | kJ/mol | Joback Method |
| hvap | 76.81 | kJ/mol | Joback Method |
| log10ws | -4.56 | | Crippen Method |
| logp | 3.425 | | Crippen Method |
| mcvol | 219.520 | ml/mol | McGowan Method |
| pc | 2121.68 | kPa | Joback Method |
| rinpol | 2270.00 | | NIST Webbook |
| tb | 803.53 | K | Joback Method |
| tc | 1027.80 | K | Joback Method |
| tf | 504.14 | K | Joback Method |
| vc | 0.838 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 619.17 | J/mol×K | 803.53 | Joback Method |
| cpg | 632.24 | J/mol×K | 840.91 | Joback Method |
| cpg | 644.17 | J/mol×K | 878.29 | Joback Method |
| cpg | 654.97 | J/mol×K | 915.66 | Joback Method |
| cpg | 664.68 | J/mol×K | 953.04 | Joback Method |
| cpg | 673.31 | J/mol×K | 990.42 | Joback Method |
| cpg | 680.88 | J/mol×K | 1027.80 | Joback Method |

# Sources

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|---|---|
| **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=U357537&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |