# Succinic acid, 2-chloro-6-fluorophenyl cis-hex-3-en-1-yl ester

**Inchi:** InChI=1S/C16H18ClFO4/c1-2-3-4-5-11-21-14(19)9-10-15(20)22-16-12(17)7-6-8-13(16)18

**InchiKey:** GWXMBNAANSITOC-ARJAWSKDSA-N

**Formula:** C16H18ClFO4

**SMILES:** CCC=CCCOC(=O)CCC(=O)Oc1c(F)cccc1Cl

**Mol. weight [g/mol]:** 328.76

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -417.37 | kJ/mol | Joback Method |
| hf | -744.21 | kJ/mol | Joback Method |
| hfus | 43.51 | kJ/mol | Joback Method |
| hvap | 76.65 | kJ/mol | Joback Method |
| log10ws | -4.87 | | Crippen Method |
| logp | 4.064 | | Crippen Method |
| mcvol | 237.130 | ml/mol | McGowan Method |
| pc | 1749.21 | kPa | Joback Method |
| rinpol | 2245.00 | | NIST Webbook |
| rinpol | 2245.00 | | NIST Webbook |
| tb | 795.56 | K | Joback Method |
| tc | 1001.35 | K | Joback Method |
| tf | 491.29 | K | Joback Method |
| vc | 0.918 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 656.06 | J/mol×K | 795.56 | Joback Method |
| cpg | 668.95 | J/mol×K | 829.86 | Joback Method |
| cpg | 680.93 | J/mol×K | 864.16 | Joback Method |
| cpg | 692.04 | J/mol×K | 898.46 | Joback Method |
| cpg | 702.29 | J/mol×K | 932.75 | Joback Method |
| cpg | 711.70 | J/mol×K | 967.05 | Joback Method |
| cpg | 720.30 | J/mol×K | 1001.35 | Joback Method |

# Sources

| | |
|---|---|
| **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=U391086&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 |
| **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 |