# Succinic acid, 3-chlorophenyl 2-bromo-4-fluorophenyl ester

**Inchi:** InChI=1S/C16H11BrClFO4/c17-13-9-11(19)4-5-14(13)23-16(21)7-6-15(20)22-12-3-1-2-1

**InchiKey:** LCZZWYZYMALDLA-UHFFFAOYSA-N

**Formula:** C16H11BrClFO4

**SMILES:** O=C(CCC(=O)Oc1ccc(F)cc1Br)Oc1cccc(Cl)c1

**Mol. weight [g/mol]:** 401.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -380.49 | kJ/mol | Joback Method |
| hf | -610.04 | kJ/mol | Joback Method |
| hfus | 42.25 | kJ/mol | Joback Method |
| hvap | 86.06 | kJ/mol | Joback Method |
| log10ws | -5.93 | | Crippen Method |
| logp | 4.533 | | Crippen Method |
| mcvol | 235.170 | ml/mol | McGowan Method |
| pc | 2361.07 | kPa | Joback Method |
| rinpol | 2585.00 | | NIST Webbook |
| rinpol | 2585.00 | | NIST Webbook |
| tb | 889.22 | K | Joback Method |
| tc | 1129.22 | K | Joback Method |
| tf | 595.11 | K | Joback Method |
| vc | 0.892 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 614.21 | J/mol×K | 889.22 | Joback Method |
| cpg | 623.79 | J/mol×K | 929.22 | Joback Method |
| cpg | 632.27 | J/mol×K | 969.22 | Joback Method |
| cpg | 639.68 | J/mol×K | 1009.22 | Joback Method |
| cpg | 646.04 | J/mol×K | 1049.22 | Joback Method |
| cpg | 651.40 | J/mol×K | 1089.22 | Joback Method |
| cpg | 655.78 | J/mol×K | 1129.22 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U389771&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |