# Succinic acid, 2-fluorophenyl 4-bromo-2-methoxyphenyl ester

**Inchi:** InChI=1S/C17H14BrFO5/c1-22-15-10-11(18)6-7-14(15)24-17(21)9-8-16(20)23-13-5-3-2-4

**InchiKey:** VZWDQIXTSMSXOV-UHFFFAOYSA-N

**Formula:** C17H14BrFO5

**SMILES:** COc1cc(Br)ccc1OC(=O)CCC(=O)Oc1ccccc1F

**Mol. weight [g/mol]:** 397.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -465.14 | kJ/mol | Joback Method |
| hf | -747.16 | kJ/mol | Joback Method |
| hfus | 41.83 | kJ/mol | Joback Method |
| hvap | 86.31 | kJ/mol | Joback Method |
| log10ws | -5.36 | | Crippen Method |
| logp | 3.888 | | Crippen Method |
| mcvol | 242.890 | ml/mol | McGowan Method |
| pc | 2195.89 | kPa | Joback Method |
| rinpol | 2711.00 | | NIST Webbook |
| rinpol | 2711.00 | | NIST Webbook |
| tb | 897.09 | K | Joback Method |
| tc | 1129.79 | K | Joback Method |
| tf | 598.69 | K | Joback Method |
| vc | 0.917 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 674.83 | J/mol×K | 897.09 | Joback Method |
| cpg | 685.29 | J/mol×K | 935.87 | Joback Method |
| cpg | 694.52 | J/mol×K | 974.66 | Joback Method |
| cpg | 702.52 | J/mol×K | 1013.44 | Joback Method |
| cpg | 709.30 | J/mol×K | 1052.22 | Joback Method |
| cpg | 714.87 | J/mol×K | 1091.00 | Joback Method |
| cpg | 719.24 | J/mol×K | 1129.79 | 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=U390918&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 |