# Fumaric acid, 4-bromophenyl 2-fluorophenyl ester

**Inchi:** InChI=1S/C16H10BrFO4/c17-11-5-7-12(8-6-11)21-15(19)9-10-16(20)22-14-4-2-1-3-13(14

**InchiKey:** PBNWQAHQQRKUNI-MDZDMXLPSA-N

**Formula:** C16H10BrFO4

**SMILES:** O=C(C=CC(=O)Oc1ccccc1F)Oc1ccc(Br)cc1

**Mol. weight [g/mol]:** 365.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -278.71 | kJ/mol | Joback Method |
| hf | -465.61 | kJ/mol | Joback Method |
| hfus | 38.64 | kJ/mol | Joback Method |
| hvap | 80.97 | kJ/mol | Joback Method |
| log10ws | -5.10 | | Crippen Method |
| logp | 3.655 | | Crippen Method |
| mcvol | 218.630 | ml/mol | McGowan Method |
| pc | 2619.09 | kPa | Joback Method |
| tb | 850.97 | K | Joback Method |
| tc | 1095.42 | K | Joback Method |
| tf | 547.59 | K | Joback Method |
| vc | 0.824 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 569.04 | J/mol×K | 850.97 | Joback Method |
| cpg | 579.46 | J/mol×K | 891.71 | Joback Method |
| cpg | 588.84 | J/mol×K | 932.45 | Joback Method |
| cpg | 597.23 | J/mol×K | 973.19 | Joback Method |
| cpg | 604.70 | J/mol×K | 1013.93 | Joback Method |
| cpg | 611.30 | J/mol×K | 1054.68 | Joback Method |
| cpg | 617.09 | J/mol×K | 1095.42 | Joback Method |

# Sources

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|---|---|
| **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=U405771&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |