# Fumaric acid, monoamide, N-(2-bromophenyl)-, 2-fluorophenyl ester

**Inchi:** InChI=1S/C16H11BrFNO3/c17-11-5-1-3-7-13(11)19-15(20)9-10-16(21)22-14-8-4-2-6-12(

**InchiKey:** FAKJERTWWPSRBD-MDZDMXLPSA-N

**Formula:** C16H11BrFNO3

**SMILES:** O=C(C=CC(=O)Oc1ccccc1F)Nc1ccccc1Br

**Mol. weight [g/mol]:** 364.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -84.32 | kJ/mol | Joback Method |
| hf | -279.92 | kJ/mol | Joback Method |
| hfus | 42.55 | kJ/mol | Joback Method |
| hvap | 85.00 | kJ/mol | Joback Method |
| log10ws | -4.99 | | Crippen Method |
| logp | 3.688 | | Crippen Method |
| mcvol | 222.740 | ml/mol | McGowan Method |
| pc | 2701.41 | kPa | Joback Method |
| rinpol | 2759.00 | | NIST Webbook |
| rinpol | 2759.00 | | NIST Webbook |
| tb | 878.72 | K | Joback Method |
| tc | 1124.02 | K | Joback Method |
| tf | 578.02 | K | Joback Method |
| vc | 0.841 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 593.11 | J/mol×K | 878.72 | Joback Method |
| cpg | 603.29 | J/mol×K | 919.60 | Joback Method |
| cpg | 612.52 | J/mol×K | 960.49 | Joback Method |
| cpg | 620.91 | J/mol×K | 1001.37 | Joback Method |
| cpg | 628.52 | J/mol×K | 1042.26 | Joback Method |
| cpg | 635.45 | J/mol×K | 1083.14 | Joback Method |
| cpg | 641.77 | J/mol×K | 1124.02 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357480&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 |

# 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 |