# Fumaric acid, monoamide, N-(2-bromophenyl)-, 2,4,6-trichlorophenyl ester

**Inchi:** InChI=1S/C16H9BrCl3NO3/c17-10-3-1-2-4-13(10)21-14(22)5-6-15(23)24-16-11(19)7-9(1

**InchiKey:** KPDQBWJRVINLGB-AATRIKPKSA-N

**Formula:** C16H9BrCl3NO3

**SMILES:** O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Nc1ccccc1Br

**Mol. weight [g/mol]:** 449.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 55.44 | kJ/mol | Joback Method |
| hf | -153.97 | kJ/mol | Joback Method |
| hfus | 51.29 | kJ/mol | Joback Method |
| hvap | 100.30 | kJ/mol | Joback Method |
| log10ws | -6.71 | | Crippen Method |
| logp | 5.510 | | Crippen Method |
| mcvol | 257.690 | ml/mol | McGowan Method |
| pc | 2450.74 | kPa | Joback Method |
| rinpol | 3240.00 | | NIST Webbook |
| tb | 1001.70 | K | Joback Method |
| tc | 1263.33 | K | Joback Method |
| tf | 692.23 | K | Joback Method |
| vc | 0.970 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 632.60 | J/mol×K | 1001.70 | Joback Method |
| cpg | 639.95 | J/mol×K | 1045.30 | Joback Method |
| cpg | 646.53 | J/mol×K | 1088.91 | Joback Method |
| cpg | 652.42 | J/mol×K | 1132.51 | Joback Method |
| cpg | 657.72 | J/mol×K | 1176.12 | Joback Method |
| cpg | 662.51 | J/mol×K | 1219.72 | Joback Method |
| cpg | 666.87 | J/mol×K | 1263.33 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U357467&Units=SI |

# 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 |