# Fumaric acid, 4-bromophenyl hex-4-yn-3-yl ester

**Inchi:** InChI=1S/C16H15BrO4/c1-3-5-13(4-2)20-15(18)10-11-16(19)21-14-8-6-12(17)7-9-14/h6-

**InchiKey:** QBCNXANJJMVLJA-ZHACJKMWSA-N

**Formula:** C16H15BrO4

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

**Mol. weight [g/mol]:** 351.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 13.68 | kJ/mol | Joback Method |
| hf | -227.54 | kJ/mol | Joback Method |
| hfus | 41.51 | kJ/mol | Joback Method |
| hvap | 80.62 | kJ/mol | Joback Method |
| log10ws | -4.92 | | Crippen Method |
| logp | 3.256 | | Crippen Method |
| mcvol | 232.020 | ml/mol | McGowan Method |
| pc | 2363.37 | kPa | Joback Method |
| rinpol | 2331.00 | | NIST Webbook |
| rinpol | 2331.00 | | NIST Webbook |
| tb | 828.60 | K | Joback Method |
| tc | 1069.41 | K | Joback Method |
| tf | 599.16 | K | Joback Method |
| vc | 0.870 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 609.90 | J/mol×K | 828.60 | Joback Method |
| cpg | 622.39 | J/mol×K | 868.73 | Joback Method |
| cpg | 633.84 | J/mol×K | 908.87 | Joback Method |
| cpg | 644.28 | J/mol×K | 949.00 | Joback Method |
| cpg | 653.76 | J/mol×K | 989.14 | Joback Method |
| cpg | 662.32 | J/mol×K | 1029.27 | Joback Method |
| cpg | 670.00 | J/mol×K | 1069.41 | 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=U405769&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |