# Succinic acid, but-3-yn-2-yl 4-bromophenyl ester

**Inchi:** InChI=1S/C14H13BrO4/c1-3-10(2)18-13(16)8-9-14(17)19-12-6-4-11(15)5-7-12/h1,4-7,10

**InchiKey:** VWFVOZUJAXCPNO-UHFFFAOYSA-N

**Formula:** C14H13BrO4

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

**Mol. weight [g/mol]:** 325.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -63.11 | kJ/mol | Joback Method |
| hf | -283.88 | kJ/mol | Joback Method |
| hfus | 35.98 | kJ/mol | Joback Method |
| hvap | 73.91 | kJ/mol | Joback Method |
| log10ws | -4.23 | | Crippen Method |
| logp | 2.700 | | Crippen Method |
| mcvol | 208.140 | ml/mol | McGowan Method |
| pc | 2687.42 | kPa | Joback Method |
| rinpol | 2083.00 | | NIST Webbook |
| rinpol | 2083.00 | | NIST Webbook |
| tb | 759.80 | K | Joback Method |
| tc | 991.79 | K | Joback Method |
| tf | 522.57 | K | Joback Method |
| vc | 0.777 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 527.44 | J/mol×K | 759.80 | Joback Method |
| cpg | 539.42 | J/mol×K | 798.46 | Joback Method |
| cpg | 550.45 | J/mol×K | 837.13 | Joback Method |
| cpg | 560.54 | J/mol×K | 875.79 | Joback Method |
| cpg | 569.74 | J/mol×K | 914.46 | Joback Method |
| cpg | 578.05 | J/mol×K | 953.12 | Joback Method |
| cpg | 585.52 | J/mol×K | 991.79 | 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=U389819&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 |