# Glutaric acid, but-3-yn-2-yl 2-chloro-5-methylphenyl ester

**Inchi:** InChI=1S/C16H17ClO4/c1-4-12(3)20-15(18)6-5-7-16(19)21-14-10-11(2)8-9-13(14)17/h1,

**InchiKey:** FHMCLXANRRHSST-UHFFFAOYSA-N

**Formula:** C16H17ClO4

**SMILES:** C#CC(C)OC(=O)CCCC(=O)Oc1cc(C)ccc1Cl

**Mol. weight [g/mol]:** 308.76

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -82.15 | kJ/mol | Joback Method |
| hf | -378.70 | kJ/mol | Joback Method |
| hfus | 39.68 | kJ/mol | Joback Method |
| hvap | 76.98 | kJ/mol | Joback Method |
| log10ws | -4.65 | | Crippen Method |
| logp | 3.289 | | Crippen Method |
| mcvol | 231.060 | ml/mol | McGowan Method |
| pc | 1989.43 | kPa | Joback Method |
| rinpol | 2149.00 | | NIST Webbook |
| rinpol | 2149.00 | | NIST Webbook |
| tb | 781.81 | K | Joback Method |
| tc | 1000.88 | K | Joback Method |
| tf | 527.75 | K | Joback Method |
| vc | 0.876 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 622.18 | J/mol×K | 781.81 | Joback Method |
| cpg | 635.33 | J/mol×K | 818.32 | Joback Method |
| cpg | 647.48 | J/mol×K | 854.83 | Joback Method |
| cpg | 658.67 | J/mol×K | 891.34 | Joback Method |
| cpg | 668.89 | J/mol×K | 927.86 | Joback Method |
| cpg | 678.18 | J/mol×K | 964.37 | Joback Method |
| cpg | 686.53 | J/mol×K | 1000.88 | 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=U393416&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 |