# Glutaric acid, but-3-yn-2-yl 4-chloro-2-methoxyphenyl ester

**Inchi:** InChI=1S/C16H17ClO5/c1-4-11(2)21-15(18)6-5-7-16(19)22-13-9-8-12(17)10-14(13)20-3/

**InchiKey:** AKEUFKOLKNHLQY-UHFFFAOYSA-N

**Formula:** C16H17ClO5

**SMILES:** C#CC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1OC

**Mol. weight [g/mol]:** 324.76

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -187.15 | kJ/mol | Joback Method |
| hf | -510.92 | kJ/mol | Joback Method |
| hfus | 40.87 | kJ/mol | Joback Method |
| hvap | 79.39 | kJ/mol | Joback Method |
| log10ws | -4.29 | | Crippen Method |
| logp | 2.989 | | Crippen Method |
| mcvol | 236.930 | ml/mol | McGowan Method |
| pc | 1959.60 | kPa | Joback Method |
| rinpol | 2255.00 | | NIST Webbook |
| rinpol | 2255.00 | | NIST Webbook |
| tb | 804.23 | K | Joback Method |
| tc | 1021.65 | K | Joback Method |
| tf | 549.98 | K | Joback Method |
| vc | 0.894 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 648.33 | J/mol×K | 804.23 | Joback Method |
| cpg | 661.07 | J/mol×K | 840.47 | Joback Method |
| cpg | 672.78 | J/mol×K | 876.70 | Joback Method |
| cpg | 683.45 | J/mol×K | 912.94 | Joback Method |
| cpg | 693.08 | J/mol×K | 949.18 | Joback Method |
| cpg | 701.68 | J/mol×K | 985.41 | Joback Method |
| cpg | 709.23 | J/mol×K | 1021.65 | 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=U393902&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 |