# Glutaric acid, but-3-yn-2-yl phenethyl ester

**Inchi:** InChI=1S/C17H20O4/c1-3-14(2)21-17(19)11-7-10-16(18)20-13-12-15-8-5-4-6-9-15/h1,4-
**InchiKey:** QSCVUFNECKYCKC-UHFFFAOYSA-N
**Formula:** C17H20O4
**SMILES:** C#CC(C)OC(=O)CCCC(=O)OCCc1ccccc1
**Mol. weight [g/mol]:** 288.34

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -42.54 | kJ/mol | Joback Method |
| hf | -360.66 | kJ/mol | Joback Method |
| hfus | 38.85 | kJ/mol | Joback Method |
| hvap | 73.49 | kJ/mol | Joback Method |
| log10ws | -3.67 | | Crippen Method |
| logp | 2.507 | | Crippen Method |
| mcvol | 232.910 | ml/mol | McGowan Method |
| pc | 1938.95 | kPa | Joback Method |
| rinpol | 2042.00 | | NIST Webbook |
| rinpol | 2042.00 | | NIST Webbook |
| tb | 757.30 | K | Joback Method |
| tc | 969.03 | K | Joback Method |
| tf | 484.06 | K | Joback Method |
| vc | 0.883 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 653.79 | J/mol×K | 757.30 | Joback Method |
| cpg | 668.63 | J/mol×K | 792.59 | Joback Method |
| cpg | 682.43 | J/mol×K | 827.88 | Joback Method |
| cpg | 695.22 | J/mol×K | 863.17 | Joback Method |
| cpg | 707.02 | J/mol×K | 898.46 | Joback Method |
| cpg | 717.87 | J/mol×K | 933.75 | Joback Method |
| cpg | 727.78 | J/mol×K | 969.03 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391786&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **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 |