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

**Inchi:** InChI=1S/C18H22O4/c1-4-9-15-10-6-7-11-16(15)22-18(20)13-8-12-17(19)21-14(3)5-2/h2

**InchiKey:** JBVFNOVTKZJBOP-UHFFFAOYSA-N

**Formula:** C18H22O4

**SMILES:** C#CC(C)OC(=O)CCCC(=O)Oc1ccccc1CCC

**Mol. weight [g/mol]:** 302.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -43.75 | kJ/mol | Joback Method |
| hf | -392.77 | kJ/mol | Joback Method |
| hfus | 41.05 | kJ/mol | Joback Method |
| hvap | 76.38 | kJ/mol | Joback Method |
| log10ws | -4.71 | | Crippen Method |
| logp | 3.280 | | Crippen Method |
| mcvol | 247.000 | ml/mol | McGowan Method |
| pc | 1762.45 | kPa | Joback Method |
| rinpol | 2068.00 | | NIST Webbook |
| rinpol | 2068.00 | | NIST Webbook |
| tb | 785.16 | K | Joback Method |
| tc | 995.53 | K | Joback Method |
| tf | 507.85 | K | Joback Method |
| vc | 0.940 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 708.37 | J/mol×K | 785.16 | Joback Method |
| cpg | 723.38 | J/mol×K | 820.22 | Joback Method |
| cpg | 737.33 | J/mol×K | 855.28 | Joback Method |
| cpg | 750.25 | J/mol×K | 890.35 | Joback Method |
| cpg | 762.17 | J/mol×K | 925.41 | Joback Method |
| cpg | 773.11 | J/mol×K | 960.47 | Joback Method |
| cpg | 783.09 | J/mol×K | 995.53 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392137&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

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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 |