

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

**Inchi:** InChI=1S/C16H22O4/c1-3-11(2)19-15(17)5-4-6-16(18)20-14-10-12-7-8-13(14)9-12/h1,11  
**InchiKey:** MZSQLNDULFIOJH-UHFFFAOYSA-N  
**Formula:** C16H22O4  
**SMILES:** C#CC(C)OC(=O)CCCC(=O)OC1CC2CCC1C2  
**Mol. weight [g/mol]:** 278.34

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -61.68  | kJ/mol               | Joback Method  |
| hf            | -457.45 | kJ/mol               | Joback Method  |
| hfus          | 37.46   | kJ/mol               | Joback Method  |
| hvap          | 68.68   | kJ/mol               | Joback Method  |
| log10ws       | -3.57   |                      | Crippen Method |
| logp          | 2.453   |                      | Crippen Method |
| mcvol         | 220.860 | ml/mol               | McGowan Method |
| pc            | 1968.30 | kPa                  | Joback Method  |
| rinpola       | 1924.00 |                      | NIST Webbook   |
| rinpola       | 1924.00 |                      | NIST Webbook   |
| tb            | 720.82  | K                    | Joback Method  |
| tc            | 930.06  | K                    | Joback Method  |
| tf            | 474.49  | K                    | Joback Method  |
| vc            | 0.841   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 659.55 | J/mol×K | 720.82          | Joback Method |
| cpg           | 676.87 | J/mol×K | 755.69          | Joback Method |
| cpg           | 693.10 | J/mol×K | 790.57          | Joback Method |
| cpg           | 708.29 | J/mol×K | 825.44          | Joback Method |
| cpg           | 722.50 | J/mol×K | 860.31          | Joback Method |
| cpg           | 735.77 | J/mol×K | 895.19          | Joback Method |
| cpg           | 748.17 | J/mol×K | 930.06          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405485&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405485&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvp:</b>     | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mvol:</b>    | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rpol:</b>    | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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