

# Glutaric acid, butyl 1-phenylethyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C17H24O4/c1-3-4-13-20-16(18)11-8-12-17(19)21-14(2)15-9-6-5-7-10-15/h5-7, |
| <b>InchiKey:</b>            | GVPCWSRHGRQQPY-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C17H24O4  |
| <b>SMILES:</b>              | CCCCOC(=O)CCCC(=O)OC(C)c1ccccc1   |
| <b>Mol. weight [g/mol]:</b> | 292.37  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -265.61 | kJ/mol               | Joback Method  |
| hf            | -652.56 | kJ/mol               | Joback Method  |
| hfus          | 35.88   | kJ/mol               | Joback Method  |
| hvap          | 73.64   | kJ/mol               | Joback Method  |
| log10ws       | -4.23   |                      | Crippen Method |
| logp          | 3.804   |                      | Crippen Method |
| mcvol         | 241.510 | ml/mol               | McGowan Method |
| pc            | 1708.95 | kPa                  | Joback Method  |
| rinpola       | 2254.00 |                      | NIST Webbook   |
| tb            | 767.18  | K                    | Joback Method  |
| tc            | 969.48  | K                    | Joback Method  |
| tf            | 437.09  | K                    | Joback Method  |
| vc            | 0.921   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 705.62    | J/molxK | 767.18          | Joback Method |
| cpg           | 773.93    | J/molxK | 935.76          | Joback Method |
| cpg           | 762.30    | J/molxK | 902.04          | Joback Method |
| cpg           | 749.67    | J/molxK | 868.33          | Joback Method |
| cpg           | 736.03    | J/molxK | 834.61          | Joback Method |
| cpg           | 721.35    | J/molxK | 800.90          | Joback Method |
| cpg           | 784.60    | J/molxK | 969.48          | Joback Method |
| dvisc         | 0.0000752 | Paxs    | 767.18          | Joback Method |
| dvisc         | 0.0000989 | Paxs    | 712.16          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001362 | Paxs | 657.15 | Joback Method |
| dvisc | 0.0001988 | Paxs | 602.13 | Joback Method |
| dvisc | 0.0003130 | Paxs | 547.12 | Joback Method |
| dvisc | 0.0005455 | Paxs | 492.11 | Joback Method |
| dvisc | 0.0010935 | Paxs | 437.09 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377513&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377513&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>dvisc:</b>   | Dynamic viscosity                               |
| <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>hvap:</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>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</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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