

# Glutaric acid, 3-methylbut-2-en-1-yl 4-biphenyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C22H24O4/c1-17(2)15-16-25-21(23)9-6-10-22(24)26-20-13-11-19(12-14-20)18 |
| <b>InchiKey:</b>            | LSKPNBMIYXPFKC-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C22H24O4   |
| <b>SMILES:</b>              | CC(C)=CCOC(=O)CCCC(=O)Oc1ccc(-c2ccccc2)cc1                                       |
| <b>Mol. weight [g/mol]:</b> | 352.42   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -46.62  | kJ/mol               | Joback Method  |
| hf            | -417.99 | kJ/mol               | Joback Method  |
| hfus          | 44.90   | kJ/mol               | Joback Method  |
| hvap          | 88.13   | kJ/mol               | Joback Method  |
| log10ws       | -6.45   |                      | Crippen Method |
| logp          | 4.939   |                      | Crippen Method |
| mcvol         | 283.900 | ml/mol               | McGowan Method |
| pc            | 1557.35 | kPa                  | Joback Method  |
| rinpol        | 2860.00 |                      | NIST Webbook   |
| rinpol        | 2860.00 |                      | NIST Webbook   |
| tb            | 917.72  | K                    | Joback Method  |
| tc            | 1146.47 | K                    | Joback Method  |
| tf            | 528.34  | K                    | Joback Method  |
| vc            | 1.081   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 869.39 | J/mol×K | 917.72          | Joback Method |
| cpg           | 883.56 | J/mol×K | 955.85          | Joback Method |
| cpg           | 896.49 | J/mol×K | 993.97          | Joback Method |
| cpg           | 908.24 | J/mol×K | 1032.10         | Joback Method |
| cpg           | 918.89 | J/mol×K | 1070.22         | Joback Method |
| cpg           | 928.49 | J/mol×K | 1108.35         | Joback Method |
| cpg           | 937.12 | J/mol×K | 1146.47         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U390122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390122&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |

# Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</b>     | Ideal gas heat capacity                         |
| <b>g<sub>f</sub>:</b>      | Standard Gibbs free energy of formation         |
| <b>h<sub>f</sub>:</b>      | Enthalpy of formation at standard conditions    |
| <b>h<sub>fus</sub>:</b>    | Enthalpy of fusion at standard conditions       |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</b>    | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>                 | Critical Pressure                               |
| <b>rin<sub>pol</sub>:</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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