

# Glutaric acid, 2-biphenyl hexyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C23H28O4/c1-2-3-4-10-18-26-22(24)16-11-17-23(25)27-21-15-9-8-14-20(21)1 |
| <b>InchiKey:</b>            | SZXMBKJMQWMLIE-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C23H28O4   |
| <b>SMILES:</b>              | CCCCCOC(=O)CCCC(=O)Oc1ccccc1-c1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 368.47   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -109.87 | kJ/mol               | Joback Method  |
| hf            | -546.06 | kJ/mol               | Joback Method  |
| hfus          | 48.59   | kJ/mol               | Joback Method  |
| hvap          | 90.32   | kJ/mol               | Joback Method  |
| log10ws       | -7.02   |                      | Crippen Method |
| logp          | 5.553   |                      | Crippen Method |
| mcvol         | 302.290 | ml/mol               | McGowan Method |
| pc            | 1385.05 | kPa                  | Joback Method  |
| rinpola       | 2773.00 |                      | NIST Webbook   |
| tb            | 936.56  | K                    | Joback Method  |
| tc            | 1158.33 | K                    | Joback Method  |
| tf            | 558.65  | K                    | Joback Method  |
| vc            | 1.155   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 957.00    | J/molxK | 936.56          | Joback Method |
| cpg           | 971.39    | J/molxK | 973.52          | Joback Method |
| cpg           | 984.43    | J/molxK | 1010.48         | Joback Method |
| cpg           | 996.18    | J/molxK | 1047.44         | Joback Method |
| cpg           | 1006.67   | J/molxK | 1084.41         | Joback Method |
| cpg           | 1015.97   | J/molxK | 1121.37         | Joback Method |
| cpg           | 1024.11   | J/molxK | 1158.33         | Joback Method |
| dvisc         | 0.0003786 | Paxs    | 558.65          | Joback Method |
| dvisc         | 0.0002108 | Paxs    | 621.63          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001307 | Paxs | 684.62 | Joback Method |
| dvisc | 0.0000879 | Paxs | 747.61 | Joback Method |
| dvisc | 0.0000628 | Paxs | 810.59 | Joback Method |
| dvisc | 0.0000472 | Paxs | 873.57 | Joback Method |
| dvisc | 0.0000368 | Paxs | 936.56 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U358970&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358970&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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