

# Glutaric acid, heptyl 2-naphthyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C22H28O4/c1-2-3-4-5-8-16-25-21(23)12-9-13-22(24)26-20-15-14-18-10-6-7-1 |
| <b>InchiKey:</b>            | ZSWVMEGLAVDGMX-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C22H28O4   |
| <b>SMILES:</b>              | CCCCCCCOC(=O)CCCC(=O)Oc1ccc2ccccc2c1   |
| <b>Mol. weight [g/mol]:</b> | 356.46   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -124.05 | kJ/mol               | Joback Method  |
| hf            | -570.88 | kJ/mol               | Joback Method  |
| hfus          | 48.98   | kJ/mol               | Joback Method  |
| hvap          | 87.46   | kJ/mol               | Joback Method  |
| log10ws       | -6.64   |                      | Crippen Method |
| logp          | 5.429   |                      | Crippen Method |
| mcvol         | 292.500 | ml/mol               | McGowan Method |
| pc            | 1395.41 | kPa                  | Joback Method  |
| rinqol        | 2955.00 |                      | NIST Webbook   |
| tb            | 905.98  | K                    | Joback Method  |
| tc            | 1119.89 | K                    | Joback Method  |
| tf            | 553.66  | K                    | Joback Method  |
| vc            | 1.129   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 920.00    | J/molxK | 905.98          | Joback Method |
| cpg           | 934.94    | J/molxK | 941.63          | Joback Method |
| cpg           | 948.76    | J/molxK | 977.28          | Joback Method |
| cpg           | 961.53    | J/molxK | 1012.93         | Joback Method |
| cpg           | 973.31    | J/molxK | 1048.59         | Joback Method |
| cpg           | 984.14    | J/molxK | 1084.24         | Joback Method |
| cpg           | 994.08    | J/molxK | 1119.89         | Joback Method |
| dvisc         | 0.0005974 | Paxs    | 553.66          | Joback Method |
| dvisc         | 0.0003677 | Paxs    | 612.38          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002463 | Paxs | 671.10 | Joback Method |
| dvisc | 0.0001760 | Paxs | 729.82 | Joback Method |
| dvisc | 0.0001322 | Paxs | 788.54 | Joback Method |
| dvisc | 0.0001034 | Paxs | 847.26 | Joback Method |
| dvisc | 0.0000834 | Paxs | 905.98 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U358783&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358783&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>                                 |

## 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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