

# Glutaric acid, ethyl heptadecyl ester

**Inchi:** InChI=1S/C24H46O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-28-24(26)21-19-20  
**InchiKey:** DHDPWFLMWKNDKA-UHFFFAOYSA-N  
**Formula:** C24H46O4  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC  
**Mol. weight [g/mol]:** 398.62

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -316.64  | kJ/mol  | Joback Method  |
| hf            | -1028.29 | kJ/mol  | Joback Method  |
| hfus          | 63.49    | kJ/mol  | Joback Method  |
| hvap          | 87.33    | kJ/mol  | Joback Method  |
| log10ws       | -7.59    |         | Crippen Method |
| logp          | 7.134    |         | Crippen Method |
| mcvol         | 363.900  | ml/mol  | McGowan Method |
| pc            | 849.99   | kPa     | Joback Method  |
| rinpol        | 2823.00  |         | NIST Webbook   |
| tb            | 901.10   | K       | Joback Method  |
| tc            | 1104.70  | K       | Joback Method  |
| tf            | 504.56   | K       | Joback Method  |
| vc            | 1.427    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1217.58   | J/molxK | 901.10          | Joback Method |
| cpg           | 1304.84   | J/molxK | 1070.77         | Joback Method |
| cpg           | 1290.07   | J/molxK | 1036.83         | Joback Method |
| cpg           | 1273.99   | J/molxK | 1002.90         | Joback Method |
| cpg           | 1256.57   | J/molxK | 968.97          | Joback Method |
| cpg           | 1237.78   | J/molxK | 935.03          | Joback Method |
| cpg           | 1318.35   | J/molxK | 1104.70         | Joback Method |
| dvisc         | 0.0000294 | Paxs    | 901.10          | Joback Method |
| dvisc         | 0.0000393 | Paxs    | 835.01          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000553 | Paxs | 768.92 | Joback Method |
| dvisc | 0.0000828 | Paxs | 702.83 | Joback Method |
| dvisc | 0.0001350 | Paxs | 636.74 | Joback Method |
| dvisc | 0.0002463 | Paxs | 570.65 | Joback Method |
| dvisc | 0.0005261 | Paxs | 504.56 | 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=U360006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360006&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>                         |

## 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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