

# Glutaric acid, 2-decyl hexyl ester

**Inchi:** InChI=1S/C21H40O4/c1-4-6-8-10-11-12-15-19(3)25-21(23)17-14-16-20(22)24-18-13-9-7  
**InchiKey:** UQEMFLVXSXCDFFG-UHFFFAOYSA-N  
**Formula:** C21H40O4  
**SMILES:** CCCCCCCCC(C)OC(=O)CCCC(=O)OCCCCC  
**Mol. weight [g/mol]:** 356.54

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -344.34 | kJ/mol  | Joback Method  |
| hf            | -971.65 | kJ/mol  | Joback Method  |
| hfus          | 52.20   | kJ/mol  | Joback Method  |
| hvap          | 80.26   | kJ/mol  | Joback Method  |
| log10ws       | -6.45   |         | Crippen Method |
| logp          | 5.963   |         | Crippen Method |
| mcvol         | 321.630 | ml/mol  | McGowan Method |
| pc            | 1018.13 | kPa     | Joback Method  |
| rinpol        | 2396.00 |         | NIST Webbook   |
| rinpol        | 2396.00 |         | NIST Webbook   |
| tb            | 832.02  | K       | Joback Method  |
| tc            | 1019.80 | K       | Joback Method  |
| tf            | 455.75  | K       | Joback Method  |
| vc            | 1.254   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1030.73   | J/mol×K | 832.02          | Joback Method |
| cpg           | 1113.31   | J/mol×K | 988.51          | Joback Method |
| cpg           | 1098.97   | J/mol×K | 957.21          | Joback Method |
| cpg           | 1083.56   | J/mol×K | 925.91          | Joback Method |
| cpg           | 1067.07   | J/mol×K | 894.61          | Joback Method |
| cpg           | 1049.46   | J/mol×K | 863.32          | Joback Method |
| cpg           | 1126.61   | J/mol×K | 1019.80         | Joback Method |
| dvisc         | 0.0000422 | Pa×s    | 832.02          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000570 | Pa×s | 769.31 | Joback Method |
| dvisc | 0.0000812 | Pa×s | 706.60 | Joback Method |
| dvisc | 0.0001238 | Pa×s | 643.88 | Joback Method |
| dvisc | 0.0002068 | Pa×s | 581.17 | Joback Method |
| dvisc | 0.0003912 | Pa×s | 518.46 | Joback Method |
| dvisc | 0.0008818 | Pa×s | 455.75 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359771&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359771&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.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>mccvol:</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                                 |

Latest version available from:

<https://www.chemeo.com/cid/49-939-6/Glutaric-acid-2-decyl-hexyl-ester.pdf>

Generated by Cheméo on 2025-12-23 09:41:47.771441092 +0000 UTC m=+6231105.301481745.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.