

# Glutaric acid, 3-octyl tridecyl ester

**Inchi:** InChI=1S/C26H50O4/c1-4-7-9-10-11-12-13-14-15-16-18-23-29-25(27)21-19-22-26(28)30

**InchiKey:** WIWAXNWQXUJABS-UHFFFAOYSA-N

**Formula:** C26H50O4

**SMILES:** CCCCCCCCCCCCCOC(=O)CCCC(=O)OC(CC)CCCC

**Mol. weight [g/mol]:** 426.67

## Physical Properties

| Property code | Value    | Unit    | Source         |
|---------------|----------|---------|----------------|
| gf            | -302.24  | kJ/mol  | Joback Method  |
| hf            | -1074.85 | kJ/mol  | Joback Method  |
| hfus          | 65.15    | kJ/mol  | Joback Method  |
| hvap          | 91.39    | kJ/mol  | Joback Method  |
| log10ws       | -8.54    |         | Crippen Method |
| logp          | 7.913    |         | Crippen Method |
| mcvol         | 392.080  | ml/mol  | McGowan Method |
| pc            | 765.64   | kPa     | Joback Method  |
| rinpol        | 2931.00  |         | NIST Webbook   |
| tb            | 946.42   | K       | Joback Method  |
| tc            | 1164.49  | K       | Joback Method  |
| tf            | 512.10   | K       | Joback Method  |
| vc            | 1.534    | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1345.59   | J/mol×K | 946.42          | Joback Method |
| cpg           | 1366.80   | J/mol×K | 982.76          | Joback Method |
| cpg           | 1386.34   | J/mol×K | 1019.11         | Joback Method |
| cpg           | 1404.25   | J/mol×K | 1055.45         | Joback Method |
| cpg           | 1420.58   | J/mol×K | 1091.80         | Joback Method |
| cpg           | 1435.40   | J/mol×K | 1128.14         | Joback Method |
| cpg           | 1448.73   | J/mol×K | 1164.49         | Joback Method |
| dvisc         | 0.0004671 | Pa×s    | 512.10          | Joback Method |
| dvisc         | 0.0001988 | Pa×s    | 584.49          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001021 | Pa×s | 656.87 | Joback Method |
| dvisc | 0.0000599 | Pa×s | 729.26 | Joback Method |
| dvisc | 0.0000387 | Pa×s | 801.65 | Joback Method |
| dvisc | 0.0000268 | Pa×s | 874.03 | Joback Method |
| dvisc | 0.0000197 | Pa×s | 946.42 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377433&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377433&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>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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