

# Glutaric acid, di(2,4-dimethylpent-3-yl) ester

**Inchi:** InChI=1S/C19H36O4/c1-12(2)18(13(3)4)22-16(20)10-9-11-17(21)23-19(14(5)6)15(7)8/h1-12,14-18,20-23,25H,13,19H2,21H3  
**InchiKey:** JDNMPNLUFYQEHO-UHFFFAOYSA-N  
**Formula:** C19H36O4  
**SMILES:** CC(C)C(OC(=O)CCCC(=O)OC(C(C)C)C(C(C)C)C(C)C)  
**Mol. weight [g/mol]:** 328.49

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -373.38 | kJ/mol  | Joback Method  |
| hf            | -956.77 | kJ/mol  | Joback Method  |
| hfus          | 29.40   | kJ/mol  | Joback Method  |
| hvap          | 73.87   | kJ/mol  | Joback Method  |
| log10ws       | -4.76   |         | Crippen Method |
| logp          | 4.604   |         | Crippen Method |
| mcvol         | 293.450 | ml/mol  | McGowan Method |
| pc            | 1187.42 | kPa     | Joback Method  |
| rinpol        | 1996.00 |         | NIST Webbook   |
| tb            | 784.06  | K       | Joback Method  |
| tc            | 973.04  | K       | Joback Method  |
| tf            | 358.21  | K       | Joback Method  |
| vc            | 1.111   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 911.80    | J/mol×K | 784.06          | Joback Method |
| cpg           | 930.47    | J/mol×K | 815.56          | Joback Method |
| cpg           | 948.01    | J/mol×K | 847.05          | Joback Method |
| cpg           | 964.45    | J/mol×K | 878.55          | Joback Method |
| cpg           | 979.81    | J/mol×K | 910.05          | Joback Method |
| cpg           | 994.10    | J/mol×K | 941.55          | Joback Method |
| cpg           | 1007.33   | J/mol×K | 973.04          | Joback Method |
| dvisc         | 0.0038652 | Pa×s    | 358.21          | Joback Method |
| dvisc         | 0.0009398 | Pa×s    | 429.19          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003414 | Pa×s | 500.16 | Joback Method |
| dvisc | 0.0001595 | Pa×s | 571.13 | Joback Method |
| dvisc | 0.0000882 | Pa×s | 642.11 | Joback Method |
| dvisc | 0.0000548 | Pa×s | 713.08 | Joback Method |
| dvisc | 0.0000372 | Pa×s | 784.06 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U359490&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359490&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>                                     |

## 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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