

# Glutaric acid, 2-methylhex-3-yl 5-methylhex-2-yl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C19H36O4/c1-7-9-17(15(4)5)23-19(21)11-8-10-18(20)22-16(6)13-12-14(2)3/h |
| <b>InchiKey:</b>            | YKGJJBICACYYKH-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H36O4   |
| <b>SMILES:</b>              | CCCC(OC(=O)CCCC(=O)OC(C)CCC(C)C)C(C)C  |
| <b>Mol. weight [g/mol]:</b> | 328.49   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -368.50 | kJ/mol               | Joback Method  |
| hf            | -946.21 | kJ/mol               | Joback Method  |
| hfus          | 36.45   | kJ/mol               | Joback Method  |
| hvap          | 74.65   | kJ/mol               | Joback Method  |
| log10ws       | -5.24   |                      | Crippen Method |
| logp          | 4.893   |                      | Crippen Method |
| mcvol         | 293.450 | ml/mol               | McGowan Method |
| pc            | 1174.44 | kPa                  | Joback Method  |
| rinpola       | 2228.00 |                      | NIST Webbook   |
| tb            | 784.94  | K                    | Joback Method  |
| tc            | 970.70  | K                    | Joback Method  |
| tf            | 388.21  | K                    | Joback Method  |
| vc            | 1.123   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 910.84    | J/molxK | 784.94          | Joback Method |
| cpg           | 992.02    | J/molxK | 939.74          | Joback Method |
| cpg           | 977.85    | J/molxK | 908.78          | Joback Method |
| cpg           | 962.66    | J/molxK | 877.82          | Joback Method |
| cpg           | 946.44    | J/molxK | 846.86          | Joback Method |
| cpg           | 929.17    | J/molxK | 815.90          | Joback Method |
| cpg           | 1005.19   | J/molxK | 970.70          | Joback Method |
| dvisc         | 0.0000439 | Paxs    | 784.94          | Joback Method |
| dvisc         | 0.0000624 | Paxs    | 718.82          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000950 | Paxs | 652.70 | Joback Method |
| dvisc | 0.0001591 | Paxs | 586.58 | Joback Method |
| dvisc | 0.0003040 | Paxs | 520.45 | Joback Method |
| dvisc | 0.0007008 | Paxs | 454.33 | Joback Method |
| dvisc | 0.0021477 | Paxs | 388.21 | 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=U377660&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377660&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>                                 |

## 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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