

# Glutaric acid, di(2-norbornyl) ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C19H28O4/c20-18(22-16-10-12-4-6-14(16)8-12)2-1-3-19(21)23-17-11-13-5-7- |
| <b>InchiKey:</b>            | QTDRNQDUODEKEV-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C19H28O4   |
| <b>SMILES:</b>              | O=C(CCCC(=O)OC1CC2CCC1C2)OC1CC2CCC1C2  |
| <b>Mol. weight [g/mol]:</b> | 320.42   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -155.36 | kJ/mol               | Joback Method  |
| hf            | -686.89 | kJ/mol               | Joback Method  |
| hfus          | 41.02   | kJ/mol               | Joback Method  |
| hvap          | 75.58   | kJ/mol               | Joback Method  |
| log10ws       | -4.34   |                      | Crippen Method |
| logp          | 3.620   |                      | Crippen Method |
| mcvol         | 250.010 | ml/mol               | McGowan Method |
| pc            | 1671.43 | kPa                  | Joback Method  |
| rinqol        | 2417.00 |                      | NIST Webbook   |
| tb            | 812.86  | K                    | Joback Method  |
| tc            | 1028.63 | K                    | Joback Method  |
| tf            | 504.45  | K                    | Joback Method  |
| vc            | 0.958   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 860.49    | J/molxK | 812.86          | Joback Method |
| cpg           | 947.42    | J/molxK | 992.67          | Joback Method |
| cpg           | 932.16    | J/molxK | 956.71          | Joback Method |
| cpg           | 915.93    | J/molxK | 920.74          | Joback Method |
| cpg           | 898.65    | J/molxK | 884.78          | Joback Method |
| cpg           | 880.20    | J/molxK | 848.82          | Joback Method |
| cpg           | 961.83    | J/molxK | 1028.63         | Joback Method |
| dvisc         | 0.0040331 | Paxs    | 812.86          | Joback Method |
| dvisc         | 0.0042760 | Paxs    | 761.46          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0045720 | Paxs | 710.06 | Joback Method |
| dvisc | 0.0049398 | Paxs | 658.65 | Joback Method |
| dvisc | 0.0054076 | Paxs | 607.25 | Joback Method |
| dvisc | 0.0060196 | Paxs | 555.85 | Joback Method |
| dvisc | 0.0068488 | Paxs | 504.45 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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.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=U405497&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405497&amp;Units=SI</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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