

# Diglycolic acid, dodecyl 3-methylbutyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C21H40O5/c1-4-5-6-7-8-9-10-11-12-13-15-25-20(22)17-24-18-21(23)26-16-14 |
| <b>InchiKey:</b>            | AQZMLXQFCDXNU-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C21H40O5   |
| <b>SMILES:</b>              | CCCCCCCCCCCCOC(=O)COCC(=O)OCCC(C)C   |
| <b>Mol. weight [g/mol]:</b> | 372.54   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -449.34  | kJ/mol               | Joback Method  |
| hf            | -1103.87 | kJ/mol               | Joback Method  |
| hfus          | 53.38    | kJ/mol               | Joback Method  |
| hvap          | 82.67    | kJ/mol               | Joback Method  |
| log10ws       | -5.18    |                      | Crippen Method |
| logp          | 5.056    |                      | Crippen Method |
| mcvol         | 327.500  | ml/mol               | McGowan Method |
| pc            | 1007.17  | kPa                  | Joback Method  |
| rinpol        | 3089.00  |                      | NIST Webbook   |
| rinpol        | 3089.00  |                      | NIST Webbook   |
| tb            | 854.44   | K                    | Joback Method  |
| tc            | 1046.32  | K                    | Joback Method  |
| tf            | 477.98   | K                    | Joback Method  |
| vc            | 1.272    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1062.62   | J/molxK | 854.44          | Joback Method |
| cpg           | 1081.09   | J/molxK | 886.42          | Joback Method |
| cpg           | 1098.34   | J/molxK | 918.40          | Joback Method |
| cpg           | 1114.36   | J/molxK | 950.38          | Joback Method |
| cpg           | 1129.16   | J/molxK | 982.36          | Joback Method |
| cpg           | 1142.77   | J/molxK | 1014.34         | Joback Method |
| cpg           | 1155.19   | J/molxK | 1046.32         | Joback Method |
| dvisc         | 0.0005916 | Paxs    | 477.98          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002731 | Paxs | 540.72 | Joback Method |
| dvisc | 0.0001480 | Paxs | 603.47 | Joback Method |
| dvisc | 0.0000901 | Paxs | 666.21 | Joback Method |
| dvisc | 0.0000597 | Paxs | 728.95 | Joback Method |
| dvisc | 0.0000422 | Paxs | 791.70 | Joback Method |
| dvisc | 0.0000314 | Paxs | 854.44 | 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=U382278&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382278&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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